Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 08:33 PM EDT

PDB ID	:	2I14
Title	:	Crystal structure of nicotinate-nucleotide pyrophosphorylase from Pyrococcus furiosus
Authors	:	Shin, D.H.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on	:	2006-08-12
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

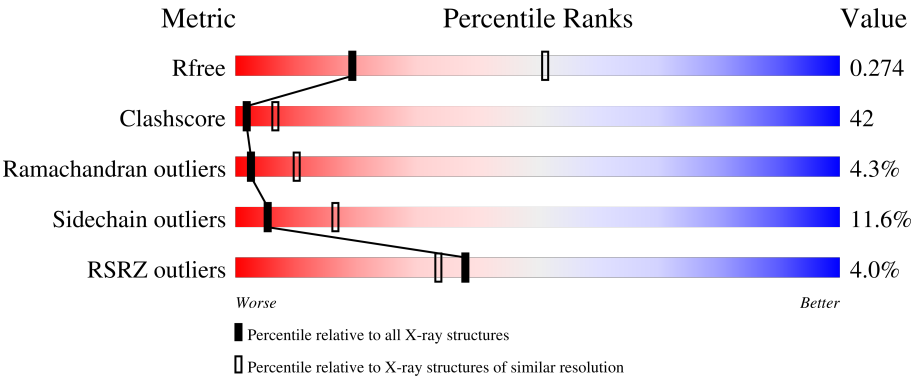
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	395	3% 41% 50% 7%
1	B	395	5% 39% 50% 9%
1	C	395	4% 41% 49% 8%
1	D	395	4% 39% 50% 8%

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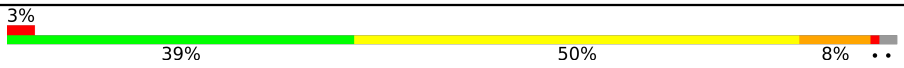
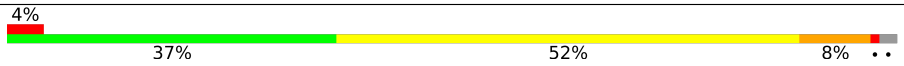
Mol	Chain	Length	Quality of chain
1	E	395	
1	F	395	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18539 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nicotinate-nucleotide pyrophosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	B	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	C	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	D	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	E	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	F	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	cloning artifact	UNP Q8TZS9
A	-4	GLY	-	cloning artifact	UNP Q8TZS9
A	-3	GLY	-	cloning artifact	UNP Q8TZS9
A	-2	GLY	-	cloning artifact	UNP Q8TZS9
A	-1	GLY	-	cloning artifact	UNP Q8TZS9
A	0	GLY	-	cloning artifact	UNP Q8TZS9
B	395	GLY	-	cloning artifact	UNP Q8TZS9
B	396	GLY	-	cloning artifact	UNP Q8TZS9
B	397	GLY	-	cloning artifact	UNP Q8TZS9
B	398	GLY	-	cloning artifact	UNP Q8TZS9
B	399	GLY	-	cloning artifact	UNP Q8TZS9
B	400	GLY	-	cloning artifact	UNP Q8TZS9
C	995	GLY	-	cloning artifact	UNP Q8TZS9
C	996	GLY	-	cloning artifact	UNP Q8TZS9
C	997	GLY	-	cloning artifact	UNP Q8TZS9
C	998	GLY	-	cloning artifact	UNP Q8TZS9
C	999	GLY	-	cloning artifact	UNP Q8TZS9

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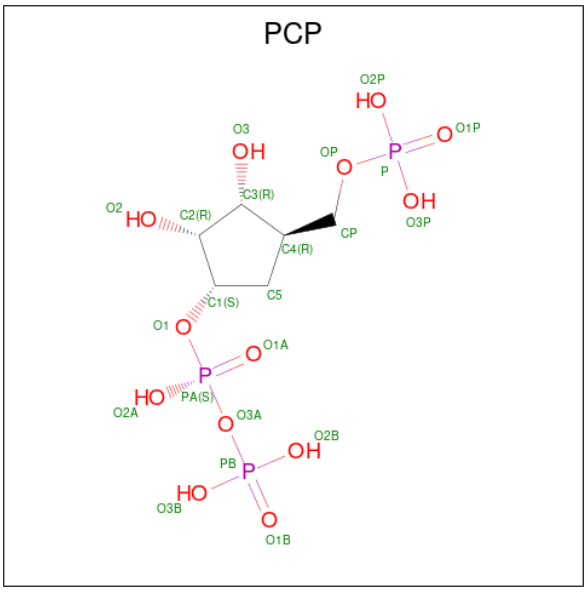
Chain	Residue	Modelled	Actual	Comment	Reference
C	1000	GLY	-	cloning artifact	UNP Q8TZS9
D	1395	GLY	-	cloning artifact	UNP Q8TZS9
D	1396	GLY	-	cloning artifact	UNP Q8TZS9
D	1397	GLY	-	cloning artifact	UNP Q8TZS9
D	1398	GLY	-	cloning artifact	UNP Q8TZS9
D	1399	GLY	-	cloning artifact	UNP Q8TZS9
D	1400	GLY	-	cloning artifact	UNP Q8TZS9
E	1995	GLY	-	cloning artifact	UNP Q8TZS9
E	1996	GLY	-	cloning artifact	UNP Q8TZS9
E	1997	GLY	-	cloning artifact	UNP Q8TZS9
E	1998	GLY	-	cloning artifact	UNP Q8TZS9
E	1999	GLY	-	cloning artifact	UNP Q8TZS9
E	2000	GLY	-	cloning artifact	UNP Q8TZS9
F	2395	GLY	-	cloning artifact	UNP Q8TZS9
F	2396	GLY	-	cloning artifact	UNP Q8TZS9
F	2397	GLY	-	cloning artifact	UNP Q8TZS9
F	2398	GLY	-	cloning artifact	UNP Q8TZS9
F	2399	GLY	-	cloning artifact	UNP Q8TZS9
F	2400	GLY	-	cloning artifact	UNP Q8TZS9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is 1-ALPHA-PYROPHOSPHORYL-2-ALPHA,3-ALPHA-DIHYDROXY-4-BETA-CYCLOPENTANE-METHANOL-5-PHOSPHATE (three-letter code: PCP) (formula: $C_6H_{15}O_{13}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			22	6	13	3		
3	B	1	Total	C	O	P	0	0
			22	6	13	3		
3	C	1	Total	C	O	P	0	0
			22	6	13	3		
3	D	1	Total	C	O	P	0	0
			22	6	13	3		
3	E	1	Total	C	O	P	0	0
			22	6	13	3		
3	F	1	Total	C	O	P	0	0
			22	6	13	3		

- Molecule 4 is water.

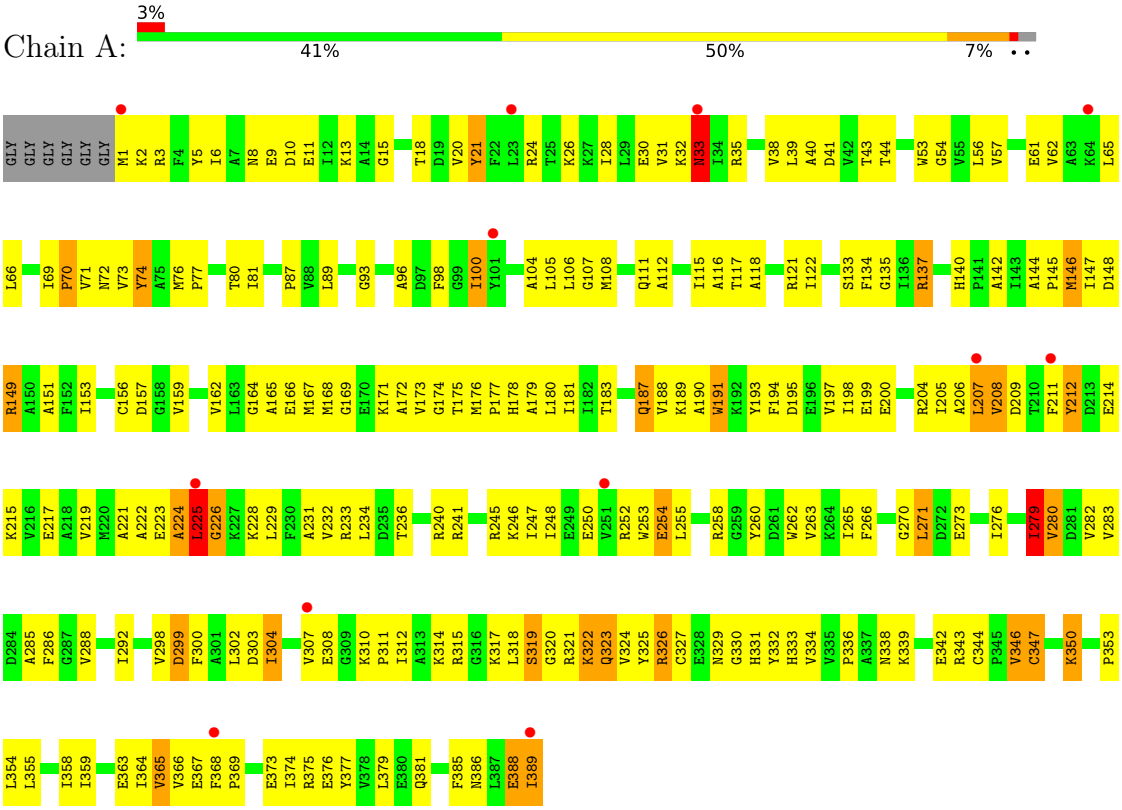
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	10	Total	O	0	0
			10	10		
4	C	9	Total	O	0	0
			9	9		
4	D	10	Total	O	0	0
			10	10		
4	E	16	Total	O	0	0
			16	16		
4	F	12	Total	O	0	0
			12	12		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

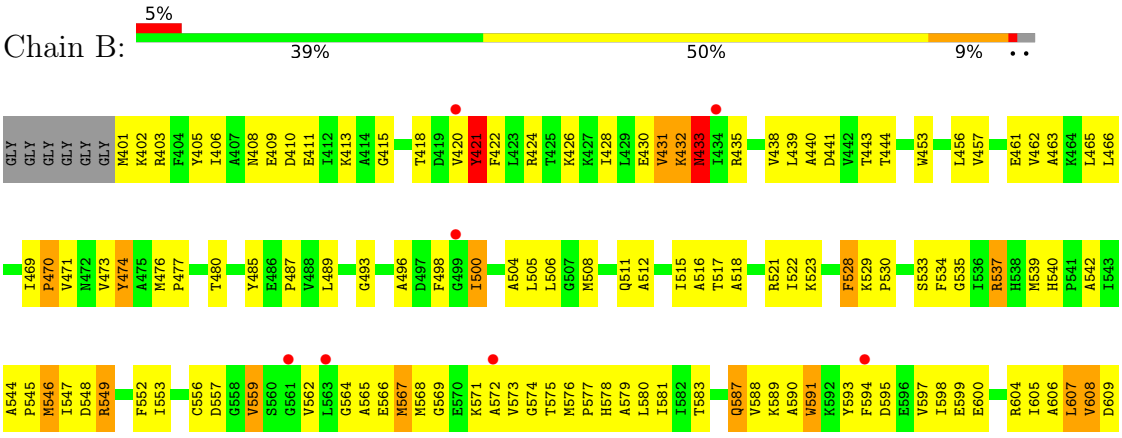
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase

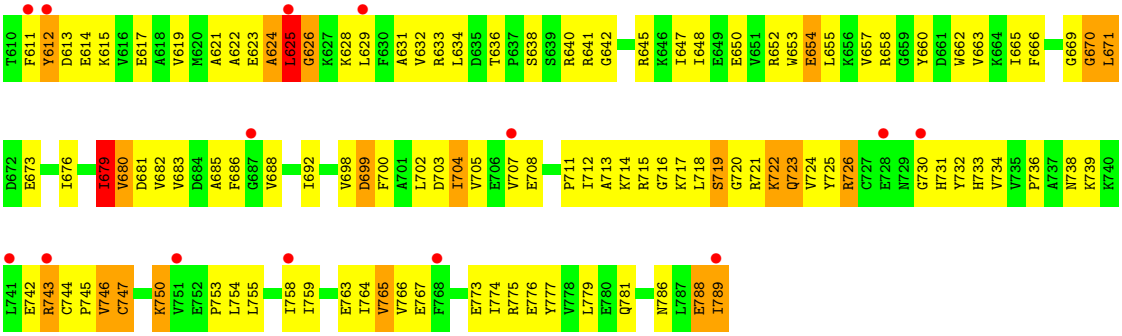
Chain A:



• Molecule 1: Nicotinate-nucleotide pyrophosphorylase

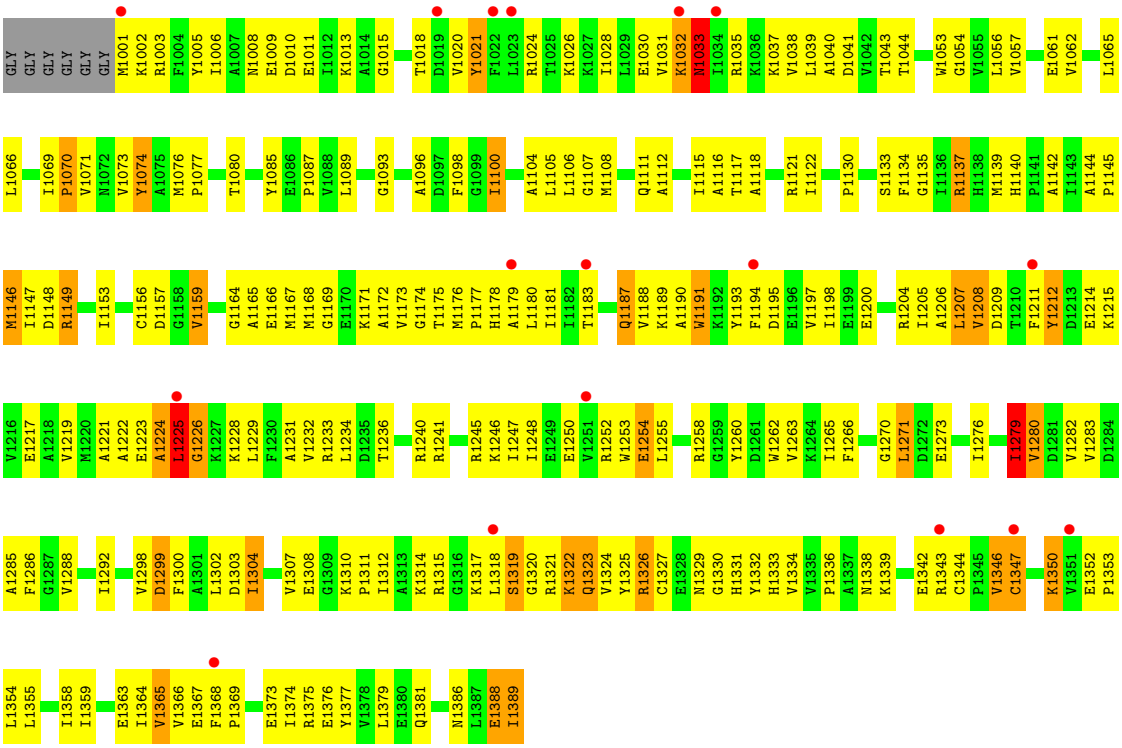
Chain B:





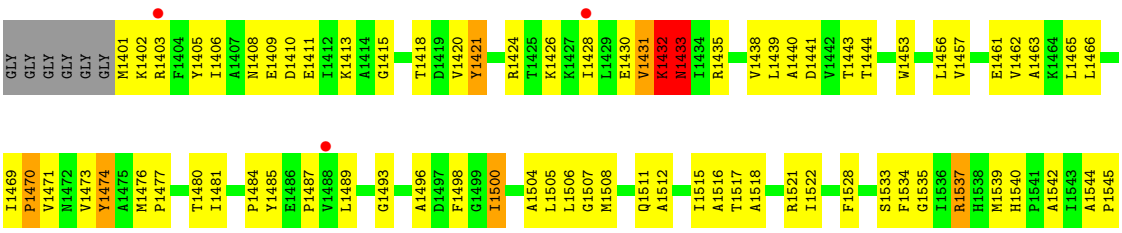
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase

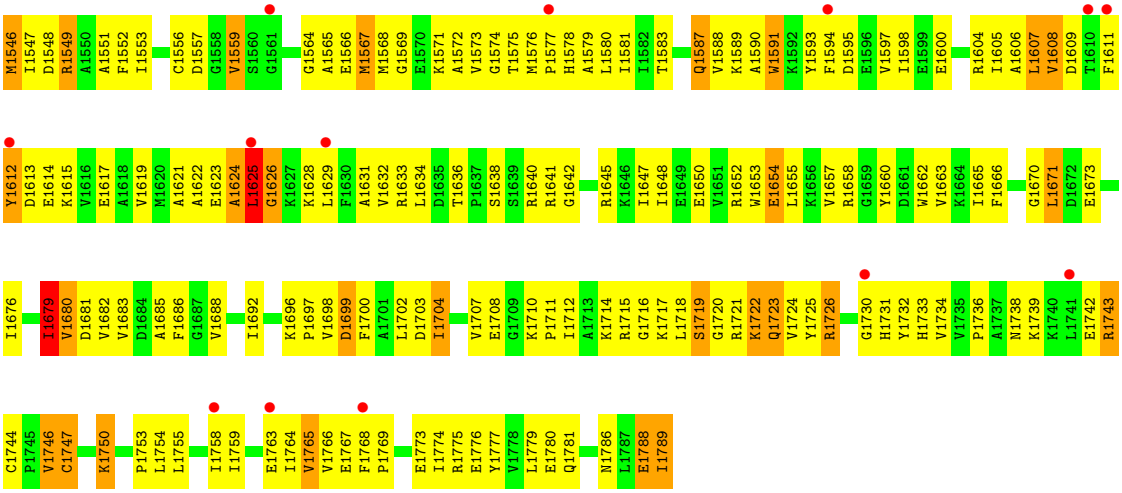
Chain C:



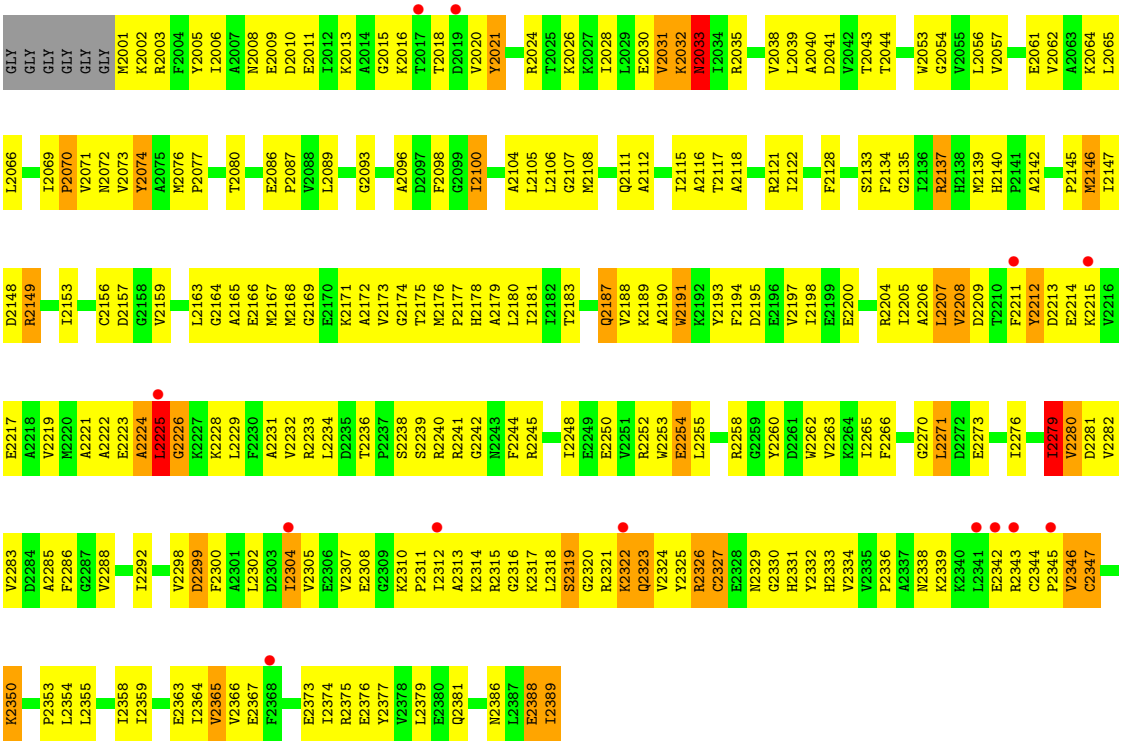
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase

Chain D:

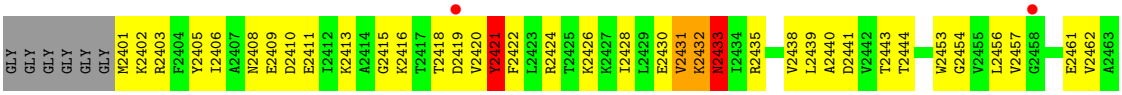


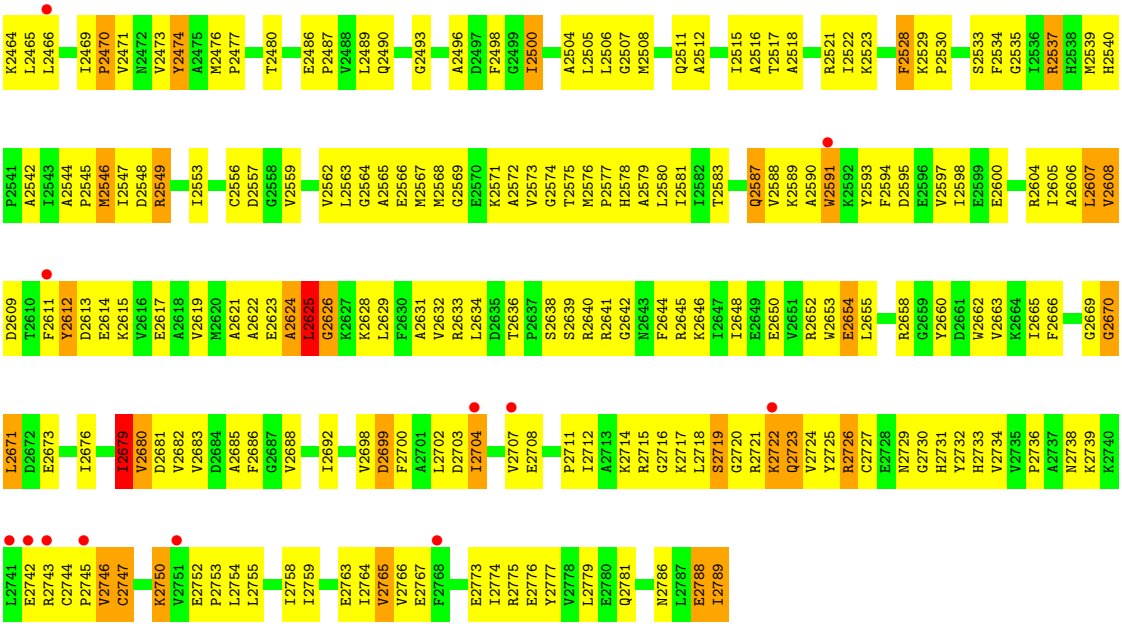


• Molecule 1: Nicotinate-nucleotide pyrophosphorylase



• Molecule 1: Nicotinate-nucleotide pyrophosphorylase




K2464 L2465 L2466 I2469 P2470 V2471 N2472 V2473 Y2474 A2475 M2476 P2477 T2480 E2486 P2487 V2488 L2489 Q2490 G2493 A2496 D2497 F2498 G2499 I2500 A2504 L2505 L2506 G2507 M2508 Q2511 A2512 I2515 A2516 T2517 A2518 R2521 I2522 K2523 F2528 K2529 P2530 S2533 F2534 G2535 I2536 R2537 H2538 M2539 H2540
P2541 A2542 I2543 A2544 P2545 M2546 I2547 D2548 R2549 I2553 C2556 D2557 G2558 V2559 V2562 L2563 G2564 A2565 E2566 M2567 M2568 G2569 E2570 K2571 A2572 V2573 G2574 T2575 M2576 P2577 H2578 A2579 L2580 I2581 I2582 T2583 Q2587 V2588 K2589 A2590 W2591 K2592 Y2593 F2594 D2595 E2596 V2597 I2598 E2599 E2600 R2604 I2605 A2606 L2607 V2608
D2609 T2610 F2611 Y2612 D2613 E2614 K2615 V2616 E2617 A2618 V2619 W2620 A2621 A2622 E2623 A2624 L2625 G2626 K2627 K2628 L2629 F2630 A2631 V2632 R2633 L2634 D2635 T2636 P2637 S2638 S2639 R2640 R2641 G2642 N2643 F2644 R2645 K2646 I2647 I2648 E2649 E2650 V2651 R2652 W2653 E2654 L2655 R2658 G2659 Y2660 D2661 W2662 V2663 K2664 I2665 F2666 G2669 G2670
L2671 D2672 E2673 I2676 I2679 V2680 D2681 V2682 V2683 D2684 A2685 F2686 G2687 V2688 I2692 V2698 D2699 F2700 A2701 L2702 D2703 I2704 V2707 E2708 P2711 I2712 A2713 K2714 R2715 G2716 K2717 L2718 S2719 G2720 R2721 K2722 Q2723 V2724 Y2725 R2726 C2727 E2728 N2729 G2730 H2731 Y2732 H2733 V2734 V2735 P2736 A2737 N2738 K2739 K2740
L2741 E2742 R2743 C2744 P2745 V2746 C2747 K2750 V2751 E2752 P2753 L2754 L2755 I2758 I2759 E2763 I2764 V2765 V2766 E2767 F2768 E2773 I2774 R2775 E2776 Y2777 V2778 L2779 E2780 Q2781 N2786 L2787 E2788 I2789

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	111.48Å 111.48Å 178.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.90 48.27 – 2.90	Depositor EDS
% Data completeness (in resolution range)	85.3 (19.99-2.90) 94.9 (48.27-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.282 0.243 , 0.274	Depositor DCC
R_{free} test set	5584 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å^2)	68.0	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.478 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18539	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2409e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.44	0/3117	0.66	2/4211 (0.0%)
1	B	0.46	0/3117	0.67	2/4211 (0.0%)
1	C	0.44	0/3117	0.66	2/4211 (0.0%)
1	D	0.45	0/3117	0.67	2/4211 (0.0%)
1	E	0.46	0/3117	0.67	2/4211 (0.0%)
1	F	0.47	0/3117	0.67	2/4211 (0.0%)
All	All	0.45	0/18702	0.67	12/25266 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1135	GLY	N-CA-C	5.59	127.08	113.10
1	B	535	GLY	N-CA-C	5.49	126.83	113.10
1	E	2135	GLY	N-CA-C	5.45	126.72	113.10
1	D	1535	GLY	N-CA-C	5.43	126.67	113.10
1	F	2535	GLY	N-CA-C	5.42	126.66	113.10
1	A	135	GLY	N-CA-C	5.41	126.63	113.10
1	B	625	LEU	CA-CB-CG	5.32	127.53	115.30
1	D	1625	LEU	CA-CB-CG	5.25	127.37	115.30
1	C	1225	LEU	CA-CB-CG	5.10	127.02	115.30
1	F	2625	LEU	CA-CB-CG	5.03	126.87	115.30
1	E	2225	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	225	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3055	0	3140	283	0
1	B	3055	0	3138	287	0
1	C	3055	0	3137	283	1
1	D	3055	0	3138	292	1
1	E	3055	0	3138	295	1
1	F	3055	0	3138	301	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	22	0	10	2	0
3	B	22	0	10	1	0
3	C	22	0	10	1	0
3	D	22	0	10	2	0
3	E	22	0	10	1	0
3	F	22	0	10	1	0
4	A	8	0	0	0	0
4	B	10	0	0	0	0
4	C	9	0	0	2	0
4	D	10	0	0	0	0
4	E	16	0	0	1	0
4	F	12	0	0	0	0
All	All	18539	0	18889	1578	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (1578) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LYS:HG3	1:A:336:PRO:HA	1.23	1.19
1:E:2322:LYS:HG3	1:E:2336:PRO:HA	1.23	1.15
1:B:722:LYS:HG3	1:B:736:PRO:HA	1.21	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2722:LYS:HG3	1:F:2736:PRO:HA	1.23	1.11
1:A:157:ASP:HA	1:A:375:ARG:HH12	1.16	1.09
1:C:1157:ASP:HA	1:C:1375:ARG:HH12	1.17	1.09
1:D:1722:LYS:HG3	1:D:1736:PRO:HA	1.22	1.09
1:C:1322:LYS:HG3	1:C:1336:PRO:HA	1.22	1.08
1:D:1557:ASP:HA	1:D:1775:ARG:HH12	1.17	1.08
1:F:2557:ASP:HA	1:F:2775:ARG:HH12	1.16	1.06
1:B:557:ASP:HA	1:B:775:ARG:HH12	1.18	1.05
1:E:2157:ASP:HA	1:E:2375:ARG:HH12	1.17	1.03
1:F:2724:VAL:HG12	1:F:2734:VAL:HG22	1.41	1.02
1:C:1346:VAL:HG22	1:C:1347:CYS:H	1.25	1.01
1:A:346:VAL:HG22	1:A:347:CYS:H	1.26	1.00
1:B:724:VAL:HG12	1:B:734:VAL:HG22	1.42	1.00
1:D:1746:VAL:HG22	1:D:1747:CYS:H	1.27	0.99
1:A:324:VAL:HG12	1:A:334:VAL:HG22	1.43	0.99
1:E:2324:VAL:HG12	1:E:2334:VAL:HG22	1.40	0.99
1:F:2746:VAL:HG22	1:F:2747:CYS:H	1.26	0.99
1:C:1044:THR:HG21	1:C:1298:VAL:HG12	1.44	0.98
1:F:2444:THR:HG21	1:F:2698:VAL:HG12	1.45	0.98
1:D:1724:VAL:HG12	1:D:1734:VAL:HG22	1.42	0.98
1:B:746:VAL:HG22	1:B:747:CYS:H	1.27	0.98
1:E:2044:THR:HG21	1:E:2298:VAL:HG12	1.45	0.97
1:C:1324:VAL:HG12	1:C:1334:VAL:HG22	1.43	0.97
1:B:444:THR:HG21	1:B:698:VAL:HG12	1.45	0.96
1:E:2346:VAL:HG22	1:E:2347:CYS:H	1.27	0.96
1:D:1444:THR:HG21	1:D:1698:VAL:HG12	1.47	0.96
1:A:44:THR:HG21	1:A:298:VAL:HG12	1.45	0.95
1:D:1750:LYS:HE3	1:D:1750:LYS:H	1.32	0.95
1:C:1350:LYS:H	1:C:1350:LYS:HE3	1.33	0.94
1:B:750:LYS:HE3	1:B:750:LYS:H	1.32	0.93
1:A:350:LYS:HE3	1:A:350:LYS:H	1.32	0.93
1:E:2350:LYS:HE3	1:E:2350:LYS:H	1.33	0.93
1:F:2750:LYS:H	1:F:2750:LYS:HE3	1.34	0.91
1:B:721:ARG:C	1:B:722:LYS:HD2	1.92	0.90
1:C:1321:ARG:C	1:C:1322:LYS:HD2	1.91	0.89
1:E:2321:ARG:C	1:E:2322:LYS:HD2	1.93	0.89
1:C:1100:ILE:HD12	1:C:1100:ILE:H	1.35	0.89
1:B:500:ILE:H	1:B:500:ILE:HD12	1.37	0.89
1:E:2100:ILE:H	1:E:2100:ILE:HD12	1.38	0.89
1:F:2721:ARG:C	1:F:2722:LYS:HD2	1.93	0.89
1:A:321:ARG:C	1:A:322:LYS:HD2	1.93	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ILE:HD12	1:A:100:ILE:H	1.36	0.89
1:D:1721:ARG:C	1:D:1722:LYS:HD2	1.93	0.88
1:F:2500:ILE:HD12	1:F:2500:ILE:H	1.39	0.86
1:E:2323:GLN:NE2	1:E:2353:PRO:HB3	1.91	0.86
1:D:1500:ILE:H	1:D:1500:ILE:HD12	1.37	0.86
1:F:2723:GLN:NE2	1:F:2753:PRO:HB3	1.90	0.85
1:B:723:GLN:NE2	1:B:753:PRO:HB3	1.92	0.85
1:C:1323:GLN:NE2	1:C:1353:PRO:HB3	1.92	0.85
1:D:1723:GLN:NE2	1:D:1753:PRO:HB3	1.91	0.85
1:E:2197:VAL:HB	1:F:2428:ILE:HD13	1.59	0.84
1:A:323:GLN:NE2	1:A:353:PRO:HB3	1.91	0.83
1:F:2537:ARG:HG2	1:F:2537:ARG:HH11	1.43	0.83
1:A:254:GLU:OE1	1:D:1719:SER:HB2	1.77	0.83
1:C:1350:LYS:H	1:C:1350:LYS:CE	1.92	0.83
1:D:1750:LYS:H	1:D:1750:LYS:CE	1.92	0.83
1:E:2018:THR:HG21	1:E:2100:ILE:O	1.80	0.82
1:C:1346:VAL:HG22	1:C:1347:CYS:N	1.95	0.82
1:F:2612:TYR:HB2	1:F:2617:GLU:HG3	1.62	0.81
1:A:350:LYS:H	1:A:350:LYS:CE	1.92	0.81
1:B:719:SER:HB2	1:C:1254:GLU:OE1	1.79	0.81
1:E:2212:TYR:HB2	1:E:2217:GLU:HG3	1.62	0.81
1:E:2350:LYS:H	1:E:2350:LYS:CE	1.92	0.81
1:A:212:TYR:HB2	1:A:217:GLU:HG3	1.63	0.81
1:A:346:VAL:HG22	1:A:347:CYS:N	1.96	0.81
1:B:750:LYS:H	1:B:750:LYS:CE	1.93	0.81
1:E:2028:ILE:HD13	1:F:2597:VAL:HB	1.60	0.81
1:F:2750:LYS:H	1:F:2750:LYS:CE	1.93	0.80
1:A:225:LEU:HB2	1:A:228:LYS:HB2	1.63	0.80
1:B:746:VAL:HG22	1:B:747:CYS:N	1.96	0.80
1:D:1746:VAL:HG22	1:D:1747:CYS:N	1.96	0.80
1:E:2346:VAL:HG22	1:E:2347:CYS:N	1.96	0.80
1:C:1212:TYR:HB2	1:C:1217:GLU:HG3	1.63	0.79
1:C:1225:LEU:HB2	1:C:1228:LYS:HB2	1.64	0.79
1:A:197:VAL:HB	1:B:428:ILE:HD13	1.64	0.79
1:B:625:LEU:HB2	1:B:628:LYS:HB2	1.64	0.79
1:C:1319:SER:HB2	1:F:2654:GLU:OE1	1.82	0.79
1:F:2746:VAL:HG22	1:F:2747:CYS:N	1.96	0.79
1:D:1625:LEU:HB2	1:D:1628:LYS:HB2	1.63	0.79
1:D:1722:LYS:HG3	1:D:1736:PRO:CA	2.10	0.79
1:D:1612:TYR:HB2	1:D:1617:GLU:HG3	1.65	0.79
1:A:18:THR:HG21	1:A:100:ILE:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2625:LEU:HB2	1:F:2628:LYS:HB2	1.64	0.78
1:B:438:VAL:HG12	1:B:707:VAL:HG13	1.66	0.78
1:B:612:TYR:HB2	1:B:617:GLU:HG3	1.65	0.78
1:C:1038:VAL:HG12	1:C:1307:VAL:HG13	1.66	0.78
1:B:722:LYS:HG3	1:B:736:PRO:CA	2.10	0.78
1:E:2137:ARG:HG2	1:E:2137:ARG:HH11	1.47	0.78
1:E:2225:LEU:HB2	1:E:2228:LYS:HB2	1.65	0.78
1:C:1018:THR:HG21	1:C:1100:ILE:O	1.84	0.78
1:D:1418:THR:HG21	1:D:1500:ILE:O	1.84	0.78
1:F:2418:THR:HG21	1:F:2500:ILE:O	1.83	0.77
1:B:418:THR:HG21	1:B:500:ILE:O	1.84	0.77
1:A:137:ARG:HH11	1:A:137:ARG:HG2	1.49	0.77
1:C:1197:VAL:HB	1:D:1428:ILE:HD13	1.65	0.77
1:E:2331:HIS:ND1	1:E:2346:VAL:HG11	2.00	0.77
1:C:1137:ARG:HH11	1:C:1137:ARG:HG2	1.48	0.77
1:B:731:HIS:ND1	1:B:746:VAL:HG11	1.99	0.77
1:E:2254:GLU:HG3	1:E:2258:ARG:HH12	1.49	0.77
1:D:1438:VAL:HG12	1:D:1707:VAL:HG13	1.67	0.77
1:E:2038:VAL:HG12	1:E:2307:VAL:HG13	1.66	0.77
1:A:146:MET:HG3	1:A:147:ILE:N	2.01	0.76
1:A:319:SER:HB2	1:E:2254:GLU:OE1	1.84	0.76
1:A:38:VAL:HG12	1:A:307:VAL:HG13	1.67	0.76
1:B:546:MET:HG3	1:B:547:ILE:N	2.01	0.76
1:D:1549:ARG:HH11	1:D:1553:ILE:HD11	1.49	0.76
1:D:1628:LYS:HA	1:D:1628:LYS:HE2	1.67	0.76
1:C:1028:ILE:HD13	1:D:1597:VAL:HB	1.67	0.76
1:D:1546:MET:HG3	1:D:1547:ILE:N	2.01	0.76
1:E:2149:ARG:HH11	1:E:2153:ILE:HD11	1.51	0.76
1:B:549:ARG:HH11	1:B:553:ILE:HD11	1.51	0.76
1:C:1100:ILE:HD12	1:C:1100:ILE:N	2.00	0.76
1:C:1228:LYS:HE2	1:C:1228:LYS:HA	1.68	0.76
1:F:2731:HIS:ND1	1:F:2746:VAL:HG11	2.00	0.76
1:E:2322:LYS:HG3	1:E:2336:PRO:CA	2.12	0.76
1:F:2546:MET:HG3	1:F:2547:ILE:N	1.99	0.75
1:A:228:LYS:HE2	1:A:228:LYS:HA	1.69	0.75
1:C:1331:HIS:ND1	1:C:1346:VAL:HG11	2.00	0.75
1:F:2654:GLU:HG3	1:F:2658:ARG:HH12	1.51	0.75
1:B:500:ILE:HD12	1:B:500:ILE:N	2.01	0.75
1:D:1731:HIS:ND1	1:D:1746:VAL:HG11	2.00	0.75
1:F:2438:VAL:HG12	1:F:2707:VAL:HG13	1.66	0.75
1:B:628:LYS:HA	1:B:628:LYS:HE2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2100:ILE:HD12	1:E:2100:ILE:N	2.02	0.75
1:D:1537:ARG:HG2	1:D:1537:ARG:HH11	1.51	0.75
1:B:615:LYS:HD3	1:B:650:GLU:OE1	1.87	0.74
1:F:2628:LYS:HE2	1:F:2628:LYS:HA	1.69	0.74
1:A:149:ARG:HH11	1:A:153:ILE:HD11	1.50	0.74
1:B:609:ASP:HB2	1:B:614:GLU:HG3	1.70	0.74
1:A:322:LYS:HG3	1:A:336:PRO:CA	2.11	0.74
1:D:1615:LYS:HD3	1:D:1650:GLU:OE1	1.87	0.74
1:F:2726:ARG:HH12	1:F:2781:GLN:HE21	1.33	0.74
1:A:100:ILE:HD12	1:A:100:ILE:N	2.03	0.74
1:D:1500:ILE:HD12	1:D:1500:ILE:N	2.02	0.74
1:F:2549:ARG:HH11	1:F:2553:ILE:HD11	1.50	0.74
1:D:1654:GLU:OE1	1:E:2319:SER:HB2	1.87	0.74
1:C:1215:LYS:HD3	1:C:1250:GLU:OE1	1.87	0.73
1:E:2146:MET:HG3	1:E:2147:ILE:N	2.02	0.73
1:A:331:HIS:ND1	1:A:346:VAL:HG11	2.02	0.73
1:F:2500:ILE:HD12	1:F:2500:ILE:N	2.02	0.73
1:C:1146:MET:HG3	1:C:1147:ILE:N	2.03	0.73
1:C:1149:ARG:HH11	1:C:1153:ILE:HD11	1.52	0.73
1:E:2228:LYS:HA	1:E:2228:LYS:HE2	1.69	0.73
1:B:650:GLU:OE2	1:F:2716:GLY:HA2	1.89	0.72
1:B:654:GLU:OE1	1:F:2719:SER:HB2	1.89	0.72
1:B:724:VAL:HG23	1:B:754:LEU:HB2	1.71	0.72
1:A:28:ILE:HD13	1:B:597:VAL:HB	1.69	0.72
1:C:1003:ARG:HG2	1:D:1409:GLU:OE2	1.89	0.72
1:E:2215:LYS:HD3	1:E:2250:GLU:OE1	1.89	0.72
1:E:2044:THR:HG21	1:E:2298:VAL:CG1	2.18	0.72
1:F:2609:ASP:HB2	1:F:2614:GLU:HG3	1.71	0.72
1:A:215:LYS:HD3	1:A:250:GLU:OE1	1.89	0.72
1:B:537:ARG:HG2	1:B:537:ARG:HH11	1.52	0.72
1:F:2615:LYS:HD3	1:F:2650:GLU:OE1	1.89	0.72
1:A:255:LEU:HD13	1:A:263:VAL:CG2	2.20	0.72
1:B:726:ARG:HH12	1:B:781:GLN:HE21	1.38	0.72
1:C:1009:GLU:OE2	1:D:1403:ARG:HG2	1.90	0.72
1:E:2209:ASP:HB2	1:E:2214:GLU:HG3	1.72	0.72
1:B:444:THR:HG21	1:B:698:VAL:CG1	2.19	0.71
1:A:254:GLU:HG3	1:A:258:ARG:HH12	1.55	0.71
1:C:1044:THR:HG21	1:C:1298:VAL:CG1	2.19	0.71
1:C:1209:ASP:HB2	1:C:1214:GLU:HG3	1.70	0.71
1:D:1609:ASP:HB2	1:D:1614:GLU:HG3	1.70	0.71
1:D:1724:VAL:HG23	1:D:1754:LEU:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2255:LEU:HD13	1:E:2263:VAL:CG2	2.20	0.71
1:E:2326:ARG:HH12	1:E:2381:GLN:HE21	1.37	0.71
1:A:9:GLU:OE2	1:B:403:ARG:HG2	1.89	0.71
1:B:465:LEU:HD22	1:B:508:MET:HE2	1.73	0.71
1:B:655:LEU:HD13	1:B:663:VAL:CG2	2.20	0.71
1:D:1588:VAL:HA	1:D:1591:TRP:NE1	2.06	0.71
1:F:2655:LEU:HD13	1:F:2663:VAL:CG2	2.21	0.71
1:F:2724:VAL:HG23	1:F:2754:LEU:HB2	1.73	0.71
1:A:3:ARG:HG2	1:B:409:GLU:OE2	1.90	0.71
1:A:209:ASP:HB2	1:A:214:GLU:HG3	1.71	0.71
1:C:1324:VAL:HG23	1:C:1354:LEU:HB2	1.72	0.71
1:C:1322:LYS:HG3	1:C:1336:PRO:CA	2.11	0.70
1:D:1726:ARG:HH12	1:D:1781:GLN:HE21	1.38	0.70
1:E:2188:VAL:HA	1:E:2191:TRP:NE1	2.06	0.70
1:E:2254:GLU:HG3	1:E:2258:ARG:NH1	2.06	0.70
1:D:1650:GLU:OE2	1:E:2316:GLY:HA2	1.90	0.70
1:F:2571:LYS:HG3	1:F:2571:LYS:O	1.91	0.70
1:F:2588:VAL:HA	1:F:2591:TRP:NE1	2.07	0.70
1:C:1255:LEU:HD13	1:C:1263:VAL:CG2	2.21	0.70
1:D:1655:LEU:HD13	1:D:1663:VAL:CG2	2.21	0.70
1:E:2171:LYS:O	1:E:2171:LYS:HG3	1.92	0.70
1:F:2654:GLU:HG3	1:F:2658:ARG:NH1	2.07	0.70
1:F:2444:THR:HG21	1:F:2698:VAL:CG1	2.20	0.69
1:A:324:VAL:HG23	1:A:354:LEU:HB2	1.73	0.69
1:B:588:VAL:HA	1:B:591:TRP:NE1	2.06	0.69
1:D:1431:VAL:C	1:D:1433:ASN:H	1.96	0.69
1:D:1465:LEU:HD22	1:D:1508:MET:HE2	1.74	0.69
1:C:1188:VAL:HA	1:C:1191:TRP:NE1	2.08	0.69
1:E:2031:VAL:C	1:E:2033:ASN:H	1.96	0.69
1:E:2065:LEU:HD22	1:E:2108:MET:HE2	1.75	0.69
1:C:1031:VAL:C	1:C:1033:ASN:H	1.96	0.69
1:D:1444:THR:HG21	1:D:1698:VAL:CG1	2.22	0.69
1:D:1654:GLU:HG3	1:D:1658:ARG:HH12	1.56	0.69
1:F:2722:LYS:HG3	1:F:2736:PRO:CA	2.12	0.69
1:F:2557:ASP:HA	1:F:2775:ARG:NH1	2.01	0.69
1:C:1005:TYR:O	1:D:1545:PRO:HG2	1.93	0.68
1:B:654:GLU:HG3	1:B:658:ARG:HH12	1.59	0.68
1:A:188:VAL:HA	1:A:191:TRP:NE1	2.08	0.68
1:C:1254:GLU:HG3	1:C:1258:ARG:HH12	1.58	0.68
1:F:2465:LEU:HD22	1:F:2508:MET:CE	2.24	0.68
1:A:44:THR:HG21	1:A:298:VAL:CG1	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:O	1:A:171:LYS:HG3	1.94	0.68
1:C:1137:ARG:HH11	1:C:1137:ARG:CG	2.07	0.68
1:F:2537:ARG:HH11	1:F:2537:ARG:CG	2.06	0.68
1:B:655:LEU:HD13	1:B:663:VAL:HG21	1.76	0.68
1:D:1595:ASP:HA	1:D:1604:ARG:HE	1.58	0.68
1:E:2324:VAL:HG23	1:E:2354:LEU:HB2	1.75	0.68
1:B:595:ASP:HA	1:B:604:ARG:HE	1.59	0.68
1:D:1655:LEU:HD13	1:D:1663:VAL:HG21	1.76	0.68
1:F:2431:VAL:C	1:F:2433:ASN:H	1.97	0.67
1:A:137:ARG:HH11	1:A:137:ARG:CG	2.07	0.67
1:B:431:VAL:C	1:B:433:ASN:H	1.95	0.67
1:E:2137:ARG:HH11	1:E:2137:ARG:CG	2.07	0.67
1:A:145:PRO:HG2	1:B:405:TYR:O	1.94	0.67
1:A:31:VAL:C	1:A:33:ASN:H	1.97	0.67
1:E:2065:LEU:HD22	1:E:2108:MET:CE	2.25	0.67
1:B:722:LYS:HZ2	1:B:736:PRO:HB3	1.60	0.67
1:D:1465:LEU:HD22	1:D:1508:MET:CE	2.25	0.66
1:E:2255:LEU:HD13	1:E:2263:VAL:HG21	1.78	0.66
1:B:465:LEU:HD22	1:B:508:MET:CE	2.25	0.66
1:A:173:VAL:HG22	1:A:174:GLY:N	2.11	0.66
1:C:1065:LEU:HD22	1:C:1108:MET:HE2	1.76	0.66
1:B:571:LYS:O	1:B:571:LYS:HG3	1.95	0.66
1:C:1255:LEU:HD13	1:C:1263:VAL:HG21	1.77	0.66
1:F:2742:GLU:OE2	1:F:2742:GLU:HA	1.96	0.66
1:A:179:ALA:HA	1:B:704:ILE:HD11	1.78	0.66
1:A:254:GLU:HG3	1:A:258:ARG:NH1	2.11	0.66
1:C:1171:LYS:HG3	1:C:1171:LYS:O	1.93	0.66
1:F:2517:THR:O	1:F:2521:ARG:HG3	1.95	0.66
1:A:5:TYR:O	1:B:545:PRO:HG2	1.95	0.65
1:C:1065:LEU:HD22	1:C:1108:MET:CE	2.26	0.65
1:D:1517:THR:O	1:D:1521:ARG:HG3	1.97	0.65
1:B:738:ASN:C	1:B:739:LYS:HD2	2.17	0.65
1:C:1117:THR:O	1:C:1121:ARG:HG3	1.95	0.65
1:A:342:GLU:OE2	1:A:342:GLU:HA	1.97	0.65
1:E:2322:LYS:CG	1:E:2336:PRO:HA	2.15	0.65
1:C:1342:GLU:OE2	1:C:1342:GLU:HA	1.97	0.65
1:D:1742:GLU:HA	1:D:1742:GLU:OE2	1.96	0.65
1:A:255:LEU:HD13	1:A:263:VAL:HG21	1.77	0.65
1:C:1145:PRO:HG2	1:D:1405:TYR:O	1.97	0.65
1:D:1654:GLU:HG3	1:D:1658:ARG:NH1	2.11	0.65
1:B:742:GLU:HA	1:B:742:GLU:OE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1573:VAL:HG22	1:D:1574:GLY:N	2.12	0.65
1:A:157:ASP:CA	1:A:375:ARG:HH12	2.03	0.64
1:A:195:ASP:HA	1:A:204:ARG:HE	1.62	0.64
1:D:1557:ASP:CA	1:D:1775:ARG:HH12	2.03	0.64
1:F:2722:LYS:CG	1:F:2736:PRO:HA	2.15	0.64
1:B:557:ASP:CA	1:B:775:ARG:HH12	2.03	0.64
1:D:1571:LYS:O	1:D:1571:LYS:HG3	1.96	0.64
1:C:1179:ALA:HA	1:D:1704:ILE:HD11	1.79	0.64
1:F:2595:ASP:HA	1:F:2604:ARG:HE	1.62	0.64
1:A:65:LEU:HD22	1:A:108:MET:CE	2.26	0.64
1:D:1537:ARG:HH11	1:D:1537:ARG:CG	2.10	0.64
1:D:1738:ASN:C	1:D:1739:LYS:HD2	2.18	0.64
1:C:1364:ILE:HG13	1:C:1364:ILE:O	1.97	0.64
1:D:1722:LYS:CG	1:D:1736:PRO:HA	2.14	0.64
1:E:2173:VAL:HG22	1:E:2174:GLY:N	2.13	0.64
1:B:573:VAL:HG22	1:B:574:GLY:N	2.13	0.64
1:F:2726:ARG:NH1	1:F:2781:GLN:HE21	1.96	0.64
1:A:157:ASP:HA	1:A:375:ARG:NH1	2.01	0.64
1:B:517:THR:O	1:B:521:ARG:HG3	1.98	0.64
1:C:1157:ASP:CA	1:C:1375:ARG:HH12	2.02	0.64
1:D:1557:ASP:HA	1:D:1775:ARG:NH1	2.02	0.64
1:E:2342:GLU:HA	1:E:2342:GLU:OE2	1.96	0.64
1:A:65:LEU:HD22	1:A:108:MET:HE2	1.79	0.64
1:A:364:ILE:HG13	1:A:364:ILE:O	1.97	0.64
1:B:654:GLU:HG3	1:B:658:ARG:NH1	2.13	0.64
1:C:1254:GLU:HG3	1:C:1258:ARG:NH1	2.12	0.64
1:E:2112:ALA:HA	1:E:2146:MET:HE1	1.80	0.64
1:C:1100:ILE:H	1:C:1100:ILE:CD1	2.10	0.63
1:F:2476:MET:CE	1:F:2724:VAL:HG21	2.28	0.63
1:B:722:LYS:CG	1:B:736:PRO:HA	2.13	0.63
1:B:537:ARG:HH11	1:B:537:ARG:CG	2.12	0.63
1:C:1326:ARG:HH12	1:C:1381:GLN:HE21	1.43	0.63
1:E:2076:MET:HE2	1:E:2324:VAL:HG21	1.81	0.63
1:A:100:ILE:H	1:A:100:ILE:CD1	2.11	0.63
1:B:521:ARG:CB	1:B:789:ILE:HD11	2.29	0.63
1:E:2195:ASP:HA	1:E:2204:ARG:HE	1.62	0.63
1:F:2489:LEU:C	1:F:2489:LEU:HD23	2.18	0.63
1:B:725:TYR:CE2	1:B:753:PRO:HG3	2.33	0.63
1:C:1173:VAL:HG22	1:C:1174:GLY:N	2.13	0.63
1:F:2465:LEU:HD22	1:F:2508:MET:HE2	1.81	0.63
1:A:173:VAL:HG22	1:A:174:GLY:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1157:ASP:HA	1:C:1375:ARG:NH1	2.02	0.63
1:C:1195:ASP:HA	1:C:1204:ARG:HE	1.62	0.63
1:A:117:THR:O	1:A:121:ARG:HG3	1.98	0.63
1:E:2117:THR:O	1:E:2121:ARG:HG3	1.99	0.63
1:A:121:ARG:CB	1:A:389:ILE:HD11	2.29	0.62
1:A:338:ASN:C	1:A:339:LYS:HD2	2.20	0.62
1:B:489:LEU:HD23	1:B:489:LEU:C	2.20	0.62
1:E:2245:ARG:N	1:E:2279:ILE:HD11	2.14	0.62
1:F:2764:ILE:HG13	1:F:2764:ILE:O	1.99	0.62
1:A:112:ALA:HA	1:A:146:MET:HE1	1.81	0.62
1:F:2573:VAL:HG22	1:F:2574:GLY:N	2.14	0.62
1:C:1112:ALA:HA	1:C:1146:MET:HE1	1.81	0.62
1:D:1774:ILE:O	1:D:1777:TYR:HB3	2.00	0.62
1:F:2512:ALA:HA	1:F:2546:MET:HE1	1.81	0.62
1:D:1764:ILE:HG13	1:D:1764:ILE:O	2.00	0.62
1:E:2197:VAL:HB	1:F:2428:ILE:CD1	2.29	0.62
1:A:245:ARG:N	1:A:279:ILE:HD11	2.15	0.62
1:D:1521:ARG:CB	1:D:1789:ILE:HD11	2.30	0.62
1:B:774:ILE:O	1:B:777:TYR:HB3	1.99	0.62
1:E:2005:TYR:O	1:F:2545:PRO:HG2	1.99	0.62
1:F:2655:LEU:HD13	1:F:2663:VAL:HG21	1.80	0.62
1:E:2076:MET:CE	1:E:2324:VAL:HG21	2.30	0.62
1:E:2364:ILE:O	1:E:2364:ILE:HG13	1.99	0.61
1:A:325:TYR:CE2	1:A:353:PRO:HG3	2.35	0.61
1:E:2089:LEU:C	1:E:2089:LEU:HD23	2.21	0.61
1:E:2326:ARG:NH1	1:E:2381:GLN:HE21	1.97	0.61
1:C:1322:LYS:CG	1:C:1336:PRO:HA	2.14	0.61
1:C:1322:LYS:HZ2	1:C:1336:PRO:HB3	1.64	0.61
1:E:2145:PRO:HG2	1:F:2405:TYR:O	1.99	0.61
1:F:2579:ALA:O	1:F:2583:THR:HG23	2.01	0.61
1:E:2179:ALA:HA	1:F:2704:ILE:HD11	1.82	0.61
1:B:671:LEU:CD1	1:B:688:VAL:HG22	2.30	0.61
1:B:764:ILE:HG13	1:B:764:ILE:O	2.01	0.61
1:C:1194:PHE:HA	1:D:1428:ILE:CD1	2.31	0.61
1:D:1725:TYR:CE2	1:D:1753:PRO:HG3	2.35	0.61
1:E:2028:ILE:CD1	1:F:2597:VAL:HB	2.28	0.61
1:F:2717:LYS:HD3	1:F:2718:LEU:H	1.65	0.61
1:B:504:ALA:O	1:B:508:MET:HG3	2.01	0.61
1:E:2338:ASN:C	1:E:2339:LYS:HD2	2.21	0.61
1:A:224:ALA:C	1:A:226:GLY:H	2.04	0.61
1:D:1500:ILE:H	1:D:1500:ILE:CD1	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2578:HIS:HE1	1:F:2609:ASP:O	1.84	0.61
1:A:89:LEU:C	1:A:89:LEU:HD23	2.22	0.60
1:C:1317:LYS:HD3	1:C:1318:LEU:H	1.66	0.60
1:A:276:ILE:O	1:A:280:VAL:HG22	2.01	0.60
1:F:2500:ILE:H	1:F:2500:ILE:CD1	2.13	0.60
1:F:2557:ASP:CA	1:F:2775:ARG:HH12	2.03	0.60
1:B:476:MET:CE	1:B:724:VAL:HG21	2.30	0.60
1:B:717:LYS:HD3	1:B:718:LEU:H	1.66	0.60
1:F:2671:LEU:CD1	1:F:2688:VAL:HG22	2.31	0.60
1:A:233:ARG:HA	1:A:266:PHE:O	2.01	0.60
1:C:1194:PHE:HA	1:D:1428:ILE:HD12	1.84	0.60
1:A:346:VAL:CG2	1:A:347:CYS:H	2.06	0.60
1:D:1476:MET:CE	1:D:1724:VAL:HG21	2.31	0.60
1:D:1573:VAL:HG22	1:D:1574:GLY:H	1.67	0.60
1:E:2100:ILE:H	1:E:2100:ILE:CD1	2.11	0.60
1:F:2504:ALA:O	1:F:2508:MET:HG3	2.01	0.60
1:F:2731:HIS:ND1	1:F:2746:VAL:CG1	2.64	0.60
1:C:1325:TYR:CE2	1:C:1353:PRO:HG3	2.36	0.60
1:E:2327:CYS:SG	1:E:2329:ASN:N	2.71	0.60
1:E:2325:TYR:CE2	1:E:2353:PRO:HG3	2.37	0.60
1:F:2521:ARG:CB	1:F:2789:ILE:HD11	2.32	0.60
1:F:2725:TYR:CE2	1:F:2753:PRO:HG3	2.36	0.60
1:A:194:PHE:HA	1:B:428:ILE:CD1	2.32	0.60
1:A:326:ARG:HH12	1:A:381:GLN:HE21	1.48	0.60
1:B:500:ILE:H	1:B:500:ILE:CD1	2.12	0.60
1:B:512:ALA:HA	1:B:546:MET:HE1	1.84	0.60
1:D:1671:LEU:CD1	1:D:1688:VAL:HG22	2.32	0.60
1:D:1717:LYS:HD3	1:D:1718:LEU:H	1.67	0.60
1:B:573:VAL:HG22	1:B:574:GLY:H	1.67	0.60
1:E:2028:ILE:HD11	1:F:2598:ILE:HG12	1.84	0.60
1:E:2157:ASP:HA	1:E:2375:ARG:NH1	2.02	0.60
1:E:2173:VAL:HG22	1:E:2174:GLY:H	1.67	0.60
1:F:2738:ASN:C	1:F:2739:LYS:HD2	2.22	0.60
1:F:2774:ILE:O	1:F:2777:TYR:HB3	2.02	0.60
1:A:271:LEU:CD1	1:A:288:VAL:HG22	2.31	0.59
1:B:619:VAL:O	1:B:623:GLU:HG2	2.02	0.59
1:C:1089:LEU:C	1:C:1089:LEU:HD23	2.22	0.59
1:C:1338:ASN:C	1:C:1339:LYS:HD2	2.21	0.59
1:C:1374:ILE:O	1:C:1377:TYR:HB3	2.02	0.59
1:E:2317:LYS:HD3	1:E:2318:LEU:H	1.66	0.59
1:C:1076:MET:CE	1:C:1324:VAL:HG21	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1104:ALA:O	1:C:1108:MET:HG3	2.01	0.59
1:D:1624:ALA:C	1:D:1626:GLY:H	2.05	0.59
1:E:2178:HIS:HE1	1:E:2209:ASP:O	1.84	0.59
1:F:2624:ALA:C	1:F:2626:GLY:H	2.05	0.59
1:E:2179:ALA:O	1:E:2183:THR:HG23	2.01	0.59
1:E:2271:LEU:CD1	1:E:2288:VAL:HG22	2.32	0.59
1:B:726:ARG:NH1	1:B:781:GLN:HE21	2.00	0.59
1:A:194:PHE:HA	1:B:428:ILE:HD12	1.85	0.59
1:C:1224:ALA:C	1:C:1226:GLY:H	2.04	0.59
1:C:1233:ARG:HA	1:C:1266:PHE:O	2.03	0.59
1:E:2331:HIS:ND1	1:E:2346:VAL:CG1	2.64	0.59
1:B:731:HIS:ND1	1:B:746:VAL:CG1	2.65	0.59
1:E:2157:ASP:CA	1:E:2375:ARG:HH12	2.04	0.59
1:E:2224:ALA:C	1:E:2226:GLY:H	2.05	0.59
1:F:2444:THR:HG23	1:F:2700:PHE:CD2	2.38	0.59
1:E:2219:VAL:O	1:E:2223:GLU:HG2	2.02	0.59
1:A:179:ALA:O	1:A:183:THR:HG23	2.02	0.59
1:C:1121:ARG:CB	1:C:1389:ILE:HD11	2.32	0.59
1:C:1173:VAL:HG22	1:C:1174:GLY:H	1.67	0.59
1:E:2198:ILE:HG12	1:F:2428:ILE:HD11	1.83	0.59
1:E:2374:ILE:O	1:E:2377:TYR:HB3	2.02	0.59
1:C:1331:HIS:ND1	1:C:1346:VAL:CG1	2.65	0.59
1:E:2304:ILE:HD11	1:F:2579:ALA:HA	1.83	0.58
1:F:2515:ILE:HG23	1:F:2692:ILE:O	2.02	0.58
1:B:624:ALA:C	1:B:626:GLY:H	2.05	0.58
1:C:1271:LEU:CD1	1:C:1288:VAL:HG22	2.32	0.58
1:D:1726:ARG:NH1	1:D:1781:GLN:HE21	2.01	0.58
1:F:2619:VAL:O	1:F:2623:GLU:HG2	2.02	0.58
1:B:579:ALA:O	1:B:583:THR:HG23	2.02	0.58
1:D:1489:LEU:HD23	1:D:1489:LEU:C	2.23	0.58
1:A:44:THR:HG23	1:A:300:PHE:CD2	2.39	0.58
1:A:317:LYS:HD3	1:A:318:LEU:H	1.68	0.58
1:B:557:ASP:HA	1:B:775:ARG:NH1	2.03	0.58
1:E:2006:ILE:HD11	1:F:2409:GLU:OE1	2.03	0.58
1:C:1044:THR:HG23	1:C:1300:PHE:CD2	2.39	0.58
1:D:1731:HIS:ND1	1:D:1746:VAL:CG1	2.66	0.58
1:D:1504:ALA:O	1:D:1508:MET:HG3	2.03	0.58
1:D:1512:ALA:HA	1:D:1546:MET:HE1	1.86	0.58
1:E:2233:ARG:HA	1:E:2266:PHE:O	2.03	0.58
1:D:1633:ARG:HA	1:D:1666:PHE:O	2.03	0.58
1:A:344:CYS:SG	1:A:346:VAL:HG12	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2121:ARG:CB	1:E:2389:ILE:HD11	2.33	0.58
1:A:331:HIS:ND1	1:A:346:VAL:CG1	2.67	0.58
1:B:744:CYS:SG	1:B:746:VAL:HG12	2.44	0.58
1:D:1444:THR:HG23	1:D:1700:PHE:CD2	2.39	0.58
1:E:2002:LYS:HD3	1:E:2006:ILE:HD12	1.86	0.58
1:B:402:LYS:HD3	1:B:406:ILE:HD12	1.86	0.58
1:D:1578:HIS:HE1	1:D:1609:ASP:O	1.86	0.58
1:F:2573:VAL:HG22	1:F:2574:GLY:H	1.69	0.58
1:D:1589:LYS:HG2	1:D:1593:TYR:CE1	2.39	0.57
1:F:2726:ARG:HH12	1:F:2781:GLN:NE2	2.02	0.57
1:C:1115:ILE:HG23	1:C:1292:ILE:O	2.04	0.57
1:D:1402:LYS:HD3	1:D:1406:ILE:HD12	1.86	0.57
1:F:2476:MET:HE2	1:F:2724:VAL:HG21	1.86	0.57
1:A:76:MET:CE	1:A:324:VAL:HG21	2.34	0.57
1:D:1619:VAL:O	1:D:1623:GLU:HG2	2.04	0.57
1:F:2645:ARG:N	1:F:2679:ILE:HD11	2.18	0.57
1:B:444:THR:HG23	1:B:700:PHE:CD2	2.37	0.57
1:B:682:VAL:HG12	1:B:682:VAL:O	2.05	0.57
1:A:133:SER:O	1:A:134:PHE:HD1	1.87	0.57
1:B:408:ASN:HB2	1:B:411:GLU:HG3	1.84	0.57
1:C:1006:ILE:HG21	1:C:1142:ALA:HB2	1.85	0.57
1:E:2006:ILE:HG21	1:E:2142:ALA:HB2	1.86	0.57
1:A:8:ASN:HB2	1:A:11:GLU:HG3	1.86	0.57
1:C:1304:ILE:HD11	1:D:1579:ALA:HA	1.85	0.57
1:C:1331:HIS:CG	1:C:1346:VAL:HG11	2.39	0.57
1:C:1178:HIS:HE1	1:C:1209:ASP:O	1.87	0.57
1:C:1208:VAL:HG13	1:C:1217:GLU:HB2	1.87	0.57
1:D:1408:ASN:HB2	1:D:1411:GLU:HG3	1.86	0.57
1:D:1579:ALA:O	1:D:1583:THR:HG23	2.03	0.57
1:C:1245:ARG:N	1:C:1279:ILE:HD11	2.19	0.57
1:A:178:HIS:HE1	1:A:209:ASP:O	1.88	0.57
1:D:1515:ILE:HD13	1:D:1547:ILE:HG23	1.86	0.57
1:D:1744:CYS:SG	1:D:1746:VAL:HG12	2.44	0.57
1:D:1676:ILE:O	1:D:1680:VAL:HG22	2.04	0.57
1:D:1682:VAL:HG12	1:D:1682:VAL:O	2.05	0.57
1:E:2276:ILE:O	1:E:2280:VAL:HG22	2.04	0.57
1:E:2373:GLU:OE2	1:E:2376:GLU:OE1	2.22	0.57
1:F:2773:GLU:OE2	1:F:2776:GLU:OE1	2.22	0.57
1:A:6:ILE:HG21	1:A:142:ALA:HB2	1.86	0.56
1:A:53:TRP:CZ3	1:A:388:GLU:O	2.58	0.56
1:A:225:LEU:O	1:A:228:LYS:N	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1179:ALA:O	1:C:1183:THR:HG23	2.05	0.56
1:F:2633:ARG:HA	1:F:2666:PHE:O	2.04	0.56
1:B:515:ILE:HD13	1:B:547:ILE:HG23	1.86	0.56
1:B:578:HIS:HE1	1:B:609:ASP:O	1.87	0.56
1:E:2175:THR:OG1	1:E:2176:MET:N	2.38	0.56
1:F:2698:VAL:O	1:F:2700:PHE:N	2.39	0.56
1:A:2:LYS:HD3	1:A:6:ILE:HD12	1.86	0.56
1:A:219:VAL:O	1:A:223:GLU:HG2	2.06	0.56
1:B:406:ILE:HG21	1:B:542:ALA:HB2	1.87	0.56
1:B:540:HIS:HD2	1:B:542:ALA:CB	2.18	0.56
1:F:2731:HIS:CG	1:F:2746:VAL:HG11	2.40	0.56
1:B:613:ASP:OD1	1:E:2240:ARG:NH1	2.39	0.56
1:D:1406:ILE:HG21	1:D:1542:ALA:HB2	1.87	0.56
1:E:2008:ASN:HB2	1:E:2011:GLU:HG3	1.88	0.56
1:E:2324:VAL:HG23	1:E:2324:VAL:O	2.06	0.56
1:B:724:VAL:CG2	1:B:754:LEU:HB2	2.36	0.56
1:C:1008:ASN:HB2	1:C:1011:GLU:HG3	1.86	0.56
1:C:1053:TRP:CZ3	1:C:1388:GLU:O	2.58	0.56
1:C:1166:GLU:O	1:C:1169:GLY:N	2.39	0.56
1:E:2009:GLU:OE1	1:F:2406:ILE:HD11	2.05	0.56
1:E:2172:ALA:HB3	1:F:2420:VAL:CG1	2.36	0.56
1:E:2208:VAL:HG13	1:E:2217:GLU:HB2	1.88	0.56
1:F:2406:ILE:HG21	1:F:2542:ALA:HB2	1.86	0.56
1:A:374:ILE:O	1:A:377:TYR:HB3	2.05	0.56
1:C:1053:TRP:CD1	1:C:1053:TRP:C	2.79	0.56
1:E:2020:VAL:CG1	1:F:2572:ALA:HB3	2.36	0.56
1:D:1645:ARG:N	1:D:1679:ILE:HD11	2.20	0.56
1:E:2057:VAL:HG21	1:E:2116:ALA:HB2	1.86	0.56
1:E:2326:ARG:HH12	1:E:2381:GLN:NE2	2.03	0.56
1:A:331:HIS:CG	1:A:346:VAL:HG11	2.40	0.56
1:E:2189:LYS:HG2	1:E:2193:TYR:CE1	2.40	0.56
1:A:189:LYS:HG2	1:A:193:TYR:CE1	2.41	0.56
1:C:1282:VAL:HG12	1:C:1282:VAL:O	2.05	0.56
1:E:2282:VAL:HG12	1:E:2282:VAL:O	2.06	0.56
1:E:2331:HIS:CG	1:E:2346:VAL:HG11	2.41	0.56
1:A:282:VAL:HG12	1:A:282:VAL:O	2.05	0.55
1:C:1008:ASN:N	1:C:1008:ASN:HD22	2.04	0.55
1:C:1344:CYS:SG	1:C:1346:VAL:HG12	2.46	0.55
1:E:2115:ILE:HG23	1:E:2292:ILE:O	2.06	0.55
1:A:304:ILE:HD11	1:B:579:ALA:HA	1.88	0.55
1:D:1722:LYS:HZ2	1:D:1736:PRO:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2311:PRO:O	1:E:2312:ILE:HG13	2.07	0.55
1:F:2580:LEU:CD2	1:F:2590:ALA:HB1	2.36	0.55
1:B:633:ARG:HA	1:B:666:PHE:O	2.06	0.55
1:B:679:ILE:O	1:B:683:VAL:HG22	2.06	0.55
1:B:731:HIS:CG	1:B:746:VAL:HG11	2.40	0.55
1:C:1324:VAL:CG2	1:C:1354:LEU:HB2	2.37	0.55
1:A:26:LYS:HD3	1:A:100:ILE:HD11	1.87	0.55
1:D:1540:HIS:HD2	1:D:1542:ALA:CB	2.19	0.55
1:E:2044:THR:HG23	1:E:2300:PHE:CD2	2.41	0.55
1:F:2589:LYS:HG2	1:F:2593:TYR:CE1	2.42	0.55
1:F:2608:VAL:HG13	1:F:2617:GLU:HB2	1.89	0.55
1:F:2727:CYS:SG	1:F:2729:ASN:N	2.74	0.55
1:A:236:THR:HB	1:A:241:ARG:HG2	1.89	0.55
1:C:1187:GLN:HG2	1:C:1217:GLU:OE1	2.07	0.55
1:C:1189:LYS:HG2	1:C:1193:TYR:CE1	2.42	0.55
1:E:2140:HIS:H	1:F:2511:GLN:NE2	2.05	0.55
1:A:71:VAL:HG12	1:A:93:GLY:HA3	1.89	0.55
1:A:111:GLN:NE2	1:B:540:HIS:H	2.05	0.55
1:C:1111:GLN:NE2	1:D:1540:HIS:H	2.05	0.55
1:C:1326:ARG:NH1	1:C:1381:GLN:HE21	2.03	0.55
1:D:1608:VAL:CG2	1:D:1632:VAL:HG13	2.37	0.55
1:D:1613:ASP:OD1	1:F:2640:ARG:NH1	2.38	0.55
1:E:2026:LYS:HD3	1:E:2100:ILE:HD11	1.89	0.55
1:E:2140:HIS:HD2	1:E:2142:ALA:CB	2.19	0.55
1:F:2408:ASN:HB2	1:F:2411:GLU:HG3	1.89	0.55
1:F:2540:HIS:HD2	1:F:2542:ALA:HB3	1.72	0.55
1:A:57:VAL:HG21	1:A:116:ALA:HB2	1.89	0.55
1:A:121:ARG:HB3	1:A:389:ILE:HD11	1.89	0.55
1:E:2104:ALA:O	1:E:2108:MET:HG3	2.07	0.55
1:F:2711:PRO:O	1:F:2712:ILE:HG13	2.07	0.55
1:F:2722:LYS:HZ2	1:F:2736:PRO:HB3	1.71	0.55
1:A:246:LYS:HD3	1:D:1485:TYR:OH	2.07	0.55
1:B:589:LYS:HG2	1:B:593:TYR:CE1	2.41	0.55
1:E:2180:LEU:CD2	1:E:2190:ALA:HB1	2.37	0.55
1:E:2298:VAL:O	1:E:2300:PHE:N	2.40	0.55
1:F:2402:LYS:HD3	1:F:2406:ILE:HD12	1.87	0.55
1:C:1026:LYS:HD3	1:C:1100:ILE:HD11	1.88	0.54
1:C:1028:ILE:CD1	1:D:1594:PHE:HA	2.37	0.54
1:C:1166:GLU:O	1:C:1168:MET:N	2.40	0.54
1:E:2140:HIS:HD2	1:E:2142:ALA:HB3	1.72	0.54
1:E:2315:ARG:NH1	1:F:2609:ASP:OD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ASN:N	1:A:8:ASN:HD22	2.04	0.54
1:A:197:VAL:HB	1:B:428:ILE:CD1	2.36	0.54
1:A:208:VAL:CG2	1:A:232:VAL:HG13	2.37	0.54
1:A:320:GLY:HA3	1:A:322:LYS:HE2	1.89	0.54
1:C:1276:ILE:O	1:C:1280:VAL:HG22	2.07	0.54
1:D:1679:ILE:O	1:D:1683:VAL:HG22	2.06	0.54
1:D:1731:HIS:CG	1:D:1746:VAL:HG11	2.42	0.54
1:A:224:ALA:O	1:A:226:GLY:N	2.40	0.54
1:A:322:LYS:CG	1:A:336:PRO:HA	2.15	0.54
1:A:326:ARG:NH1	1:A:381:GLN:HE21	2.06	0.54
1:B:473:VAL:HB	1:B:759:ILE:HB	1.90	0.54
1:C:1002:LYS:HD3	1:C:1006:ILE:HD12	1.87	0.54
1:E:2208:VAL:CG2	1:E:2232:VAL:HG13	2.37	0.54
1:E:2365:VAL:HG12	1:E:2365:VAL:O	2.08	0.54
1:F:2566:GLU:O	1:F:2569:GLY:N	2.41	0.54
1:F:2765:VAL:HG12	1:F:2765:VAL:O	2.08	0.54
1:D:1426:LYS:HD3	1:D:1500:ILE:HD11	1.89	0.54
1:F:2608:VAL:CG2	1:F:2632:VAL:HG13	2.37	0.54
1:C:1180:LEU:C	1:C:1180:LEU:HD23	2.28	0.54
1:D:1534:PHE:HB3	3:D:1792:PCP:H3	1.90	0.54
1:D:1724:VAL:CG2	1:D:1754:LEU:HB2	2.37	0.54
1:A:149:ARG:NH1	1:A:153:ILE:HD11	2.22	0.54
1:B:647:ILE:HD11	1:E:2239:SER:O	2.08	0.54
1:A:187:GLN:HG2	1:A:217:GLU:OE1	2.08	0.54
1:A:208:VAL:HG12	1:A:209:ASP:N	2.23	0.54
1:B:431:VAL:C	1:B:433:ASN:N	2.61	0.54
1:B:676:ILE:O	1:B:680:VAL:HG22	2.08	0.54
1:C:1219:VAL:O	1:C:1223:GLU:HG2	2.08	0.54
1:C:1320:GLY:HA3	1:C:1322:LYS:HE2	1.89	0.54
1:D:1608:VAL:HG13	1:D:1617:GLU:HB2	1.90	0.54
1:F:2724:VAL:HG23	1:F:2724:VAL:O	2.07	0.54
1:A:180:LEU:C	1:A:180:LEU:HD23	2.28	0.54
1:A:208:VAL:HG13	1:A:217:GLU:HB2	1.89	0.54
1:A:208:VAL:HG21	1:A:232:VAL:HG13	1.90	0.54
1:D:1660:TYR:HA	1:D:1662:TRP:CZ3	2.43	0.54
1:E:2317:LYS:HD3	1:E:2318:LEU:N	2.23	0.54
1:E:2324:VAL:CG2	1:E:2354:LEU:HB2	2.38	0.54
1:A:198:ILE:HG12	1:B:428:ILE:HD11	1.90	0.54
1:C:1279:ILE:O	1:C:1283:VAL:HG22	2.08	0.54
1:C:1298:VAL:O	1:C:1300:PHE:N	2.40	0.54
1:C:1311:PRO:O	1:C:1312:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2426:LYS:HD3	1:F:2500:ILE:HD11	1.89	0.54
1:F:2453:TRP:CD1	1:F:2453:TRP:C	2.81	0.54
1:F:2717:LYS:HD3	1:F:2718:LEU:N	2.22	0.54
1:A:28:ILE:CD1	1:B:594:PHE:HA	2.38	0.54
1:A:365:VAL:HG12	1:A:365:VAL:O	2.08	0.54
1:B:765:VAL:HG12	1:B:765:VAL:O	2.08	0.54
1:D:1726:ARG:HH12	1:D:1781:GLN:NE2	2.05	0.54
1:E:2133:SER:O	1:E:2134:PHE:HD1	1.91	0.54
1:F:2540:HIS:HD2	1:F:2542:ALA:CB	2.20	0.54
1:B:645:ARG:N	1:B:679:ILE:HD11	2.22	0.53
1:B:766:VAL:HG12	1:B:767:GLU:N	2.23	0.53
1:C:1224:ALA:O	1:C:1226:GLY:N	2.41	0.53
1:E:2156:CYS:O	1:E:2375:ARG:NH1	2.41	0.53
1:F:2566:GLU:O	1:F:2568:MET:N	2.41	0.53
1:C:1208:VAL:CG2	1:C:1232:VAL:HG13	2.39	0.53
1:F:2457:VAL:HG21	1:F:2516:ALA:HB2	1.90	0.53
1:E:2209:ASP:OD2	1:F:2715:ARG:NH1	2.41	0.53
1:F:2724:VAL:CG2	1:F:2754:LEU:HB2	2.37	0.53
1:A:322:LYS:HD2	1:A:322:LYS:N	2.24	0.53
1:B:515:ILE:HG23	1:B:692:ILE:O	2.07	0.53
1:B:608:VAL:HG13	1:B:617:GLU:HB2	1.90	0.53
1:D:1431:VAL:C	1:D:1433:ASN:N	2.61	0.53
1:F:2722:LYS:HD2	1:F:2722:LYS:N	2.24	0.53
1:A:311:PRO:O	1:A:312:ILE:HG13	2.07	0.53
1:B:426:LYS:HD3	1:B:500:ILE:HD11	1.91	0.53
1:B:717:LYS:HD3	1:B:718:LEU:N	2.23	0.53
1:B:720:GLY:HA3	1:B:722:LYS:HE2	1.90	0.53
1:D:1625:LEU:CB	1:D:1628:LYS:HB2	2.38	0.53
1:E:2322:LYS:HD2	1:E:2322:LYS:N	2.23	0.53
1:E:2343:ARG:HG2	1:E:2343:ARG:HH11	1.74	0.53
1:F:2676:ILE:O	1:F:2680:VAL:HG22	2.09	0.53
1:F:2473:VAL:HB	1:F:2759:ILE:HB	1.90	0.53
1:F:2549:ARG:NH1	1:F:2553:ILE:HD11	2.22	0.53
1:F:2575:THR:OG1	1:F:2576:MET:N	2.41	0.53
1:B:587:GLN:HG2	1:B:617:GLU:OE1	2.09	0.53
1:B:653:TRP:CG	1:F:2718:LEU:HD22	2.44	0.53
1:D:1608:VAL:HG21	1:D:1632:VAL:HG13	1.90	0.53
1:D:1739:LYS:HD2	1:D:1739:LYS:N	2.23	0.53
1:F:2682:VAL:HG12	1:F:2682:VAL:O	2.08	0.53
1:A:140:HIS:HD2	1:A:142:ALA:CB	2.22	0.53
1:B:471:VAL:HG12	1:B:493:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:ARG:HE	1:B:779:LEU:HD11	1.73	0.53
1:D:1471:VAL:HG12	1:D:1493:GLY:HA3	1.89	0.53
1:F:2743:ARG:HG2	1:F:2743:ARG:HH11	1.74	0.53
1:B:739:LYS:HD2	1:B:739:LYS:N	2.23	0.53
1:C:1028:ILE:CD1	1:D:1597:VAL:HB	2.38	0.53
1:C:1140:HIS:HD2	1:C:1142:ALA:HB3	1.73	0.53
1:C:1197:VAL:HB	1:D:1428:ILE:CD1	2.37	0.53
1:D:1457:VAL:HG21	1:D:1516:ALA:HB2	1.90	0.53
1:D:1625:LEU:O	1:D:1628:LYS:N	2.32	0.53
1:E:2073:VAL:HB	1:E:2359:ILE:HB	1.91	0.53
1:F:2587:GLN:HG2	1:F:2617:GLU:OE1	2.09	0.53
1:F:2720:GLY:HA3	1:F:2722:LYS:HE2	1.91	0.53
1:A:6:ILE:HD11	1:B:409:GLU:OE1	2.09	0.53
1:B:625:LEU:O	1:B:628:LYS:N	2.33	0.53
1:E:2073:VAL:O	1:E:2358:ILE:HG12	2.09	0.53
1:E:2074:TYR:N	1:E:2074:TYR:CD1	2.76	0.53
1:B:474:TYR:CD1	1:B:474:TYR:N	2.77	0.52
1:C:1073:VAL:HB	1:C:1359:ILE:HB	1.90	0.52
1:C:1137:ARG:HB3	1:C:1137:ARG:NH1	2.23	0.52
1:C:1198:ILE:HG12	1:D:1428:ILE:HD11	1.90	0.52
1:F:2444:THR:HG22	1:F:2699:ASP:O	2.09	0.52
1:F:2474:TYR:CD1	1:F:2474:TYR:N	2.77	0.52
1:B:540:HIS:HD2	1:B:542:ALA:HB3	1.74	0.52
1:B:721:ARG:O	1:B:722:LYS:HD2	2.10	0.52
1:D:1548:ASP:HB3	1:D:1559:VAL:HG21	1.92	0.52
1:D:1717:LYS:HD3	1:D:1718:LEU:N	2.24	0.52
1:D:1746:VAL:CG2	1:D:1747:CYS:H	2.06	0.52
1:F:2608:VAL:HG21	1:F:2632:VAL:HG13	1.90	0.52
1:A:21:TYR:CD1	1:B:577:PRO:HG3	2.44	0.52
1:A:209:ASP:OD2	1:B:715:ARG:NH1	2.43	0.52
1:B:556:CYS:O	1:B:775:ARG:NH1	2.42	0.52
1:B:566:GLU:O	1:B:569:GLY:N	2.42	0.52
1:C:1031:VAL:C	1:C:1033:ASN:N	2.62	0.52
1:C:1140:HIS:HD2	1:C:1142:ALA:CB	2.22	0.52
1:F:2612:TYR:CD1	1:F:2612:TYR:N	2.77	0.52
1:A:134:PHE:HB3	3:A:392:PCP:H3	1.91	0.52
1:A:324:VAL:CG2	1:A:354:LEU:HB2	2.38	0.52
1:A:339:LYS:HD2	1:A:339:LYS:N	2.24	0.52
1:B:534:PHE:HB3	3:B:792:PCP:H3	1.91	0.52
1:C:1365:VAL:HG12	1:C:1365:VAL:O	2.09	0.52
1:D:1723:GLN:HE21	1:D:1753:PRO:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1775:ARG:HE	1:D:1779:LEU:HD11	1.73	0.52
1:E:2134:PHE:HB3	3:E:2392:PCP:H3	1.91	0.52
1:E:2176:MET:HE2	1:E:2181:ILE:HD11	1.91	0.52
1:E:2194:PHE:HA	1:F:2428:ILE:HD12	1.92	0.52
1:E:2248:ILE:HD13	1:E:2283:VAL:CG1	2.40	0.52
1:F:2431:VAL:C	1:F:2433:ASN:N	2.62	0.52
1:F:2556:CYS:O	1:F:2775:ARG:NH1	2.42	0.52
1:A:53:TRP:CD1	1:A:53:TRP:C	2.82	0.52
1:B:666:PHE:CD2	1:B:685:ALA:HB3	2.45	0.52
1:D:1408:ASN:HD22	1:D:1408:ASN:N	2.08	0.52
1:D:1711:PRO:O	1:D:1712:ILE:HG13	2.10	0.52
1:E:2053:TRP:CD1	1:E:2053:TRP:C	2.82	0.52
1:E:2071:VAL:HG12	1:E:2093:GLY:HA3	1.92	0.52
1:E:2208:VAL:HG21	1:E:2232:VAL:HG13	1.90	0.52
1:A:180:LEU:CD2	1:A:190:ALA:HB1	2.40	0.52
1:A:317:LYS:HD3	1:A:318:LEU:N	2.25	0.52
1:C:1006:ILE:HD11	1:D:1409:GLU:OE1	2.10	0.52
1:D:1453:TRP:CZ3	1:D:1788:GLU:O	2.62	0.52
1:D:1587:GLN:HG2	1:D:1617:GLU:OE1	2.10	0.52
1:D:1743:ARG:HH11	1:D:1743:ARG:HG2	1.74	0.52
1:A:175:THR:OG1	1:A:176:MET:N	2.42	0.52
1:B:625:LEU:CB	1:B:628:LYS:HB2	2.38	0.52
1:C:1209:ASP:OD2	1:D:1715:ARG:NH1	2.43	0.52
1:C:1212:TYR:N	1:C:1212:TYR:CD1	2.78	0.52
1:D:1426:LYS:HG2	1:D:1430:GLU:OE1	2.10	0.52
1:D:1766:VAL:HG12	1:D:1767:GLU:N	2.24	0.52
1:E:2115:ILE:HD13	1:E:2147:ILE:HG23	1.92	0.52
1:E:2187:GLN:HG2	1:E:2217:GLU:OE1	2.09	0.52
1:F:2473:VAL:O	1:F:2758:ILE:HG12	2.09	0.52
1:F:2625:LEU:O	1:F:2628:LYS:N	2.35	0.52
1:A:148:ASP:HB3	1:A:159:VAL:HG21	1.92	0.52
1:B:608:VAL:CG2	1:B:632:VAL:HG13	2.39	0.52
1:B:660:TYR:HA	1:B:662:TRP:CZ3	2.45	0.52
1:C:1322:LYS:HD2	1:C:1322:LYS:N	2.23	0.52
1:D:1575:THR:OG1	1:D:1576:MET:N	2.42	0.52
1:D:1720:GLY:HA3	1:D:1722:LYS:HE2	1.91	0.52
1:E:2053:TRP:CZ3	1:E:2388:GLU:O	2.63	0.52
1:E:2236:THR:HB	1:E:2241:ARG:HG2	1.92	0.52
1:A:104:ALA:O	1:A:108:MET:HG3	2.09	0.52
1:A:323:GLN:OE1	1:A:355:LEU:HD23	2.10	0.52
1:B:476:MET:HE2	1:B:724:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1118:ALA:O	1:C:1122:ILE:HD13	2.10	0.52
1:C:1180:LEU:CD2	1:C:1190:ALA:HB1	2.40	0.52
1:A:31:VAL:C	1:A:33:ASN:N	2.62	0.52
1:B:566:GLU:O	1:B:568:MET:N	2.43	0.52
1:C:1073:VAL:O	1:C:1358:ILE:HG12	2.09	0.52
1:D:1473:VAL:HB	1:D:1759:ILE:HB	1.91	0.52
1:E:2320:GLY:HA3	1:E:2322:LYS:HE2	1.92	0.52
1:A:166:GLU:O	1:A:169:GLY:N	2.42	0.51
1:A:321:ARG:O	1:A:322:LYS:NZ	2.40	0.51
1:B:726:ARG:HH12	1:B:781:GLN:NE2	2.06	0.51
1:D:1765:VAL:HG12	1:D:1765:VAL:O	2.08	0.51
1:E:2111:GLN:NE2	1:F:2540:HIS:H	2.07	0.51
1:E:2260:TYR:HA	1:E:2262:TRP:CZ3	2.45	0.51
1:A:156:CYS:O	1:A:375:ARG:NH1	2.43	0.51
1:A:212:TYR:N	1:A:212:TYR:CD1	2.78	0.51
1:A:323:GLN:HE21	1:A:353:PRO:HB3	1.74	0.51
1:C:1134:PHE:HB3	3:C:1392:PCP:H3	1.92	0.51
1:C:1156:CYS:O	1:C:1375:ARG:NH1	2.43	0.51
1:D:1624:ALA:O	1:D:1626:GLY:N	2.43	0.51
1:A:73:VAL:O	1:A:358:ILE:HG12	2.11	0.51
1:A:324:VAL:HG23	1:A:324:VAL:O	2.10	0.51
1:B:698:VAL:O	1:B:700:PHE:N	2.42	0.51
1:C:1009:GLU:OE1	1:D:1406:ILE:HD11	2.10	0.51
1:C:1208:VAL:HG12	1:C:1209:ASP:N	2.24	0.51
1:C:1236:THR:HB	1:C:1241:ARG:HG2	1.93	0.51
1:E:2009:GLU:OE2	1:F:2403:ARG:HG2	2.10	0.51
1:E:2224:ALA:O	1:E:2226:GLY:N	2.43	0.51
1:E:2339:LYS:HD2	1:E:2339:LYS:N	2.25	0.51
1:F:2465:LEU:HD22	1:F:2508:MET:HE1	1.92	0.51
1:F:2679:ILE:O	1:F:2683:VAL:HG22	2.10	0.51
1:A:73:VAL:HB	1:A:359:ILE:HB	1.92	0.51
1:A:248:ILE:HD13	1:A:283:VAL:CG1	2.40	0.51
1:B:580:LEU:CD2	1:B:590:ALA:HB1	2.40	0.51
1:C:1076:MET:HE1	1:C:1324:VAL:HG21	1.92	0.51
1:C:1115:ILE:HD13	1:C:1147:ILE:HG23	1.92	0.51
1:D:1474:TYR:CD1	1:D:1474:TYR:N	2.77	0.51
1:D:1647:ILE:HD11	1:F:2639:SER:O	2.11	0.51
1:E:2003:ARG:HB2	1:F:2464:LYS:HD3	1.92	0.51
1:F:2624:ALA:O	1:F:2626:GLY:N	2.43	0.51
1:B:518:ALA:O	1:B:522:ILE:HD13	2.10	0.51
1:B:743:ARG:HH11	1:B:743:ARG:HG2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1339:LYS:HD2	1:C:1339:LYS:N	2.25	0.51
1:D:1657:VAL:HG22	1:E:2322:LYS:HE3	1.92	0.51
1:E:2038:VAL:CG1	1:E:2307:VAL:HG13	2.40	0.51
1:E:2225:LEU:O	1:E:2228:LYS:N	2.34	0.51
1:A:140:HIS:HD2	1:A:142:ALA:HB3	1.75	0.51
1:A:298:VAL:O	1:A:300:PHE:N	2.43	0.51
1:D:1580:LEU:CD2	1:D:1590:ALA:HB1	2.41	0.51
1:F:2533:SER:O	1:F:2534:PHE:HD1	1.93	0.51
1:A:137:ARG:HB3	1:A:137:ARG:NH1	2.26	0.51
1:B:548:ASP:HB3	1:B:559:VAL:HG21	1.92	0.51
1:C:1021:TYR:HB2	1:D:1575:THR:O	2.10	0.51
1:C:1026:LYS:HG2	1:C:1030:GLU:OE1	2.11	0.51
1:C:1175:THR:O	1:D:1421:TYR:HB2	2.11	0.51
1:D:1556:CYS:O	1:D:1775:ARG:NH1	2.43	0.51
1:D:1588:VAL:HA	1:D:1591:TRP:HE1	1.74	0.51
1:E:2140:HIS:HE1	1:F:2461:GLU:OE1	1.94	0.51
1:F:2471:VAL:HG12	1:F:2493:GLY:HA3	1.93	0.51
1:F:2534:PHE:HB3	3:F:2792:PCP:H3	1.93	0.51
1:B:453:TRP:CD1	1:B:453:TRP:C	2.83	0.51
1:C:1317:LYS:HD3	1:C:1318:LEU:N	2.25	0.51
1:D:1453:TRP:CD1	1:D:1453:TRP:C	2.84	0.51
1:E:2212:TYR:N	1:E:2212:TYR:CD1	2.78	0.51
1:A:26:LYS:HG2	1:A:30:GLU:OE1	2.11	0.51
1:A:175:THR:O	1:B:421:TYR:HB2	2.10	0.51
1:A:366:VAL:HG12	1:A:367:GLU:N	2.25	0.51
1:C:1366:VAL:HG12	1:C:1367:GLU:N	2.25	0.51
1:D:1612:TYR:CD1	1:D:1612:TYR:N	2.79	0.51
1:F:2660:TYR:HA	1:F:2662:TRP:CZ3	2.46	0.51
1:F:2744:CYS:SG	1:F:2746:VAL:HG12	2.51	0.51
1:F:2775:ARG:HE	1:F:2779:LEU:HD11	1.76	0.51
1:B:612:TYR:CD1	1:B:612:TYR:N	2.79	0.51
1:C:1225:LEU:O	1:C:1228:LYS:N	2.33	0.51
1:C:1260:TYR:HA	1:C:1262:TRP:CZ3	2.46	0.51
1:D:1566:GLU:O	1:D:1569:GLY:N	2.44	0.51
1:D:1653:TRP:CG	1:E:2318:LEU:HD22	2.46	0.51
1:F:2515:ILE:HD13	1:F:2547:ILE:HG23	1.94	0.51
1:C:1057:VAL:HG21	1:C:1116:ALA:HB2	1.92	0.50
1:D:1476:MET:HE1	1:D:1724:VAL:HG21	1.91	0.50
1:D:1666:PHE:CD2	1:D:1685:ALA:HB3	2.46	0.50
1:E:2031:VAL:C	1:E:2033:ASN:N	2.62	0.50
1:E:2344:CYS:SG	1:E:2346:VAL:HG12	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1133:SER:O	1:C:1134:PHE:HD1	1.94	0.50
1:E:2166:GLU:O	1:E:2169:GLY:N	2.44	0.50
1:F:2739:LYS:HD2	1:F:2739:LYS:N	2.27	0.50
1:B:408:ASN:HD22	1:B:408:ASN:N	2.07	0.50
1:B:683:VAL:HG21	1:B:686:PHE:CZ	2.45	0.50
1:C:1148:ASP:HB3	1:C:1159:VAL:HG21	1.93	0.50
1:C:1248:ILE:CG2	1:C:1282:VAL:HG12	2.42	0.50
1:E:2137:ARG:CG	1:E:2137:ARG:NH1	2.73	0.50
1:E:2149:ARG:NH2	1:F:2405:TYR:CE1	2.79	0.50
1:E:2208:VAL:HG12	1:E:2209:ASP:N	2.26	0.50
1:F:2453:TRP:CZ3	1:F:2788:GLU:O	2.64	0.50
1:B:476:MET:HE1	1:B:724:VAL:HG21	1.94	0.50
1:B:624:ALA:O	1:B:626:GLY:N	2.44	0.50
1:C:1071:VAL:HG12	1:C:1093:GLY:HA3	1.92	0.50
1:D:1621:ALA:O	1:D:1629:LEU:HD22	2.11	0.50
1:D:1721:ARG:O	1:D:1722:LYS:HD2	2.12	0.50
1:F:2408:ASN:N	1:F:2408:ASN:HD22	2.10	0.50
1:A:9:GLU:OE1	1:B:406:ILE:HD11	2.10	0.50
1:A:26:LYS:HD2	1:A:96:ALA:O	2.11	0.50
1:A:140:HIS:H	1:B:511:GLN:NE2	2.10	0.50
1:B:722:LYS:HD2	1:B:722:LYS:N	2.25	0.50
1:C:1028:ILE:HD12	1:D:1594:PHE:HA	1.92	0.50
1:D:1722:LYS:HD2	1:D:1722:LYS:N	2.26	0.50
1:B:426:LYS:HG2	1:B:430:GLU:OE1	2.10	0.50
1:B:521:ARG:HB3	1:B:789:ILE:HD11	1.92	0.50
1:B:575:THR:OG1	1:B:576:MET:N	2.45	0.50
1:F:2426:LYS:HG2	1:F:2430:GLU:OE1	2.11	0.50
1:A:248:ILE:CG2	1:A:282:VAL:HG12	2.41	0.50
1:B:426:LYS:O	1:B:430:GLU:HB2	2.12	0.50
1:D:1608:VAL:HG12	1:D:1609:ASP:N	2.27	0.50
1:A:74:TYR:N	1:A:74:TYR:CD1	2.80	0.50
1:A:260:TYR:HA	1:A:262:TRP:CZ3	2.46	0.50
1:B:722:LYS:HG2	1:C:1253:TRP:CH2	2.46	0.50
1:C:1026:LYS:HD2	1:C:1096:ALA:O	2.12	0.50
1:C:1026:LYS:O	1:C:1030:GLU:HB2	2.12	0.50
1:C:1077:PRO:HG2	1:C:1080:THR:OG1	2.12	0.50
1:E:2266:PHE:CD2	1:E:2285:ALA:HB3	2.46	0.50
1:F:2588:VAL:HA	1:F:2591:TRP:HE1	1.77	0.50
1:A:28:ILE:HD12	1:B:594:PHE:HA	1.94	0.50
1:B:426:LYS:HD2	1:B:496:ALA:O	2.12	0.50
1:B:453:TRP:CZ3	1:B:788:GLU:O	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:VAL:CG1	1:B:767:GLU:N	2.75	0.50
1:D:1636:THR:HB	1:D:1641:ARG:HG2	1.93	0.50
1:E:2028:ILE:HD12	1:F:2594:PHE:HA	1.94	0.50
1:A:77:PRO:HG2	1:A:80:THR:OG1	2.12	0.49
1:A:373:GLU:OE2	1:A:376:GLU:OE1	2.30	0.49
1:B:485:TYR:OH	1:C:1246:LYS:HD3	2.11	0.49
1:C:1037:LYS:NZ	4:C:16:HOH:O	2.44	0.49
1:D:1473:VAL:O	1:D:1758:ILE:HG12	2.11	0.49
1:E:2026:LYS:HD2	1:E:2096:ALA:O	2.12	0.49
1:E:2228:LYS:HA	1:E:2228:LYS:CE	2.41	0.49
1:A:28:ILE:CD1	1:B:597:VAL:HB	2.40	0.49
1:C:1146:MET:HE2	1:C:1147:ILE:HA	1.94	0.49
1:C:1266:PHE:CD2	1:C:1285:ALA:HB3	2.47	0.49
1:C:1323:GLN:OE1	1:C:1355:LEU:HD23	2.11	0.49
1:E:2061:GLU:OE1	1:F:2540:HIS:HE1	1.94	0.49
1:F:2477:PRO:HG2	1:F:2480:THR:OG1	2.12	0.49
1:C:1121:ARG:HB3	1:C:1389:ILE:HD11	1.93	0.49
1:C:1228:LYS:HA	1:C:1228:LYS:CE	2.40	0.49
1:D:1515:ILE:HG23	1:D:1692:ILE:O	2.12	0.49
1:F:2426:LYS:HD2	1:F:2496:ALA:O	2.12	0.49
1:F:2625:LEU:CB	1:F:2628:LYS:HB2	2.40	0.49
1:F:2683:VAL:HG21	1:F:2686:PHE:CZ	2.48	0.49
1:A:26:LYS:O	1:A:30:GLU:HB2	2.13	0.49
1:A:38:VAL:CG1	1:A:307:VAL:HG13	2.40	0.49
1:A:166:GLU:O	1:A:168:MET:N	2.45	0.49
1:A:221:ALA:O	1:A:229:LEU:HD22	2.12	0.49
1:B:588:VAL:HA	1:B:591:TRP:HE1	1.73	0.49
1:B:608:VAL:HG21	1:B:632:VAL:HG13	1.94	0.49
1:B:711:PRO:O	1:B:712:ILE:HG13	2.12	0.49
1:C:1283:VAL:HG21	1:C:1286:PHE:CZ	2.48	0.49
1:D:1426:LYS:HD2	1:D:1496:ALA:O	2.12	0.49
1:D:1521:ARG:HB3	1:D:1789:ILE:HD11	1.93	0.49
1:E:2069:ILE:HG23	1:E:2070:PRO:HD2	1.93	0.49
1:F:2608:VAL:HG12	1:F:2609:ASP:N	2.26	0.49
1:A:115:ILE:HD13	1:A:147:ILE:HG23	1.94	0.49
1:C:1208:VAL:HG21	1:C:1232:VAL:HG13	1.93	0.49
1:C:1324:VAL:HG23	1:C:1324:VAL:O	2.12	0.49
1:E:2121:ARG:NH1	1:E:2273:GLU:OE2	2.44	0.49
1:E:2194:PHE:HA	1:F:2428:ILE:CD1	2.42	0.49
1:E:2221:ALA:O	1:E:2229:LEU:HD22	2.12	0.49
1:E:2366:VAL:HG12	1:E:2367:GLU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2666:PHE:CD2	1:F:2685:ALA:HB3	2.47	0.49
1:A:253:TRP:HD1	1:A:254:GLU:OE2	1.96	0.49
1:A:279:ILE:O	1:A:283:VAL:HG22	2.13	0.49
1:B:457:VAL:HG21	1:B:516:ALA:HB2	1.94	0.49
1:B:537:ARG:NH1	1:B:537:ARG:HB3	2.28	0.49
1:D:1549:ARG:NH1	1:D:1553:ILE:HD11	2.23	0.49
1:F:2469:ILE:HG23	1:F:2470:PRO:HD2	1.94	0.49
1:A:105:LEU:HD12	1:A:106:LEU:N	2.26	0.49
1:B:444:THR:HG22	1:B:699:ASP:O	2.13	0.49
1:B:642:GLY:HA3	1:E:2238:SER:O	2.12	0.49
1:B:657:VAL:HG22	1:F:2722:LYS:HE3	1.93	0.49
1:E:2008:ASN:HD22	1:E:2008:ASN:N	2.10	0.49
1:E:2322:LYS:HZ2	1:E:2336:PRO:HB3	1.77	0.49
1:A:253:TRP:CH2	1:D:1722:LYS:HG2	2.48	0.49
1:B:473:VAL:O	1:B:758:ILE:HG12	2.12	0.49
1:B:671:LEU:HD12	1:B:688:VAL:HG22	1.93	0.49
1:C:1315:ARG:NH1	1:D:1609:ASP:OD2	2.46	0.49
1:E:2026:LYS:HG2	1:E:2030:GLU:OE1	2.12	0.49
1:F:2537:ARG:NH1	1:F:2537:ARG:HB3	2.27	0.49
1:A:118:ALA:O	1:A:122:ILE:HD13	2.12	0.49
1:A:315:ARG:NH1	1:B:609:ASP:OD2	2.46	0.49
1:D:1469:ILE:HG23	1:D:1470:PRO:HD2	1.95	0.49
1:E:2021:TYR:CD1	1:F:2577:PRO:HG3	2.47	0.49
1:E:2137:ARG:NH1	1:E:2137:ARG:HB3	2.27	0.49
1:F:2521:ARG:HB3	1:F:2789:ILE:HD11	1.95	0.49
1:A:137:ARG:CG	1:A:137:ARG:NH1	2.73	0.49
1:B:608:VAL:HG12	1:B:609:ASP:N	2.26	0.49
1:D:1476:MET:HE2	1:D:1724:VAL:HG21	1.95	0.49
1:D:1683:VAL:HG21	1:D:1686:PHE:CZ	2.48	0.49
1:F:2621:ALA:O	1:F:2629:LEU:HD22	2.13	0.49
1:B:628:LYS:HA	1:B:628:LYS:CE	2.40	0.48
1:C:1074:TYR:N	1:C:1074:TYR:CD1	2.80	0.48
1:C:1193:TYR:HB3	1:D:1428:ILE:HG23	1.95	0.48
1:D:1580:LEU:C	1:D:1580:LEU:HD23	2.34	0.48
1:D:1766:VAL:CG1	1:D:1767:GLU:N	2.76	0.48
1:C:1221:ALA:O	1:C:1229:LEU:HD22	2.13	0.48
1:C:1271:LEU:HD12	1:C:1288:VAL:HG22	1.96	0.48
1:D:1444:THR:HG22	1:D:1699:ASP:O	2.12	0.48
1:D:1628:LYS:HA	1:D:1628:LYS:CE	2.40	0.48
1:E:2003:ARG:HG2	1:F:2409:GLU:OE2	2.12	0.48
1:F:2723:GLN:HE21	1:F:2753:PRO:HB3	1.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:HE2	1:A:324:VAL:HG21	1.95	0.48
1:C:1248:ILE:HD13	1:C:1283:VAL:CG1	2.43	0.48
1:E:2077:PRO:HG2	1:E:2080:THR:OG1	2.13	0.48
1:E:2166:GLU:O	1:E:2168:MET:N	2.45	0.48
1:F:2424:ARG:O	1:F:2428:ILE:HG12	2.14	0.48
1:A:15:GLY:O	1:A:18:THR:HG23	2.13	0.48
1:A:20:VAL:HG23	1:A:21:TYR:N	2.29	0.48
1:A:225:LEU:CB	1:A:228:LYS:HB2	2.39	0.48
1:B:580:LEU:C	1:B:580:LEU:HD23	2.34	0.48
1:B:636:THR:HB	1:B:641:ARG:HG2	1.95	0.48
1:C:1015:GLY:O	1:C:1018:THR:HG23	2.14	0.48
1:C:1165:ALA:HB2	1:C:1172:ALA:HB2	1.95	0.48
1:D:1698:VAL:O	1:D:1700:PHE:N	2.45	0.48
1:E:2148:ASP:HB3	1:E:2159:VAL:HG21	1.94	0.48
1:B:621:ALA:O	1:B:629:LEU:HD22	2.13	0.48
1:B:724:VAL:HG23	1:B:724:VAL:O	2.13	0.48
1:C:1028:ILE:HG23	1:D:1593:TYR:HB3	1.95	0.48
1:C:1149:ARG:NH1	1:C:1153:ILE:HD11	2.23	0.48
1:D:1671:LEU:HD12	1:D:1688:VAL:HG22	1.95	0.48
1:D:1744:CYS:SG	1:D:1746:VAL:CG1	3.02	0.48
1:E:2180:LEU:C	1:E:2180:LEU:HD23	2.34	0.48
1:F:2469:ILE:O	1:F:2471:VAL:N	2.41	0.48
1:F:2723:GLN:OE1	1:F:2755:LEU:HD23	2.14	0.48
1:B:716:GLY:HA2	1:C:1250:GLU:OE2	2.13	0.48
1:B:744:CYS:SG	1:B:746:VAL:CG1	3.01	0.48
1:C:1069:ILE:HG23	1:C:1070:PRO:HD2	1.96	0.48
1:C:1105:LEU:HD12	1:C:1106:LEU:N	2.28	0.48
1:C:1175:THR:OG1	1:C:1176:MET:N	2.46	0.48
1:D:1724:VAL:HG23	1:D:1724:VAL:O	2.13	0.48
1:E:2149:ARG:NH1	1:E:2153:ILE:HD11	2.23	0.48
1:A:21:TYR:HB2	1:B:575:THR:O	2.14	0.48
1:A:69:ILE:HG23	1:A:70:PRO:HD2	1.95	0.48
1:A:248:ILE:HG22	1:A:282:VAL:HG12	1.96	0.48
1:A:266:PHE:CD2	1:A:285:ALA:HB3	2.49	0.48
1:C:1021:TYR:CD1	1:D:1577:PRO:HG3	2.48	0.48
1:C:1137:ARG:CG	1:C:1137:ARG:NH1	2.73	0.48
1:C:1140:HIS:H	1:D:1511:GLN:NE2	2.11	0.48
1:F:2476:MET:HE1	1:F:2724:VAL:HG21	1.96	0.48
1:A:180:LEU:HD23	1:A:181:ILE:N	2.29	0.48
1:B:648:ILE:HD13	1:B:683:VAL:CG1	2.44	0.48
1:C:1205:ILE:HA	1:C:1231:ALA:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1566:GLU:O	1:D:1568:MET:N	2.47	0.48
1:D:1642:GLY:HA3	1:F:2638:SER:O	2.12	0.48
1:E:2064:LYS:HD3	1:F:2403:ARG:HB2	1.95	0.48
1:E:2330:GLY:O	1:E:2332:TYR:HD1	1.97	0.48
1:F:2619:VAL:HG11	1:F:2658:ARG:HD2	1.96	0.48
1:A:343:ARG:HG2	1:A:343:ARG:HH11	1.79	0.48
1:A:375:ARG:HE	1:A:379:LEU:HD11	1.79	0.48
1:B:722:LYS:HZ2	1:B:736:PRO:CB	2.24	0.48
1:C:1253:TRP:HD1	1:C:1254:GLU:OE2	1.97	0.48
1:D:1537:ARG:NH1	1:D:1537:ARG:HB3	2.29	0.48
1:D:1648:ILE:HD13	1:D:1683:VAL:CG1	2.44	0.48
1:E:2026:LYS:O	1:E:2030:GLU:HB2	2.14	0.48
1:E:2028:ILE:CD1	1:F:2594:PHE:HA	2.44	0.48
1:E:2107:GLY:HA3	1:F:2539:MET:O	2.14	0.48
1:E:2321:ARG:O	1:E:2322:LYS:NZ	2.38	0.48
1:F:2648:ILE:HD13	1:F:2683:VAL:CG1	2.44	0.48
1:A:165:ALA:HB2	1:A:172:ALA:HB2	1.96	0.47
1:A:344:CYS:SG	1:A:346:VAL:CG1	3.01	0.47
1:B:477:PRO:HG2	1:B:480:THR:OG1	2.14	0.47
1:C:1219:VAL:HG11	1:C:1258:ARG:HD2	1.95	0.47
1:E:2105:LEU:HD12	1:E:2106:LEU:N	2.29	0.47
1:F:2721:ARG:O	1:F:2722:LYS:HD2	2.14	0.47
1:F:2766:VAL:HG12	1:F:2767:GLU:N	2.28	0.47
1:A:76:MET:HE1	1:A:324:VAL:HG21	1.97	0.47
1:A:146:MET:HE2	1:A:147:ILE:HA	1.96	0.47
1:A:172:ALA:HB3	1:B:420:VAL:CG1	2.44	0.47
1:B:424:ARG:O	1:B:428:ILE:HG12	2.14	0.47
1:B:653:TRP:HD1	1:B:654:GLU:OE2	1.97	0.47
1:C:1069:ILE:HA	1:C:1070:PRO:HD3	1.78	0.47
1:D:1477:PRO:HG2	1:D:1480:THR:OG1	2.14	0.47
1:D:1533:SER:O	1:D:1534:PHE:HD1	1.97	0.47
1:E:2283:VAL:HG21	1:E:2286:PHE:CZ	2.49	0.47
1:B:648:ILE:CG2	1:B:682:VAL:HG12	2.44	0.47
1:D:1540:HIS:HD2	1:D:1542:ALA:HB3	1.78	0.47
1:E:2044:THR:HG22	1:E:2299:ASP:O	2.14	0.47
1:F:2521:ARG:NH1	1:F:2673:GLU:OE2	2.44	0.47
1:A:271:LEU:HD12	1:A:288:VAL:HG22	1.95	0.47
1:B:723:GLN:HE21	1:B:753:PRO:HB3	1.76	0.47
1:C:1248:ILE:HG22	1:C:1282:VAL:HG12	1.97	0.47
1:D:1426:LYS:O	1:D:1430:GLU:HB2	2.13	0.47
1:D:1723:GLN:OE1	1:D:1755:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2139:MET:O	1:F:2507:GLY:HA3	2.14	0.47
1:A:28:ILE:HG23	1:B:593:TYR:HB3	1.95	0.47
1:C:1020:VAL:HG23	1:C:1021:TYR:N	2.29	0.47
1:C:1180:LEU:HD23	1:C:1181:ILE:N	2.29	0.47
1:E:2208:VAL:HG13	1:E:2217:GLU:CB	2.45	0.47
1:F:2648:ILE:CG2	1:F:2682:VAL:HG12	2.44	0.47
1:C:1069:ILE:O	1:C:1071:VAL:N	2.40	0.47
1:F:2426:LYS:O	1:F:2430:GLU:HB2	2.13	0.47
1:F:2469:ILE:HA	1:F:2470:PRO:HD3	1.76	0.47
1:F:2636:THR:HB	1:F:2641:ARG:HG2	1.96	0.47
1:A:39:LEU:HD23	1:A:321:ARG:HB2	1.97	0.47
1:A:193:TYR:HB3	1:B:428:ILE:HG23	1.97	0.47
1:A:205:ILE:HA	1:A:231:ALA:O	2.14	0.47
1:A:326:ARG:HH12	1:A:381:GLN:NE2	2.12	0.47
1:B:549:ARG:NH1	1:B:553:ILE:HD11	2.24	0.47
1:C:1043:THR:HG22	1:C:1087:PRO:HA	1.97	0.47
1:C:1208:VAL:HG13	1:C:1217:GLU:CB	2.44	0.47
1:C:1343:ARG:HG2	1:C:1343:ARG:HH11	1.79	0.47
1:C:1366:VAL:CG1	1:C:1367:GLU:N	2.78	0.47
1:E:2323:GLN:OE1	1:E:2355:LEU:HD23	2.14	0.47
1:E:2375:ARG:HE	1:E:2379:LEU:HD11	1.78	0.47
1:F:2518:ALA:O	1:F:2522:ILE:HD13	2.14	0.47
1:F:2605:ILE:HD12	1:F:2605:ILE:N	2.29	0.47
1:F:2608:VAL:HG13	1:F:2617:GLU:CB	2.45	0.47
1:A:44:THR:CG2	1:A:298:VAL:HG12	2.32	0.47
1:A:176:MET:HE2	1:A:181:ILE:HD11	1.97	0.47
1:A:191:TRP:CE3	1:A:206:ALA:HB1	2.50	0.47
1:A:326:ARG:HH11	1:A:385:PHE:HZ	1.61	0.47
1:C:1024:ARG:O	1:C:1028:ILE:HG12	2.15	0.47
1:C:1076:MET:HE2	1:C:1324:VAL:HG21	1.96	0.47
1:C:1321:ARG:O	1:C:1322:LYS:HD2	2.12	0.47
1:D:1424:ARG:O	1:D:1428:ILE:HG12	2.15	0.47
1:D:1652:ARG:HD2	1:D:1682:VAL:HG13	1.97	0.47
1:E:2219:VAL:HG11	1:E:2258:ARG:HD2	1.97	0.47
1:E:2271:LEU:HD12	1:E:2288:VAL:HG22	1.96	0.47
1:A:222:ALA:HB1	1:A:260:TYR:CD2	2.50	0.47
1:B:546:MET:HE2	1:B:547:ILE:HA	1.97	0.47
1:D:1440:ALA:HA	1:D:1704:ILE:HA	1.97	0.47
1:D:1653:TRP:HD1	1:D:1654:GLU:OE2	1.97	0.47
1:E:2343:ARG:HG2	1:E:2343:ARG:NH1	2.30	0.47
1:A:9:GLU:HG2	1:B:403:ARG:HE	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLY:O	1:A:332:TYR:HD1	1.98	0.47
1:B:440:ALA:HA	1:B:704:ILE:HA	1.96	0.47
1:D:1722:LYS:HZ2	1:D:1736:PRO:CA	2.28	0.47
1:E:2165:ALA:HB2	1:E:2172:ALA:HB2	1.95	0.47
1:F:2420:VAL:HG23	1:F:2421:TYR:N	2.30	0.47
1:F:2440:ALA:HA	1:F:2704:ILE:HA	1.96	0.47
1:A:228:LYS:HA	1:A:228:LYS:CE	2.40	0.46
1:C:1330:GLY:O	1:C:1332:TYR:HD1	1.98	0.46
1:E:2327:CYS:SG	1:E:2329:ASN:HB2	2.55	0.46
1:F:2611:PHE:HB2	1:F:2612:TYR:HD1	1.80	0.46
1:A:30:GLU:HG3	1:A:35:ARG:NH1	2.31	0.46
1:A:208:VAL:HG13	1:A:217:GLU:CB	2.45	0.46
1:B:469:ILE:HG23	1:B:470:PRO:HD2	1.95	0.46
1:C:1225:LEU:CB	1:C:1228:LYS:HB2	2.39	0.46
1:D:1648:ILE:CG2	1:D:1682:VAL:HG12	2.46	0.46
1:E:2188:VAL:HA	1:E:2191:TRP:HE1	1.77	0.46
1:E:2191:TRP:CE3	1:E:2206:ALA:HB1	2.50	0.46
1:E:2212:TYR:N	1:E:2212:TYR:HD1	2.13	0.46
1:E:2222:ALA:HB1	1:E:2260:TYR:CD2	2.50	0.46
1:F:2580:LEU:HD23	1:F:2580:LEU:C	2.35	0.46
1:F:2612:TYR:N	1:F:2612:TYR:HD1	2.13	0.46
1:A:65:LEU:HD22	1:A:108:MET:HE1	1.98	0.46
1:A:247:ILE:HG12	1:C:1240:ARG:HE	1.80	0.46
1:B:420:VAL:HG23	1:B:421:TYR:N	2.30	0.46
1:B:634:LEU:HD23	1:B:665:ILE:HG23	1.97	0.46
1:C:1177:PRO:HG3	1:D:1421:TYR:CD1	2.50	0.46
1:E:2003:ARG:NH2	4:E:42:HOH:O	2.39	0.46
1:E:2020:VAL:HG23	1:E:2021:TYR:N	2.30	0.46
1:E:2024:ARG:O	1:E:2028:ILE:HG12	2.15	0.46
1:E:2322:LYS:HZ2	1:E:2336:PRO:CA	2.27	0.46
1:F:2438:VAL:CG1	1:F:2707:VAL:HG13	2.41	0.46
1:F:2600:GLU:OE1	1:F:2600:GLU:HA	2.14	0.46
1:F:2634:LEU:HD23	1:F:2665:ILE:HG23	1.97	0.46
1:A:43:THR:HG22	1:A:87:PRO:HA	1.97	0.46
1:B:438:VAL:CG1	1:B:707:VAL:HG13	2.40	0.46
1:C:1044:THR:CG2	1:C:1298:VAL:HG12	2.32	0.46
1:C:1344:CYS:SG	1:C:1346:VAL:CG1	3.03	0.46
1:E:2200:GLU:HA	1:E:2200:GLU:OE1	2.15	0.46
1:E:2323:GLN:HE21	1:E:2353:PRO:HB3	1.75	0.46
1:A:252:ARG:HD2	1:A:282:VAL:HG13	1.98	0.46
1:B:439:LEU:HD23	1:B:721:ARG:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ILE:N	1:B:605:ILE:HD12	2.31	0.46
1:D:1591:TRP:CE3	1:D:1606:ALA:HB1	2.50	0.46
1:E:2005:TYR:CE1	1:F:2549:ARG:NH2	2.82	0.46
1:E:2040:ALA:HA	1:E:2304:ILE:HA	1.98	0.46
1:F:2565:ALA:HB2	1:F:2572:ALA:HB2	1.96	0.46
1:F:2594:PHE:CE1	1:F:2598:ILE:HG13	2.50	0.46
1:A:188:VAL:HA	1:A:191:TRP:HE1	1.78	0.46
1:B:457:VAL:CG1	1:B:512:ALA:HB1	2.46	0.46
1:B:521:ARG:NH1	1:B:673:GLU:OE2	2.48	0.46
1:C:1172:ALA:HB3	1:D:1420:VAL:CG1	2.46	0.46
1:C:1211:PHE:HB2	1:C:1212:TYR:HD1	1.80	0.46
1:E:2304:ILE:H	1:E:2304:ILE:HG12	1.58	0.46
1:F:2628:LYS:HA	1:F:2628:LYS:CE	2.41	0.46
1:B:622:ALA:HB1	1:B:660:TYR:CD2	2.51	0.46
1:B:648:ILE:HG22	1:B:682:VAL:HG12	1.98	0.46
1:B:702:LEU:HD13	1:B:702:LEU:C	2.35	0.46
1:D:1608:VAL:HG13	1:D:1617:GLU:CB	2.46	0.46
1:F:2743:ARG:HG2	1:F:2743:ARG:NH1	2.31	0.46
1:A:164:GLY:O	1:A:168:MET:HG3	2.15	0.46
1:A:212:TYR:N	1:A:212:TYR:HD1	2.14	0.46
1:A:302:LEU:HD13	1:A:302:LEU:C	2.36	0.46
1:B:469:ILE:HA	1:B:470:PRO:HD3	1.78	0.46
1:B:611:PHE:HB2	1:B:612:TYR:HD1	1.81	0.46
1:C:1038:VAL:CG1	1:C:1307:VAL:HG13	2.40	0.46
1:C:1375:ARG:HE	1:C:1379:LEU:HD11	1.81	0.46
1:D:1580:LEU:HD23	1:D:1581:ILE:N	2.30	0.46
1:D:1622:ALA:HB1	1:D:1660:TYR:CD2	2.51	0.46
1:E:2211:PHE:HB2	1:E:2212:TYR:HD1	1.81	0.46
1:E:2283:VAL:HG21	1:E:2286:PHE:CE2	2.51	0.46
1:F:2415:GLY:O	1:F:2418:THR:HG23	2.16	0.46
1:F:2605:ILE:HA	1:F:2631:ALA:O	2.15	0.46
1:A:321:ARG:O	1:A:322:LYS:HD2	2.14	0.46
1:B:591:TRP:CE3	1:B:606:ALA:HB1	2.50	0.46
1:C:1040:ALA:HA	1:C:1304:ILE:HA	1.98	0.46
1:C:1194:PHE:CE1	1:C:1198:ILE:HG13	2.51	0.46
1:C:1222:ALA:HB1	1:C:1260:TYR:CD2	2.51	0.46
1:D:1576:MET:HE3	1:D:1580:LEU:HD22	1.98	0.46
1:E:2043:THR:HG22	1:E:2087:PRO:HA	1.98	0.46
1:E:2205:ILE:HA	1:E:2231:ALA:O	2.15	0.46
1:E:2366:VAL:CG1	1:E:2367:GLU:N	2.79	0.46
1:F:2505:LEU:HD12	1:F:2506:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:PHE:HB2	1:A:212:TYR:HD1	1.81	0.46
1:A:322:LYS:HZ2	1:A:336:PRO:CA	2.28	0.46
1:B:533:SER:O	1:B:534:PHE:HD1	1.98	0.46
1:B:652:ARG:HD2	1:B:682:VAL:HG13	1.96	0.46
1:B:723:GLN:OE1	1:B:755:LEU:HD23	2.14	0.46
1:C:1028:ILE:HD11	1:D:1598:ILE:HG12	1.98	0.46
1:C:1121:ARG:NH1	1:C:1273:GLU:OE2	2.49	0.46
1:D:1443:THR:HG22	1:D:1487:PRO:HA	1.98	0.46
1:D:1605:ILE:HA	1:D:1631:ALA:O	2.16	0.46
1:E:2121:ARG:HB3	1:E:2389:ILE:HD11	1.97	0.46
1:E:2177:PRO:HG3	1:F:2421:TYR:CD1	2.51	0.46
1:F:2648:ILE:HG22	1:F:2682:VAL:HG12	1.98	0.46
1:F:2721:ARG:O	1:F:2722:LYS:NZ	2.35	0.46
1:A:115:ILE:HG23	1:A:292:ILE:O	2.16	0.45
1:A:200:GLU:OE1	1:A:200:GLU:HA	2.17	0.45
1:A:224:ALA:C	1:A:226:GLY:N	2.68	0.45
1:A:240:ARG:HE	1:C:1247:ILE:HG12	1.80	0.45
1:A:322:LYS:HZ2	1:A:336:PRO:HB3	1.80	0.45
1:A:366:VAL:CG1	1:A:367:GLU:N	2.78	0.45
1:B:580:LEU:HD23	1:B:581:ILE:N	2.30	0.45
1:B:600:GLU:HA	1:B:600:GLU:OE1	2.16	0.45
1:C:1164:GLY:O	1:C:1168:MET:HG3	2.15	0.45
1:E:2030:GLU:HG3	1:E:2035:ARG:NH1	2.31	0.45
1:A:219:VAL:HG11	1:A:258:ARG:HD2	1.97	0.45
1:A:250:GLU:OE2	1:D:1716:GLY:HA2	2.16	0.45
1:C:1071:VAL:HG11	1:C:1098:PHE:CD2	2.51	0.45
1:C:1107:GLY:HA3	1:D:1539:MET:O	2.16	0.45
1:C:1373:GLU:OE2	1:C:1376:GLU:OE1	2.34	0.45
1:E:2279:ILE:O	1:E:2283:VAL:HG22	2.16	0.45
1:E:2322:LYS:HZ2	1:E:2336:PRO:HA	1.82	0.45
1:F:2746:VAL:CG2	1:F:2747:CYS:H	2.06	0.45
1:A:173:VAL:CG2	1:A:174:GLY:N	2.78	0.45
1:A:234:LEU:N	1:A:234:LEU:HD22	2.32	0.45
1:B:430:GLU:HG3	1:B:435:ARG:NH1	2.32	0.45
1:D:1505:LEU:HD12	1:D:1506:LEU:N	2.31	0.45
1:D:1605:ILE:N	1:D:1605:ILE:HD12	2.31	0.45
1:D:1648:ILE:HG22	1:D:1682:VAL:HG12	1.98	0.45
1:F:2671:LEU:HD12	1:F:2688:VAL:HG22	1.98	0.45
1:F:2683:VAL:HG21	1:F:2686:PHE:CE2	2.51	0.45
1:C:1346:VAL:CG2	1:C:1347:CYS:N	2.67	0.45
1:C:1368:PHE:HA	1:C:1369:PRO:HD2	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1438:VAL:CG1	1:D:1707:VAL:HG13	2.41	0.45
1:D:1439:LEU:HD23	1:D:1721:ARG:HB2	1.98	0.45
1:D:1747:CYS:O	1:D:1747:CYS:SG	2.75	0.45
1:E:2205:ILE:N	1:E:2205:ILE:HD12	2.31	0.45
1:E:2234:LEU:HD23	1:E:2265:ILE:HG23	1.99	0.45
1:F:2443:THR:HG22	1:F:2487:PRO:HA	1.98	0.45
1:F:2730:GLY:O	1:F:2732:TYR:HD1	1.98	0.45
1:A:283:VAL:HG21	1:A:286:PHE:CZ	2.52	0.45
1:B:443:THR:HG22	1:B:487:PRO:HA	1.98	0.45
1:B:594:PHE:CE1	1:B:598:ILE:HG13	2.52	0.45
1:B:605:ILE:HA	1:B:631:ALA:O	2.16	0.45
1:B:726:ARG:HG3	1:B:732:TYR:CE1	2.51	0.45
1:E:2173:VAL:CG2	1:E:2174:GLY:N	2.80	0.45
1:E:2194:PHE:CE1	1:E:2198:ILE:HG13	2.51	0.45
1:F:2622:ALA:HB1	1:F:2660:TYR:CD2	2.52	0.45
1:B:505:LEU:HD12	1:B:506:LEU:N	2.30	0.45
1:B:609:ASP:C	1:B:609:ASP:OD1	2.55	0.45
1:C:1030:GLU:HG3	1:C:1035:ARG:NH1	2.31	0.45
1:C:1173:VAL:CG2	1:C:1174:GLY:N	2.80	0.45
1:D:1726:ARG:HG3	1:D:1732:TYR:CE1	2.52	0.45
1:D:1773:GLU:OE2	1:D:1776:GLU:OE1	2.34	0.45
1:F:2564:GLY:O	1:F:2568:MET:HG3	2.17	0.45
1:F:2609:ASP:OD1	1:F:2609:ASP:C	2.55	0.45
1:B:608:VAL:HG13	1:B:617:GLU:CB	2.46	0.45
1:C:1144:ALA:N	1:C:1145:PRO:HD2	2.32	0.45
1:C:1322:LYS:HZ2	1:C:1336:PRO:CB	2.27	0.45
1:D:1611:PHE:HB2	1:D:1612:TYR:HD1	1.81	0.45
1:E:2016:LYS:O	1:F:2563:LEU:HB2	2.17	0.45
1:E:2039:LEU:HD23	1:E:2321:ARG:HB2	1.99	0.45
1:F:2624:ALA:C	1:F:2626:GLY:N	2.70	0.45
1:B:773:GLU:OE2	1:B:776:GLU:OE1	2.34	0.45
1:C:1003:ARG:HD3	4:C:36:HOH:O	2.17	0.45
1:C:1326:ARG:HG3	1:C:1332:TYR:CE1	2.52	0.45
1:D:1589:LYS:HG2	1:D:1593:TYR:CZ	2.52	0.45
1:D:1634:LEU:HD23	1:D:1665:ILE:HG23	1.98	0.45
1:D:1652:ARG:HD2	1:D:1682:VAL:CG1	2.47	0.45
1:E:2020:VAL:HG11	1:F:2572:ALA:HB3	1.99	0.45
1:E:2033:ASN:HD22	1:E:2033:ASN:HA	1.60	0.45
1:F:2537:ARG:CG	1:F:2537:ARG:NH1	2.71	0.45
1:F:2704:ILE:H	1:F:2704:ILE:HG12	1.58	0.45
1:A:40:ALA:HA	1:A:304:ILE:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:THR:HG22	1:A:299:ASP:O	2.17	0.45
1:B:544:ALA:N	1:B:545:PRO:HD2	2.32	0.45
1:B:612:TYR:N	1:B:612:TYR:HD1	2.14	0.45
1:C:1100:ILE:O	1:C:1100:ILE:HG22	2.17	0.45
1:C:1200:GLU:OE1	1:C:1200:GLU:HA	2.16	0.45
1:D:1537:ARG:CG	1:D:1537:ARG:NH1	2.75	0.45
1:D:1609:ASP:C	1:D:1609:ASP:OD1	2.55	0.45
1:D:1624:ALA:C	1:D:1626:GLY:N	2.70	0.45
1:D:1722:LYS:HZ2	1:D:1736:PRO:CB	2.30	0.45
1:E:2248:ILE:CG2	1:E:2282:VAL:HG12	2.47	0.45
1:F:2430:GLU:HG3	1:F:2435:ARG:NH1	2.31	0.45
1:B:573:VAL:CG2	1:B:574:GLY:N	2.80	0.45
1:B:619:VAL:HG11	1:B:658:ARG:HD2	1.99	0.45
1:C:1176:MET:HB2	1:C:1207:LEU:HB2	1.99	0.45
1:C:1234:LEU:HD23	1:C:1265:ILE:HG23	1.97	0.45
1:C:1252:ARG:HD2	1:C:1282:VAL:HG13	1.98	0.45
1:D:1444:THR:CG2	1:D:1698:VAL:HG12	2.33	0.45
1:D:1594:PHE:CE1	1:D:1598:ILE:HG13	2.52	0.45
1:E:2003:ARG:CB	1:F:2464:LYS:HD3	2.47	0.45
1:A:53:TRP:HZ3	1:A:388:GLU:O	2.00	0.44
1:A:198:ILE:O	1:A:204:ARG:NH2	2.50	0.44
1:D:1518:ALA:O	1:D:1522:ILE:HD13	2.17	0.44
1:E:2188:VAL:HA	1:E:2191:TRP:CD1	2.52	0.44
1:F:2591:TRP:CE3	1:F:2606:ALA:HB1	2.52	0.44
1:B:730:GLY:O	1:B:732:TYR:HD1	2.00	0.44
1:C:1212:TYR:N	1:C:1212:TYR:HD1	2.13	0.44
1:D:1576:MET:HB2	1:D:1607:LEU:HB2	2.00	0.44
1:D:1600:GLU:HA	1:D:1600:GLU:OE1	2.17	0.44
1:D:1612:TYR:N	1:D:1612:TYR:HD1	2.14	0.44
1:E:2044:THR:CG2	1:E:2298:VAL:HG12	2.31	0.44
1:E:2163:LEU:HB2	1:F:2416:LYS:O	2.17	0.44
1:F:2655:LEU:HD13	1:F:2663:VAL:HG23	1.97	0.44
1:F:2727:CYS:SG	1:F:2729:ASN:HB2	2.56	0.44
1:A:322:LYS:HZ2	1:A:336:PRO:HA	1.82	0.44
1:B:743:ARG:HG2	1:B:743:ARG:NH1	2.33	0.44
1:C:1044:THR:HG22	1:C:1299:ASP:O	2.17	0.44
1:C:1118:ALA:O	1:C:1122:ILE:CD1	2.66	0.44
1:C:1139:MET:O	1:D:1507:GLY:HA3	2.18	0.44
1:C:1166:GLU:C	1:C:1168:MET:N	2.70	0.44
1:C:1224:ALA:C	1:C:1226:GLY:N	2.68	0.44
1:D:1430:GLU:HG3	1:D:1435:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2164:GLY:O	1:E:2168:MET:HG3	2.17	0.44
1:E:2180:LEU:HD23	1:E:2181:ILE:N	2.32	0.44
1:E:2225:LEU:CB	1:E:2228:LYS:HB2	2.41	0.44
1:E:2248:ILE:HG22	1:E:2282:VAL:HG12	1.99	0.44
1:F:2548:ASP:HB3	1:F:2559:VAL:HG21	2.00	0.44
1:C:1061:GLU:OE1	1:D:1540:HIS:HE1	2.01	0.44
1:C:1145:PRO:O	1:C:1146:MET:C	2.55	0.44
1:C:1188:VAL:HA	1:C:1191:TRP:HE1	1.78	0.44
1:D:1598:ILE:O	1:D:1604:ARG:NH2	2.50	0.44
1:F:2546:MET:HE2	1:F:2547:ILE:HA	2.00	0.44
1:A:194:PHE:CE1	1:A:198:ILE:HG13	2.52	0.44
1:A:347:CYS:SG	1:A:347:CYS:O	2.76	0.44
1:C:1176:MET:HE2	1:C:1181:ILE:HD11	2.00	0.44
1:C:1191:TRP:CE3	1:C:1206:ALA:HB1	2.52	0.44
1:C:1205:ILE:HD12	1:C:1205:ILE:N	2.32	0.44
1:D:1420:VAL:HG23	1:D:1421:TYR:N	2.31	0.44
1:D:1702:LEU:HD13	1:D:1702:LEU:C	2.38	0.44
1:E:2071:VAL:HG11	1:E:2098:PHE:CD2	2.53	0.44
1:E:2198:ILE:O	1:E:2204:ARG:NH2	2.50	0.44
1:A:26:LYS:HD3	1:A:100:ILE:CD1	2.48	0.44
1:A:57:VAL:CG1	1:A:112:ALA:HB1	2.48	0.44
1:A:177:PRO:HG3	1:B:421:TYR:CD1	2.53	0.44
1:B:537:ARG:CG	1:B:537:ARG:NH1	2.76	0.44
1:C:1327:CYS:SG	1:C:1329:ASN:HB2	2.58	0.44
1:D:1546:MET:HE2	1:D:1547:ILE:HA	1.99	0.44
1:E:2252:ARG:HD2	1:E:2282:VAL:CG1	2.47	0.44
1:A:71:VAL:HG11	1:A:98:PHE:CD2	2.53	0.44
1:B:549:ARG:O	1:B:553:ILE:HG13	2.18	0.44
1:B:566:GLU:C	1:B:568:MET:N	2.71	0.44
1:B:576:MET:HE2	1:B:581:ILE:HD11	2.00	0.44
1:B:576:MET:HE3	1:B:580:LEU:HD22	1.99	0.44
1:C:1283:VAL:HG21	1:C:1286:PHE:CE2	2.53	0.44
1:C:1352:GLU:HA	1:C:1353:PRO:HD3	1.86	0.44
1:D:1565:ALA:HB2	1:D:1572:ALA:HB2	2.00	0.44
1:E:2054:GLY:HA2	1:E:2117:THR:HG23	2.00	0.44
1:F:2652:ARG:HD2	1:F:2682:VAL:HG13	2.00	0.44
1:F:2722:LYS:HZ2	1:F:2736:PRO:CB	2.31	0.44
1:A:166:GLU:C	1:A:168:MET:N	2.72	0.44
1:B:598:ILE:O	1:B:604:ARG:NH2	2.51	0.44
1:B:747:CYS:O	1:B:747:CYS:SG	2.76	0.44
1:C:1039:LEU:HD23	1:C:1321:ARG:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1222:ALA:O	1:C:1226:GLY:HA2	2.18	0.44
1:D:1471:VAL:HG11	1:D:1498:PHE:CD2	2.53	0.44
1:D:1544:ALA:N	1:D:1545:PRO:HD2	2.32	0.44
1:E:2175:THR:O	1:F:2421:TYR:HB2	2.18	0.44
1:F:2766:VAL:CG1	1:F:2767:GLU:N	2.80	0.44
1:C:1302:LEU:HD13	1:C:1302:LEU:C	2.39	0.43
1:D:1465:LEU:HD22	1:D:1508:MET:HE1	2.00	0.43
1:D:1521:ARG:NH1	1:D:1673:GLU:OE2	2.47	0.43
1:D:1607:LEU:HD22	1:D:1607:LEU:HA	1.86	0.43
1:F:2566:GLU:C	1:F:2568:MET:N	2.70	0.43
1:F:2588:VAL:HA	1:F:2591:TRP:CD1	2.53	0.43
1:F:2653:TRP:HD1	1:F:2654:GLU:OE2	2.01	0.43
1:A:176:MET:HB2	1:A:207:LEU:HB2	1.99	0.43
1:B:431:VAL:O	1:B:433:ASN:N	2.51	0.43
1:B:576:MET:HB2	1:B:607:LEU:HB2	1.99	0.43
1:A:5:TYR:HA	1:B:567:MET:HE1	2.00	0.43
1:A:205:ILE:HD12	1:A:205:ILE:N	2.33	0.43
1:C:1065:LEU:HD22	1:C:1108:MET:HE1	2.00	0.43
1:E:2209:ASP:C	1:E:2209:ASP:OD1	2.56	0.43
1:A:24:ARG:O	1:A:28:ILE:HG12	2.18	0.43
1:A:28:ILE:HD11	1:B:598:ILE:HG12	2.00	0.43
1:A:69:ILE:O	1:A:71:VAL:N	2.43	0.43
1:C:1054:GLY:HA2	1:C:1117:THR:HG23	2.01	0.43
1:C:1209:ASP:OD1	1:C:1209:ASP:C	2.57	0.43
1:C:1326:ARG:HH12	1:C:1381:GLN:NE2	2.11	0.43
1:D:1683:VAL:HG21	1:D:1686:PHE:CE2	2.53	0.43
1:F:2722:LYS:HZ2	1:F:2736:PRO:CA	2.30	0.43
1:B:471:VAL:HG11	1:B:498:PHE:CD2	2.53	0.43
1:B:565:ALA:HB2	1:B:572:ALA:HB2	2.00	0.43
1:C:1062:VAL:HG11	1:C:1089:LEU:HD11	1.99	0.43
1:C:1198:ILE:O	1:C:1204:ARG:NH2	2.51	0.43
1:D:1457:VAL:CG1	1:D:1512:ALA:HB1	2.48	0.43
1:D:1463:ALA:HB2	1:D:1758:ILE:HD12	2.00	0.43
1:D:1730:GLY:O	1:D:1732:TYR:HD1	2.01	0.43
1:E:2172:ALA:HB3	1:F:2420:VAL:HG11	1.99	0.43
1:E:2252:ARG:HD2	1:E:2282:VAL:HG13	2.00	0.43
1:F:2726:ARG:HG3	1:F:2732:TYR:CE1	2.53	0.43
1:A:107:GLY:HA3	1:B:539:MET:O	2.19	0.43
1:C:1057:VAL:CG1	1:C:1112:ALA:HB1	2.48	0.43
1:D:1743:ARG:HG2	1:D:1743:ARG:NH1	2.31	0.43
1:E:2321:ARG:O	1:E:2322:LYS:HD2	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ARG:NH1	1:A:273:GLU:OE2	2.50	0.43
1:B:521:ARG:HA	1:B:789:ILE:HD11	2.00	0.43
1:C:1346:VAL:HG13	1:C:1347:CYS:N	2.34	0.43
1:E:2166:GLU:C	1:E:2168:MET:N	2.72	0.43
1:E:2176:MET:HB2	1:E:2207:LEU:HB2	2.01	0.43
1:F:2471:VAL:HG11	1:F:2498:PHE:CD2	2.53	0.43
1:B:652:ARG:HD2	1:B:682:VAL:CG1	2.48	0.43
1:B:746:VAL:HG13	1:B:747:CYS:N	2.34	0.43
1:C:1026:LYS:HD3	1:C:1100:ILE:CD1	2.48	0.43
1:C:1252:ARG:HD2	1:C:1282:VAL:CG1	2.49	0.43
1:C:1347:CYS:SG	1:C:1347:CYS:O	2.77	0.43
1:D:1573:VAL:CG2	1:D:1574:GLY:N	2.79	0.43
1:E:2064:LYS:HD3	1:F:2403:ARG:CB	2.49	0.43
1:B:721:ARG:O	1:B:722:LYS:NZ	2.37	0.43
1:C:1003:ARG:HE	1:D:1409:GLU:HG2	1.84	0.43
1:C:1020:VAL:CG1	1:D:1572:ALA:HB3	2.49	0.43
1:F:2426:LYS:HD3	1:F:2500:ILE:CD1	2.49	0.43
1:A:188:VAL:HA	1:A:191:TRP:CD1	2.54	0.43
1:A:222:ALA:O	1:A:226:GLY:HA2	2.19	0.43
1:B:725:TYR:HE2	1:B:753:PRO:HG3	1.82	0.43
1:E:2310:LYS:HA	1:E:2311:PRO:HD3	1.88	0.43
1:B:683:VAL:CG2	1:B:686:PHE:CZ	3.01	0.42
1:D:1426:LYS:HD3	1:D:1500:ILE:CD1	2.49	0.42
1:E:2069:ILE:HA	1:E:2070:PRO:HD3	1.76	0.42
1:E:2197:VAL:CB	1:F:2428:ILE:HD13	2.39	0.42
1:E:2224:ALA:C	1:E:2225:LEU:HD23	2.40	0.42
1:E:2344:CYS:SG	1:E:2346:VAL:CG1	3.07	0.42
1:F:2420:VAL:O	1:F:2422:PHE:N	2.52	0.42
1:B:545:PRO:O	1:B:546:MET:C	2.54	0.42
1:B:552:PHE:O	1:B:553:ILE:C	2.57	0.42
1:B:589:LYS:HG2	1:B:593:TYR:CZ	2.54	0.42
1:B:683:VAL:HG21	1:B:686:PHE:CE2	2.54	0.42
1:D:1551:ALA:O	1:D:1556:CYS:HB2	2.19	0.42
1:D:1564:GLY:O	1:D:1568:MET:HG3	2.19	0.42
1:D:1634:LEU:N	1:D:1634:LEU:HD22	2.34	0.42
1:D:1746:VAL:HG13	1:D:1747:CYS:N	2.34	0.42
1:E:2069:ILE:O	1:E:2071:VAL:N	2.44	0.42
1:E:2302:LEU:HD13	1:E:2302:LEU:C	2.39	0.42
1:F:2454:GLY:HA2	1:F:2517:THR:HG23	2.01	0.42
1:D:1573:VAL:CG2	1:D:1574:GLY:H	2.31	0.42
1:D:1652:ARG:CD	1:D:1682:VAL:HG13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2028:ILE:HD13	1:F:2597:VAL:CB	2.39	0.42
1:E:2359:ILE:O	1:E:2359:ILE:HG22	2.19	0.42
1:F:2580:LEU:HD23	1:F:2581:ILE:N	2.35	0.42
1:F:2744:CYS:SG	1:F:2746:VAL:CG1	3.07	0.42
1:A:234:LEU:HD23	1:A:265:ILE:HG23	2.00	0.42
1:A:310:LYS:HA	1:A:311:PRO:HD3	1.89	0.42
1:C:1322:LYS:HZ2	1:C:1336:PRO:CA	2.33	0.42
1:F:2544:ALA:N	1:F:2545:PRO:HD2	2.35	0.42
1:F:2702:LEU:C	1:F:2702:LEU:HD13	2.40	0.42
1:C:1085:TYR:OH	1:F:2646:LYS:HD3	2.20	0.42
1:C:1130:PRO:HA	1:C:1157:ASP:OD1	2.19	0.42
1:C:1327:CYS:SG	1:C:1329:ASN:N	2.82	0.42
1:D:1588:VAL:HA	1:D:1591:TRP:CD1	2.54	0.42
1:E:2350:LYS:CE	1:E:2350:LYS:N	2.73	0.42
1:F:2457:VAL:CG1	1:F:2512:ALA:HB1	2.49	0.42
1:A:263:VAL:O	1:A:263:VAL:HG23	2.19	0.42
1:A:326:ARG:HG3	1:A:332:TYR:CE1	2.55	0.42
1:B:444:THR:CG2	1:B:698:VAL:HG12	2.32	0.42
1:B:576:MET:HA	1:B:577:PRO:HD3	1.83	0.42
1:C:1009:GLU:HG2	1:D:1403:ARG:HE	1.85	0.42
1:C:1283:VAL:CG2	1:C:1286:PHE:CZ	3.03	0.42
1:E:2057:VAL:CG1	1:E:2112:ALA:HB1	2.49	0.42
1:E:2118:ALA:O	1:E:2122:ILE:HD13	2.19	0.42
1:E:2146:MET:HE2	1:E:2147:ILE:HA	2.01	0.42
1:F:2752:GLU:HA	1:F:2753:PRO:HD3	1.88	0.42
1:A:327:CYS:SG	1:A:329:ASN:HB2	2.60	0.42
1:B:415:GLY:O	1:B:418:THR:HG23	2.19	0.42
1:B:564:GLY:O	1:B:568:MET:HG3	2.19	0.42
1:C:1053:TRP:HZ3	1:C:1388:GLU:O	2.01	0.42
1:C:1255:LEU:HD13	1:C:1263:VAL:HG23	2.00	0.42
1:D:1638:SER:O	1:F:2642:GLY:HA3	2.20	0.42
1:E:2020:VAL:HG13	1:F:2572:ALA:HB3	2.01	0.42
1:E:2189:LYS:HG2	1:E:2193:TYR:CZ	2.54	0.42
1:E:2207:LEU:HD21	1:E:2233:ARG:NH2	2.34	0.42
1:F:2486:GLU:HG2	1:F:2734:VAL:CG2	2.50	0.42
1:F:2489:LEU:HD23	1:F:2490:GLN:N	2.35	0.42
1:F:2500:ILE:O	1:F:2500:ILE:HG22	2.20	0.42
1:A:62:VAL:HG11	1:A:89:LEU:HD11	2.01	0.42
1:A:368:PHE:HA	1:A:369:PRO:HD2	1.84	0.42
1:B:462:VAL:HG11	1:B:489:LEU:HD11	2.01	0.42
1:B:640:ARG:NH1	1:E:2213:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1696:LYS:HA	1:D:1697:PRO:HD3	1.94	0.42
1:E:2086:GLU:HG2	1:E:2334:VAL:CG2	2.50	0.42
1:A:61:GLU:OE1	1:B:540:HIS:HE1	2.03	0.42
1:A:176:MET:HA	1:A:177:PRO:HD3	1.85	0.42
1:B:588:VAL:HA	1:B:591:TRP:CD1	2.55	0.42
1:F:2529:LYS:HB3	1:F:2530:PRO:HD2	2.01	0.42
1:F:2652:ARG:HD2	1:F:2682:VAL:CG1	2.49	0.42
1:A:252:ARG:HD2	1:A:282:VAL:CG1	2.49	0.42
1:A:282:VAL:O	1:A:282:VAL:CG1	2.68	0.42
1:B:465:LEU:HD22	1:B:508:MET:HE1	2.01	0.42
1:D:1431:VAL:O	1:D:1433:ASN:N	2.52	0.42
1:D:1608:VAL:HG12	1:D:1614:GLU:HA	2.02	0.42
1:D:1655:LEU:HD13	1:D:1663:VAL:HG23	2.00	0.42
1:D:1768:PHE:HA	1:D:1769:PRO:HD2	1.84	0.42
1:E:2064:LYS:HB3	1:F:2403:ARG:HB2	2.02	0.42
1:E:2233:ARG:HG3	1:E:2266:PHE:HD1	1.85	0.42
1:F:2546:MET:HE2	1:F:2546:MET:O	2.20	0.42
1:F:2573:VAL:CG2	1:F:2574:GLY:N	2.82	0.42
1:C:1188:VAL:HA	1:C:1191:TRP:CD1	2.54	0.41
1:C:1310:LYS:HA	1:C:1311:PRO:HD3	1.88	0.41
1:D:1625:LEU:O	1:D:1628:LYS:HB2	2.20	0.41
1:D:1663:VAL:HG23	1:D:1663:VAL:O	2.19	0.41
1:D:1750:LYS:CE	1:D:1750:LYS:N	2.73	0.41
1:E:2234:LEU:HD22	1:E:2234:LEU:N	2.34	0.41
1:F:2439:LEU:HD23	1:F:2721:ARG:HB2	2.01	0.41
1:F:2521:ARG:HA	1:F:2789:ILE:HD11	2.01	0.41
1:F:2624:ALA:C	1:F:2625:LEU:HD23	2.41	0.41
1:A:162:VAL:HG22	1:B:420:VAL:HG12	2.01	0.41
1:A:209:ASP:C	1:A:209:ASP:OD1	2.58	0.41
1:B:653:TRP:CD1	1:F:2718:LEU:HD22	2.55	0.41
1:B:669:GLY:O	1:B:670:GLY:C	2.58	0.41
1:F:2454:GLY:HA2	1:F:2517:THR:CG2	2.50	0.41
1:F:2607:LEU:HD22	1:F:2607:LEU:HA	1.86	0.41
1:F:2744:CYS:O	1:F:2745:PRO:C	2.59	0.41
1:A:252:ARG:CD	1:A:282:VAL:HG13	2.51	0.41
1:C:1350:LYS:CE	1:C:1350:LYS:N	2.73	0.41
1:E:2208:VAL:HG12	1:E:2214:GLU:HA	2.03	0.41
1:E:2283:VAL:CG2	1:E:2286:PHE:CZ	3.04	0.41
1:F:2576:MET:HB2	1:F:2607:LEU:HB2	2.01	0.41
1:F:2628:LYS:HE2	1:F:2628:LYS:CA	2.44	0.41
1:F:2683:VAL:CG2	1:F:2686:PHE:CZ	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:VAL:CG1	1:B:572:ALA:HB3	2.50	0.41
1:A:121:ARG:HA	1:A:389:ILE:HD11	2.02	0.41
1:A:144:ALA:N	1:A:145:PRO:HD2	2.35	0.41
1:A:212:TYR:HB2	1:A:217:GLU:CG	2.44	0.41
1:A:343:ARG:HG2	1:A:343:ARG:NH1	2.35	0.41
1:C:1189:LYS:HG2	1:C:1193:TYR:CZ	2.56	0.41
1:D:1552:PHE:O	1:D:1553:ILE:C	2.58	0.41
1:D:1566:GLU:C	1:D:1568:MET:N	2.73	0.41
1:D:1619:VAL:HG11	1:D:1658:ARG:HD2	2.02	0.41
1:E:2253:TRP:HD1	1:E:2254:GLU:OE2	2.03	0.41
1:E:2344:CYS:O	1:E:2345:PRO:C	2.59	0.41
1:F:2462:VAL:HG11	1:F:2489:LEU:HD11	2.02	0.41
1:F:2750:LYS:CE	1:F:2750:LYS:N	2.73	0.41
1:A:173:VAL:CG2	1:A:174:GLY:H	2.30	0.41
1:A:346:VAL:HG13	1:A:347:CYS:N	2.34	0.41
1:E:2021:TYR:HB2	1:F:2575:THR:O	2.19	0.41
1:E:2026:LYS:HD3	1:E:2100:ILE:CD1	2.50	0.41
1:E:2054:GLY:HA2	1:E:2117:THR:CG2	2.51	0.41
1:A:187:GLN:H	1:A:187:GLN:NE2	2.19	0.41
1:A:283:VAL:HG21	1:A:286:PHE:CE2	2.55	0.41
1:B:744:CYS:O	1:B:745:PRO:C	2.59	0.41
1:D:1462:VAL:HG11	1:D:1489:LEU:HD11	2.03	0.41
1:D:1469:ILE:O	1:D:1471:VAL:N	2.46	0.41
1:D:1683:VAL:CG2	1:D:1686:PHE:CZ	3.04	0.41
1:E:2062:VAL:HG11	1:E:2089:LEU:HD11	2.02	0.41
1:A:208:VAL:HG21	1:A:232:VAL:CG1	2.51	0.41
1:A:304:ILE:H	1:A:304:ILE:HG12	1.57	0.41
1:B:521:ARG:CG	1:B:789:ILE:HD11	2.50	0.41
1:C:1208:VAL:HG12	1:C:1214:GLU:HA	2.03	0.41
1:D:1415:GLY:O	1:D:1418:THR:HG23	2.20	0.41
1:D:1537:ARG:CZ	3:D:1792:PCP:O2	2.69	0.41
1:D:1608:VAL:HG21	1:D:1632:VAL:CG1	2.51	0.41
1:D:1722:LYS:HZ2	1:D:1736:PRO:HA	1.85	0.41
1:D:1724:VAL:HG22	1:D:1755:LEU:CD2	2.50	0.41
1:E:2031:VAL:O	1:E:2033:ASN:N	2.54	0.41
1:E:2326:ARG:HG3	1:E:2332:TYR:CE1	2.56	0.41
1:F:2576:MET:HE2	1:F:2581:ILE:HD11	2.01	0.41
1:F:2598:ILE:O	1:F:2604:ARG:NH2	2.53	0.41
1:F:2622:ALA:O	1:F:2626:GLY:HA2	2.21	0.41
1:F:2703:ASP:HB2	1:F:2717:LYS:HE3	2.03	0.41
1:A:346:VAL:CG2	1:A:347:CYS:N	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:LYS:HZ2	1:B:736:PRO:CA	2.34	0.41
1:C:1343:ARG:HG2	1:C:1343:ARG:NH1	2.35	0.41
1:D:1521:ARG:CG	1:D:1789:ILE:HD11	2.50	0.41
1:D:1622:ALA:O	1:D:1626:GLY:HA2	2.21	0.41
1:D:1789:ILE:HD12	1:D:1789:ILE:HA	1.85	0.41
1:E:2121:ARG:CG	1:E:2389:ILE:HD11	2.51	0.41
1:E:2252:ARG:CD	1:E:2282:VAL:HG13	2.51	0.41
1:F:2549:ARG:O	1:F:2553:ILE:HG13	2.21	0.41
1:F:2624:ALA:O	1:F:2625:LEU:HG	2.21	0.41
1:F:2759:ILE:O	1:F:2759:ILE:HG22	2.20	0.41
1:A:20:VAL:HG12	1:B:562:VAL:HG22	2.02	0.41
1:A:54:GLY:HA2	1:A:117:THR:HG23	2.02	0.41
1:A:81:ILE:H	1:A:381:GLN:HE22	1.68	0.41
1:A:140:HIS:HE1	1:B:461:GLU:OE1	2.04	0.41
1:A:151:ALA:O	1:A:156:CYS:HB2	2.21	0.41
1:A:225:LEU:O	1:A:228:LYS:HB2	2.21	0.41
1:B:463:ALA:HB2	1:B:758:ILE:HD12	2.02	0.41
1:B:682:VAL:O	1:B:682:VAL:CG1	2.68	0.41
1:B:704:ILE:H	1:B:704:ILE:HG12	1.57	0.41
1:B:724:VAL:HG22	1:B:755:LEU:CD2	2.51	0.41
1:C:1005:TYR:HA	1:D:1567:MET:HE1	2.02	0.41
1:C:1303:ASP:HB2	1:C:1317:LYS:HE3	2.02	0.41
1:C:1324:VAL:HG22	1:C:1355:LEU:CD2	2.51	0.41
1:D:1703:ASP:HB2	1:D:1717:LYS:HE3	2.03	0.41
1:E:2003:ARG:HB2	1:F:2464:LYS:HB3	2.02	0.41
1:E:2065:LEU:HD22	1:E:2108:MET:HE1	2.01	0.41
1:E:2172:ALA:HB3	1:F:2420:VAL:HG13	2.02	0.41
1:E:2222:ALA:O	1:E:2226:GLY:HA2	2.21	0.41
1:E:2255:LEU:HD13	1:E:2263:VAL:HG23	1.98	0.41
1:E:2346:VAL:HG13	1:E:2347:CYS:N	2.36	0.41
1:F:2431:VAL:O	1:F:2433:ASN:N	2.53	0.41
1:F:2576:MET:HE3	1:F:2580:LEU:HD22	2.02	0.41
1:F:2669:GLY:O	1:F:2670:GLY:C	2.59	0.41
1:A:26:LYS:CD	1:A:100:ILE:HD11	2.51	0.41
1:A:208:VAL:HG12	1:A:214:GLU:HA	2.03	0.41
1:A:233:ARG:HG3	1:A:266:PHE:HD1	1.86	0.41
1:B:420:VAL:O	1:B:422:PHE:N	2.54	0.41
1:B:523:LYS:HE3	1:B:528:PHE:HA	2.03	0.41
1:B:624:ALA:O	1:B:625:LEU:HG	2.21	0.41
1:C:1028:ILE:HD11	1:D:1594:PHE:HA	2.03	0.41
1:C:1140:HIS:HE1	1:D:1461:GLU:OE1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1173:VAL:CG2	1:C:1174:GLY:H	2.33	0.41
1:D:1481:ILE:H	1:D:1781:GLN:HE22	1.69	0.41
1:D:1640:ARG:NH1	1:F:2613:ASP:OD1	2.53	0.41
1:A:100:ILE:O	1:A:100:ILE:HG22	2.21	0.40
1:A:236:THR:HB	1:A:241:ARG:CG	2.51	0.40
1:B:530:PRO:HA	1:B:557:ASP:OD1	2.21	0.40
1:B:652:ARG:CD	1:B:682:VAL:HG13	2.50	0.40
1:B:653:TRP:CZ2	1:F:2722:LYS:HG2	2.57	0.40
1:C:1191:TRP:HZ3	1:C:1207:LEU:O	2.04	0.40
1:C:1194:PHE:HA	1:D:1428:ILE:HD11	2.01	0.40
1:C:1208:VAL:CG1	1:C:1217:GLU:HB2	2.51	0.40
1:D:1521:ARG:HA	1:D:1789:ILE:HD11	2.03	0.40
1:F:2521:ARG:CG	1:F:2789:ILE:HD11	2.51	0.40
1:A:303:ASP:HB2	1:A:317:LYS:HE3	2.03	0.40
1:B:529:LYS:HB3	1:B:530:PRO:HD2	2.03	0.40
1:B:573:VAL:CG2	1:B:574:GLY:H	2.32	0.40
1:B:638:SER:O	1:E:2242:GLY:HA3	2.20	0.40
1:B:705:VAL:HA	1:B:713:ALA:HB2	2.04	0.40
1:D:1710:LYS:HA	1:D:1711:PRO:HD3	1.87	0.40
1:D:1759:ILE:O	1:D:1759:ILE:HG22	2.20	0.40
1:E:2173:VAL:CG2	1:E:2174:GLY:H	2.32	0.40
1:E:2224:ALA:C	1:E:2226:GLY:N	2.70	0.40
1:F:2419:ASP:HB2	1:F:2421:TYR:CE2	2.56	0.40
1:F:2444:THR:HG22	1:F:2699:ASP:C	2.41	0.40
1:F:2523:LYS:HE3	1:F:2528:PHE:HA	2.03	0.40
1:A:137:ARG:CZ	3:A:392:PCP:O2	2.69	0.40
1:A:189:LYS:HG2	1:A:193:TYR:CZ	2.55	0.40
1:B:426:LYS:HD3	1:B:500:ILE:CD1	2.51	0.40
1:B:613:ASP:CG	1:E:2240:ARG:NH1	2.74	0.40
1:C:1031:VAL:O	1:C:1033:ASN:N	2.54	0.40
1:C:1193:TYR:CE2	1:D:1432:LYS:HD3	2.56	0.40
1:D:1576:MET:HA	1:D:1577:PRO:HD3	1.82	0.40
1:D:1647:ILE:HG12	1:F:2640:ARG:HE	1.87	0.40
1:E:2208:VAL:HG21	1:E:2232:VAL:CG1	2.51	0.40
1:F:2581:ILE:HG23	1:F:2587:GLN:HA	2.04	0.40
1:F:2746:VAL:HG13	1:F:2747:CYS:N	2.36	0.40
1:A:315:ARG:HE	1:B:640:ARG:NH1	2.20	0.40
1:A:324:VAL:HG22	1:A:355:LEU:CD2	2.51	0.40
1:B:625:LEU:O	1:B:628:LYS:HB2	2.21	0.40
1:C:1032:LYS:HD3	1:D:1593:TYR:CE2	2.56	0.40
1:C:1323:GLN:HE21	1:C:1353:PRO:HB3	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2015:GLY:O	1:E:2018:THR:HG23	2.21	0.40
1:E:2072:ASN:HA	1:E:2359:ILE:O	2.21	0.40
1:E:2121:ARG:HA	1:E:2389:ILE:HD11	2.02	0.40
1:E:2305:VAL:HA	1:E:2313:ALA:HB2	2.03	0.40
1:E:2330:GLY:O	1:E:2332:TYR:CD1	2.75	0.40
1:F:2608:VAL:HG12	1:F:2614:GLU:HA	2.03	0.40
1:A:72:ASN:HA	1:A:359:ILE:O	2.22	0.40
1:B:608:VAL:HG12	1:B:614:GLU:HA	2.04	0.40
1:B:703:ASP:HB2	1:B:717:LYS:HE3	2.03	0.40
1:B:722:LYS:HG2	1:C:1253:TRP:HH2	1.86	0.40
1:C:1121:ARG:HA	1:C:1389:ILE:HD11	2.03	0.40
1:C:1224:ALA:O	1:C:1225:LEU:HG	2.20	0.40
1:D:1484:PRO:O	1:D:1485:TYR:HB2	2.22	0.40
1:D:1576:MET:HE2	1:D:1581:ILE:HD11	2.02	0.40
1:E:2053:TRP:HZ3	1:E:2388:GLU:O	2.05	0.40
1:E:2324:VAL:HG23	1:E:2354:LEU:HD12	2.03	0.40
1:E:2346:VAL:CG2	1:E:2347:CYS:H	2.06	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2376:GLU:OE1	1:F:2776:GLU:OE1[3_884]	1.90	0.30
1:C:1373:GLU:OE2	1:D:1780:GLU:OE1[2_865]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	387/395 (98%)	329 (85%)	44 (11%)	14 (4%)	3 14
1	B	387/395 (98%)	328 (85%)	40 (10%)	19 (5%)	2 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	387/395 (98%)	329 (85%)	45 (12%)	13 (3%)	3 15
1	D	387/395 (98%)	329 (85%)	41 (11%)	17 (4%)	2 10
1	E	387/395 (98%)	330 (85%)	40 (10%)	17 (4%)	2 10
1	F	387/395 (98%)	326 (84%)	42 (11%)	19 (5%)	2 8
All	All	2322/2370 (98%)	1971 (85%)	252 (11%)	99 (4%)	2 10

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	VAL
1	B	746	VAL
1	C	1346	VAL
1	D	1746	VAL
1	E	2346	VAL
1	F	2746	VAL
1	A	70	PRO
1	A	167	MET
1	A	208	VAL
1	A	225	LEU
1	A	226	GLY
1	A	299	ASP
1	A	347	CYS
1	B	470	PRO
1	B	567	MET
1	B	608	VAL
1	B	626	GLY
1	C	1070	PRO
1	C	1167	MET
1	C	1208	VAL
1	C	1225	LEU
1	C	1226	GLY
1	C	1299	ASP
1	C	1347	CYS
1	D	1470	PRO
1	D	1528	PHE
1	D	1567	MET
1	D	1608	VAL
1	D	1625	LEU
1	D	1626	GLY
1	D	1699	ASP
1	E	2070	PRO

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Mol	Chain	Res	Type
1	E	2167	MET
1	E	2208	VAL
1	E	2225	LEU
1	E	2226	GLY
1	E	2270	GLY
1	E	2299	ASP
1	E	2347	CYS
1	F	2470	PRO
1	F	2567	MET
1	F	2608	VAL
1	F	2625	LEU
1	F	2626	GLY
1	F	2670	GLY
1	F	2747	CYS
1	A	33	ASN
1	A	270	GLY
1	B	433	ASN
1	B	528	PHE
1	B	625	LEU
1	B	670	GLY
1	B	699	ASP
1	B	747	CYS
1	C	1033	ASN
1	C	1224	ALA
1	D	1433	ASN
1	D	1670	GLY
1	D	1747	CYS
1	E	2033	ASN
1	E	2128	PHE
1	E	2224	ALA
1	F	2433	ASN
1	F	2624	ALA
1	F	2699	ASP
1	A	224	ALA
1	B	624	ALA
1	B	679	ILE
1	C	1270	GLY
1	D	1624	ALA
1	D	1679	ILE
1	E	2281	ASP
1	F	2528	PHE
1	A	279	ILE

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Mol	Chain	Res	Type
1	B	421	TYR
1	B	432	LYS
1	B	765	VAL
1	C	1279	ILE
1	C	1365	VAL
1	D	1681	ASP
1	F	2421	TYR
1	F	2432	LYS
1	F	2765	VAL
1	A	199	GLU
1	A	365	VAL
1	B	599	GLU
1	B	681	ASP
1	D	1432	LYS
1	D	1765	VAL
1	E	2032	LYS
1	E	2279	ILE
1	E	2365	VAL
1	F	2681	ASP
1	F	2679	ILE
1	F	2562	VAL
1	E	2031	VAL
1	F	2431	VAL
1	B	431	VAL
1	D	1431	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	321/321 (100%)	285 (89%)	36 (11%)	6 18
1	B	321/321 (100%)	283 (88%)	38 (12%)	5 16
1	C	321/321 (100%)	284 (88%)	37 (12%)	5 17
1	D	321/321 (100%)	283 (88%)	38 (12%)	5 16
1	E	321/321 (100%)	283 (88%)	38 (12%)	5 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	321/321 (100%)	284 (88%)	37 (12%)	5 17
All	All	1926/1926 (100%)	1702 (88%)	224 (12%)	5 16

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	ASP
1	A	13	LYS
1	A	21	TYR
1	A	32	LYS
1	A	33	ASN
1	A	41	ASP
1	A	56	LEU
1	A	66	LEU
1	A	74	TYR
1	A	100	ILE
1	A	137	ARG
1	A	146	MET
1	A	149	ARG
1	A	187	GLN
1	A	191	TRP
1	A	207	LEU
1	A	212	TYR
1	A	225	LEU
1	A	254	GLU
1	A	271	LEU
1	A	279	ILE
1	A	280	VAL
1	A	304	ILE
1	A	308	GLU
1	A	314	LYS
1	A	319	SER
1	A	322	LYS
1	A	323	GLN
1	A	326	ARG
1	A	333	HIS
1	A	350	LYS
1	A	363	GLU
1	A	386	ASN
1	A	388	GLU
1	A	389	ILE

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Mol	Chain	Res	Type
1	B	401	MET
1	B	410	ASP
1	B	413	LYS
1	B	421	TYR
1	B	432	LYS
1	B	433	ASN
1	B	441	ASP
1	B	456	LEU
1	B	466	LEU
1	B	474	TYR
1	B	500	ILE
1	B	537	ARG
1	B	546	MET
1	B	549	ARG
1	B	559	VAL
1	B	587	GLN
1	B	591	TRP
1	B	607	LEU
1	B	612	TYR
1	B	625	LEU
1	B	654	GLU
1	B	671	LEU
1	B	679	ILE
1	B	680	VAL
1	B	704	ILE
1	B	708	GLU
1	B	714	LYS
1	B	719	SER
1	B	722	LYS
1	B	723	GLN
1	B	726	ARG
1	B	733	HIS
1	B	743	ARG
1	B	750	LYS
1	B	763	GLU
1	B	786	ASN
1	B	788	GLU
1	B	789	ILE
1	C	1001	MET
1	C	1010	ASP
1	C	1013	LYS
1	C	1021	TYR

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Mol	Chain	Res	Type
1	C	1032	LYS
1	C	1033	ASN
1	C	1041	ASP
1	C	1056	LEU
1	C	1066	LEU
1	C	1074	TYR
1	C	1100	ILE
1	C	1137	ARG
1	C	1146	MET
1	C	1149	ARG
1	C	1159	VAL
1	C	1187	GLN
1	C	1191	TRP
1	C	1207	LEU
1	C	1212	TYR
1	C	1225	LEU
1	C	1254	GLU
1	C	1271	LEU
1	C	1279	ILE
1	C	1280	VAL
1	C	1304	ILE
1	C	1308	GLU
1	C	1314	LYS
1	C	1319	SER
1	C	1322	LYS
1	C	1323	GLN
1	C	1326	ARG
1	C	1333	HIS
1	C	1350	LYS
1	C	1363	GLU
1	C	1386	ASN
1	C	1388	GLU
1	C	1389	ILE
1	D	1401	MET
1	D	1410	ASP
1	D	1413	LYS
1	D	1421	TYR
1	D	1432	LYS
1	D	1433	ASN
1	D	1441	ASP
1	D	1456	LEU
1	D	1466	LEU

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Mol	Chain	Res	Type
1	D	1474	TYR
1	D	1500	ILE
1	D	1537	ARG
1	D	1546	MET
1	D	1549	ARG
1	D	1559	VAL
1	D	1587	GLN
1	D	1591	TRP
1	D	1607	LEU
1	D	1612	TYR
1	D	1625	LEU
1	D	1654	GLU
1	D	1671	LEU
1	D	1679	ILE
1	D	1680	VAL
1	D	1704	ILE
1	D	1708	GLU
1	D	1714	LYS
1	D	1719	SER
1	D	1722	LYS
1	D	1723	GLN
1	D	1726	ARG
1	D	1733	HIS
1	D	1743	ARG
1	D	1750	LYS
1	D	1763	GLU
1	D	1786	ASN
1	D	1788	GLU
1	D	1789	ILE
1	E	2001	MET
1	E	2010	ASP
1	E	2013	LYS
1	E	2021	TYR
1	E	2032	LYS
1	E	2033	ASN
1	E	2041	ASP
1	E	2056	LEU
1	E	2066	LEU
1	E	2074	TYR
1	E	2100	ILE
1	E	2137	ARG
1	E	2146	MET

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Mol	Chain	Res	Type
1	E	2149	ARG
1	E	2187	GLN
1	E	2191	TRP
1	E	2207	LEU
1	E	2212	TYR
1	E	2225	LEU
1	E	2244	PHE
1	E	2254	GLU
1	E	2271	LEU
1	E	2279	ILE
1	E	2280	VAL
1	E	2304	ILE
1	E	2308	GLU
1	E	2314	LYS
1	E	2319	SER
1	E	2322	LYS
1	E	2323	GLN
1	E	2326	ARG
1	E	2327	CYS
1	E	2333	HIS
1	E	2350	LYS
1	E	2363	GLU
1	E	2386	ASN
1	E	2388	GLU
1	E	2389	ILE
1	F	2401	MET
1	F	2410	ASP
1	F	2413	LYS
1	F	2421	TYR
1	F	2432	LYS
1	F	2433	ASN
1	F	2441	ASP
1	F	2456	LEU
1	F	2466	LEU
1	F	2474	TYR
1	F	2500	ILE
1	F	2537	ARG
1	F	2546	MET
1	F	2549	ARG
1	F	2587	GLN
1	F	2591	TRP
1	F	2607	LEU

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Mol	Chain	Res	Type
1	F	2612	TYR
1	F	2625	LEU
1	F	2644	PHE
1	F	2654	GLU
1	F	2671	LEU
1	F	2679	ILE
1	F	2680	VAL
1	F	2704	ILE
1	F	2708	GLU
1	F	2714	LYS
1	F	2719	SER
1	F	2722	LYS
1	F	2723	GLN
1	F	2726	ARG
1	F	2733	HIS
1	F	2750	LYS
1	F	2763	GLU
1	F	2786	ASN
1	F	2788	GLU
1	F	2789	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	33	ASN
1	A	50	ASN
1	A	83	HIS
1	A	111	GLN
1	A	140	HIS
1	A	178	HIS
1	A	187	GLN
1	A	333	HIS
1	A	381	GLN
1	A	386	ASN
1	B	408	ASN
1	B	433	ASN
1	B	450	ASN
1	B	483	HIS
1	B	511	GLN
1	B	540	HIS
1	B	578	HIS

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Mol	Chain	Res	Type
1	B	587	GLN
1	B	733	HIS
1	B	781	GLN
1	B	786	ASN
1	C	1008	ASN
1	C	1033	ASN
1	C	1050	ASN
1	C	1083	HIS
1	C	1111	GLN
1	C	1140	HIS
1	C	1178	HIS
1	C	1187	GLN
1	C	1333	HIS
1	C	1381	GLN
1	C	1386	ASN
1	D	1408	ASN
1	D	1433	ASN
1	D	1450	ASN
1	D	1483	HIS
1	D	1511	GLN
1	D	1540	HIS
1	D	1578	HIS
1	D	1587	GLN
1	D	1733	HIS
1	D	1781	GLN
1	D	1786	ASN
1	E	2008	ASN
1	E	2033	ASN
1	E	2050	ASN
1	E	2083	HIS
1	E	2111	GLN
1	E	2140	HIS
1	E	2178	HIS
1	E	2187	GLN
1	E	2333	HIS
1	E	2381	GLN
1	E	2386	ASN
1	F	2408	ASN
1	F	2433	ASN
1	F	2450	ASN
1	F	2483	HIS
1	F	2511	GLN

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Mol	Chain	Res	Type
1	F	2540	HIS
1	F	2578	HIS
1	F	2587	GLN
1	F	2733	HIS
1	F	2781	GLN
1	F	2786	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PCP	B	792	-	20,22,22	1.28	3 (15%)	29,35,35	1.43	3 (10%)
3	PCP	A	392	-	20,22,22	1.29	3 (15%)	29,35,35	1.42	2 (6%)
3	PCP	F	2792	-	20,22,22	1.26	3 (15%)	29,35,35	1.46	3 (10%)
3	PCP	D	1792	-	20,22,22	1.31	3 (15%)	29,35,35	1.45	3 (10%)
3	PCP	E	2392	-	20,22,22	1.27	3 (15%)	29,35,35	1.43	3 (10%)
3	PCP	C	1392	-	20,22,22	1.29	3 (15%)	29,35,35	1.41	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCP	B	792	-	-	4/17/33/33	0/1/1/1
3	PCP	A	392	-	-	4/17/33/33	0/1/1/1
3	PCP	F	2792	-	-	4/17/33/33	0/1/1/1
3	PCP	D	1792	-	-	4/17/33/33	0/1/1/1
3	PCP	E	2392	-	-	4/17/33/33	0/1/1/1
3	PCP	C	1392	-	-	4/17/33/33	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1792	PCP	O1-C1	2.79	1.53	1.46
3	A	392	PCP	O1-C1	2.72	1.53	1.46
3	B	792	PCP	O1-C1	2.66	1.52	1.46
3	F	2792	PCP	O1-C1	2.63	1.52	1.46
3	C	1392	PCP	O1-C1	2.60	1.52	1.46
3	E	2392	PCP	O1-C1	2.56	1.52	1.46
3	C	1392	PCP	CP-C4	2.55	1.56	1.51
3	E	2392	PCP	CP-C4	2.53	1.56	1.51
3	B	792	PCP	CP-C4	2.52	1.56	1.51
3	E	2392	PCP	PB-O2B	-2.50	1.45	1.54
3	D	1792	PCP	CP-C4	2.50	1.56	1.51
3	D	1792	PCP	PB-O2B	-2.50	1.45	1.54
3	A	392	PCP	PB-O2B	-2.46	1.45	1.54
3	F	2792	PCP	CP-C4	2.42	1.56	1.51
3	A	392	PCP	CP-C4	2.41	1.56	1.51
3	B	792	PCP	PB-O2B	-2.36	1.45	1.54
3	F	2792	PCP	PB-O2B	-2.36	1.45	1.54
3	C	1392	PCP	PB-O2B	-2.35	1.45	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2792	PCP	C4-C5-C1	5.80	113.24	103.77
3	D	1792	PCP	C4-C5-C1	5.72	113.11	103.77
3	B	792	PCP	C4-C5-C1	5.72	113.11	103.77
3	E	2392	PCP	C4-C5-C1	5.67	113.02	103.77
3	A	392	PCP	C4-C5-C1	5.64	112.98	103.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1392	PCP	C4-C5-C1	5.64	112.97	103.77
3	B	792	PCP	O3B-PB-O3A	2.20	112.02	104.64
3	A	392	PCP	O2B-PB-O3A	2.18	111.96	104.64
3	F	2792	PCP	O3B-PB-O3A	2.13	111.79	104.64
3	D	1792	PCP	O3B-PB-O3A	2.12	111.74	104.64
3	D	1792	PCP	O2B-PB-O3A	2.12	111.74	104.64
3	F	2792	PCP	O2B-PB-O3A	2.11	111.72	104.64
3	C	1392	PCP	O2B-PB-O3A	2.09	111.66	104.64
3	C	1392	PCP	O3B-PB-O3A	2.07	111.58	104.64
3	E	2392	PCP	O3B-PB-O3A	2.06	111.55	104.64
3	E	2392	PCP	O2B-PB-O3A	2.06	111.54	104.64
3	B	792	PCP	O2B-PB-O3A	2.05	111.51	104.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	392	PCP	CP-OP-P-O1P
3	A	392	PCP	CP-OP-P-O2P
3	A	392	PCP	CP-OP-P-O3P
3	B	792	PCP	CP-OP-P-O1P
3	B	792	PCP	CP-OP-P-O2P
3	B	792	PCP	CP-OP-P-O3P
3	C	1392	PCP	CP-OP-P-O1P
3	C	1392	PCP	CP-OP-P-O2P
3	C	1392	PCP	CP-OP-P-O3P
3	D	1792	PCP	CP-OP-P-O1P
3	D	1792	PCP	CP-OP-P-O2P
3	D	1792	PCP	CP-OP-P-O3P
3	E	2392	PCP	CP-OP-P-O1P
3	E	2392	PCP	CP-OP-P-O2P
3	E	2392	PCP	CP-OP-P-O3P
3	F	2792	PCP	CP-OP-P-O1P
3	F	2792	PCP	CP-OP-P-O2P
3	F	2792	PCP	CP-OP-P-O3P
3	A	392	PCP	PB-O3A-PA-O1
3	B	792	PCP	PB-O3A-PA-O1
3	C	1392	PCP	PB-O3A-PA-O1
3	D	1792	PCP	PB-O3A-PA-O1
3	E	2392	PCP	PB-O3A-PA-O1
3	F	2792	PCP	PB-O3A-PA-O1

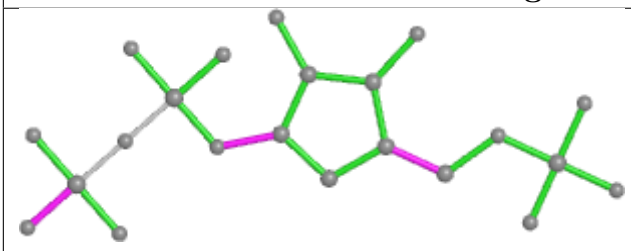
There are no ring outliers.

6 monomers are involved in 8 short contacts:

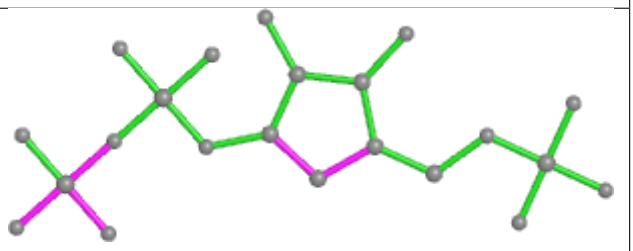
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	792	PCP	1	0
3	A	392	PCP	2	0
3	F	2792	PCP	1	0
3	D	1792	PCP	2	0
3	E	2392	PCP	1	0
3	C	1392	PCP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

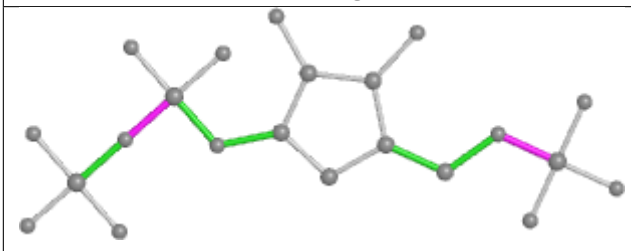
Ligand PCP B 792



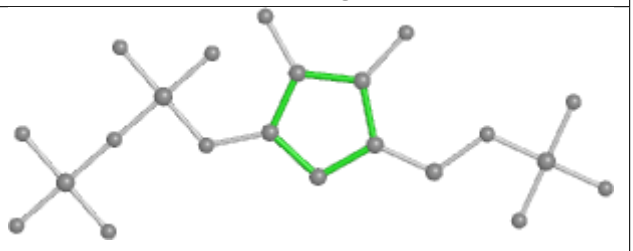
Bond lengths



Bond angles

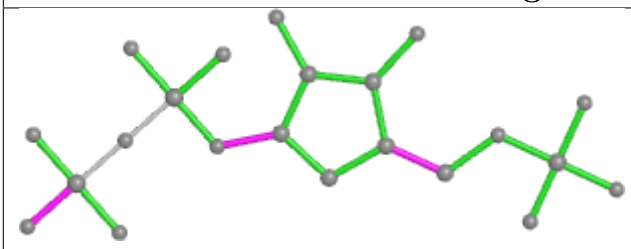


Torsions

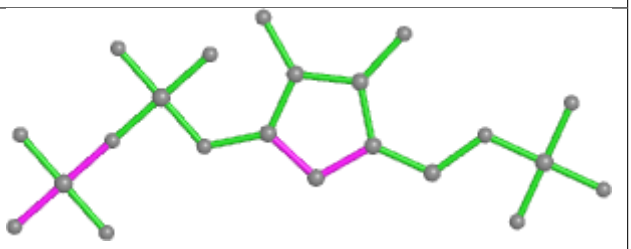


Rings

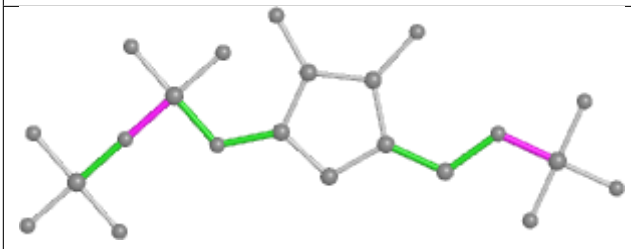
Ligand PCP A 392



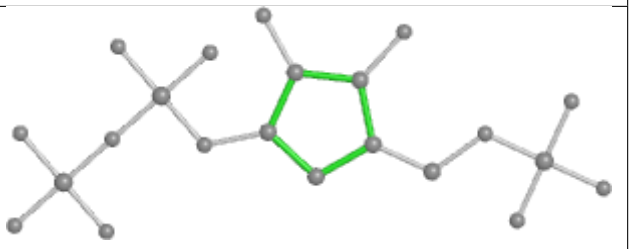
Bond lengths



Bond angles

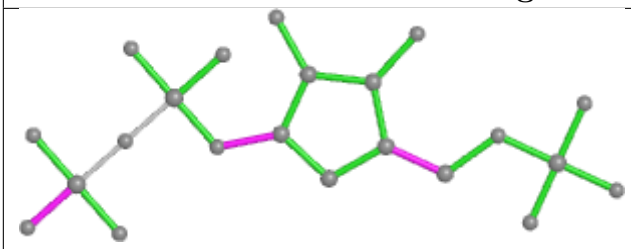


Torsions

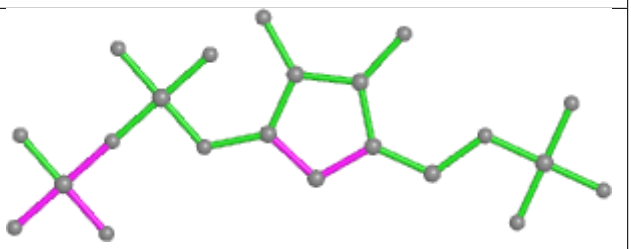


Rings

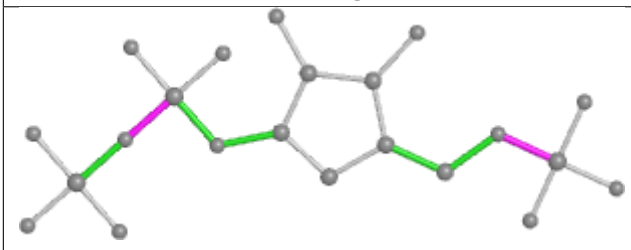
Ligand PCP F 2792



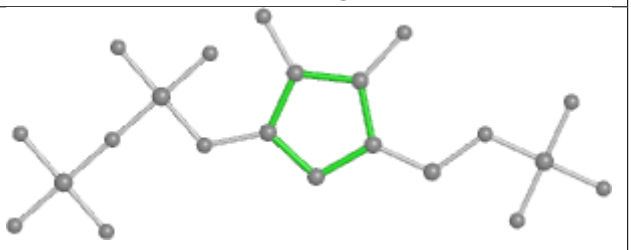
Bond lengths



Bond angles

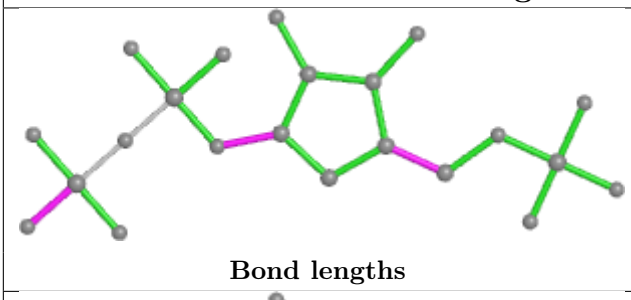


Torsions

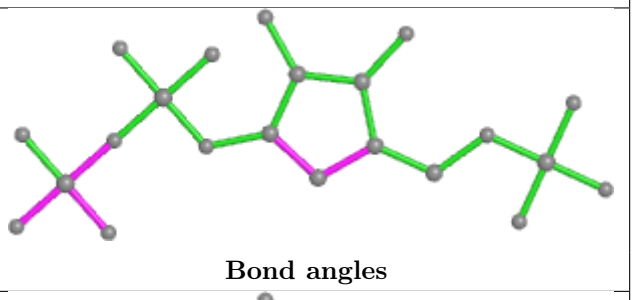


Rings

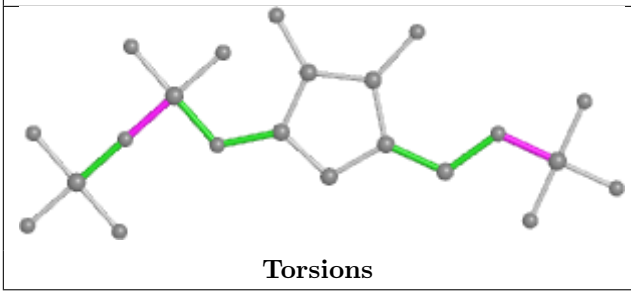
Ligand PCP D 1792



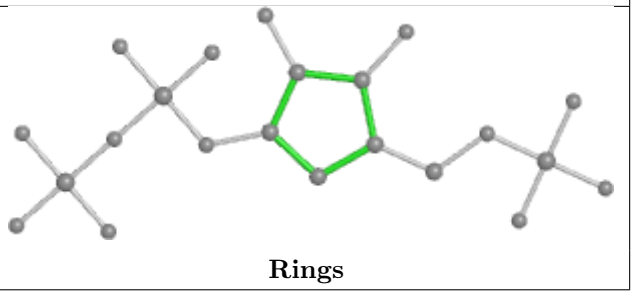
Bond lengths



Bond angles

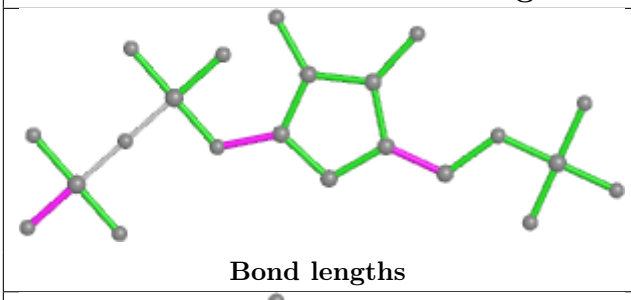


Torsions

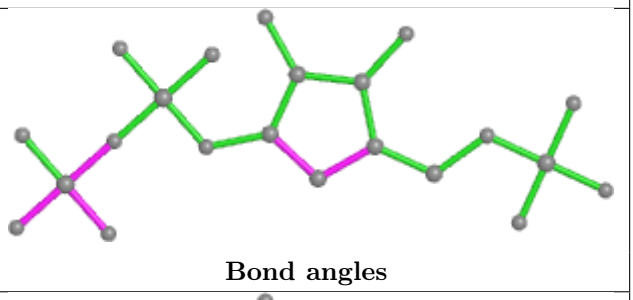


Rings

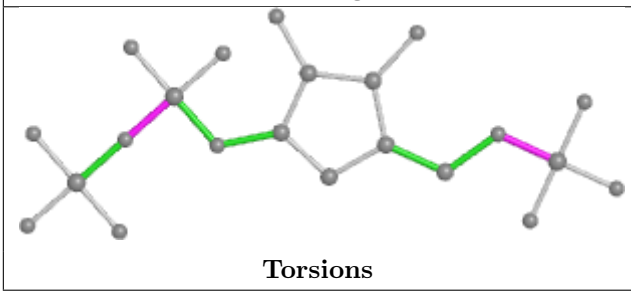
Ligand PCP E 2392



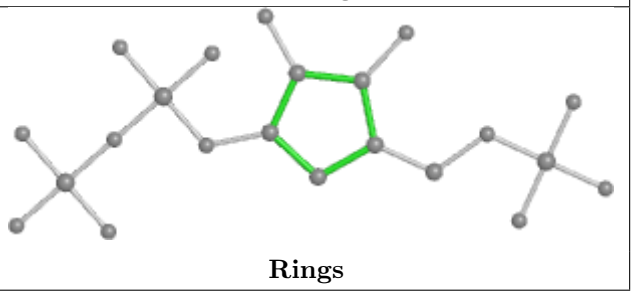
Bond lengths



Bond angles

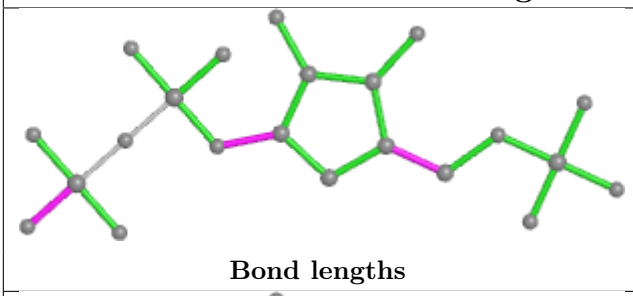


Torsions

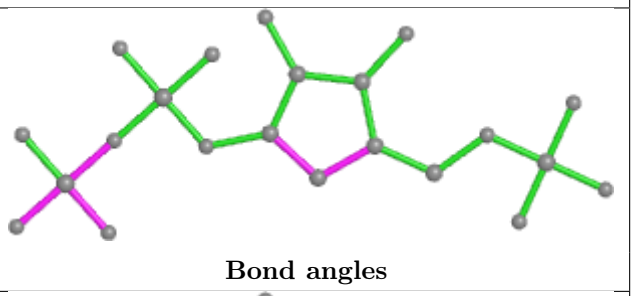


Rings

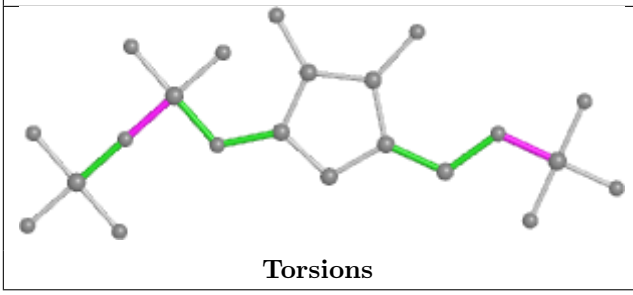
Ligand PCP C 1392



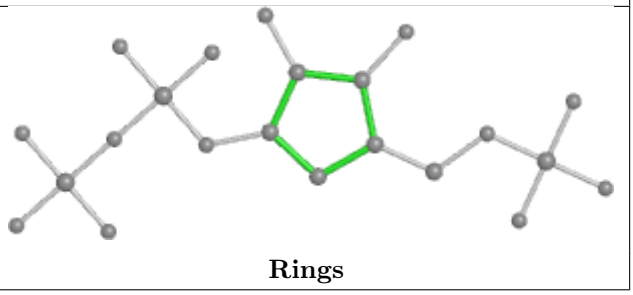
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	389/395 (98%)	0.43	12 (3%)	49	44	32, 65, 86, 105	0
1	B	389/395 (98%)	0.52	21 (5%)	25	22	34, 66, 86, 106	0
1	C	389/395 (98%)	0.47	17 (4%)	34	30	31, 65, 85, 105	0
1	D	389/395 (98%)	0.46	16 (4%)	37	32	35, 66, 86, 106	0
1	E	389/395 (98%)	0.45	13 (3%)	46	41	32, 65, 86, 106	0
1	F	389/395 (98%)	0.48	14 (3%)	42	37	32, 65, 86, 106	0
All	All	2334/2370 (98%)	0.47	93 (3%)	38	33	31, 65, 87, 106	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2741	LEU	5.9
1	E	2341	LEU	5.3
1	C	1211	PHE	4.7
1	D	1741	LEU	4.5
1	B	625	LEU	4.5
1	B	768	PHE	4.3
1	C	1034	ILE	4.1
1	B	730	GLY	4.1
1	A	211	PHE	3.8
1	B	741	LEU	3.5
1	D	1629	LEU	3.5
1	D	1610	THR	3.4
1	D	1768	PHE	3.3
1	B	611	PHE	3.2
1	D	1625	LEU	3.1
1	C	1183	THR	3.0
1	A	64	LYS	3.0
1	F	2611	PHE	2.9
1	B	594	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	1611	PHE	2.9
1	A	207	LEU	2.9
1	B	707	VAL	2.8
1	B	629	LEU	2.8
1	B	751	VAL	2.8
1	D	1730	GLY	2.8
1	C	1022	PHE	2.8
1	A	1	MET	2.7
1	B	561	GLY	2.7
1	F	2742	GLU	2.7
1	F	2419	ASP	2.7
1	B	612	TYR	2.7
1	C	1347	CYS	2.7
1	B	563	LEU	2.6
1	C	1019	ASP	2.6
1	F	2707	VAL	2.6
1	F	2751	VAL	2.6
1	D	1594	PHE	2.6
1	A	251	VAL	2.6
1	F	2743	ARG	2.5
1	B	434	ILE	2.5
1	F	2768	PHE	2.5
1	B	743	ARG	2.5
1	B	758	ILE	2.5
1	B	420	VAL	2.5
1	E	2342	GLU	2.5
1	A	389	ILE	2.5
1	E	2019	ASP	2.5
1	B	687	GLY	2.5
1	D	1612	TYR	2.5
1	B	499	GLY	2.4
1	E	2225	LEU	2.4
1	A	23	LEU	2.4
1	B	728	GLU	2.4
1	C	1194	PHE	2.4
1	C	1001	MET	2.3
1	F	2466	LEU	2.3
1	F	2591	TRP	2.3
1	D	1577	PRO	2.3
1	F	2722	LYS	2.3
1	E	2312	ILE	2.3
1	D	1488	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1343	ARG	2.3
1	F	2745	PRO	2.3
1	F	2704	ILE	2.3
1	E	2322	LYS	2.3
1	E	2343	ARG	2.2
1	D	1758	ILE	2.2
1	A	225	LEU	2.2
1	F	2458	GLY	2.2
1	A	368	PHE	2.2
1	A	101	TYR	2.2
1	C	1032	LYS	2.2
1	C	1023	LEU	2.2
1	C	1225	LEU	2.2
1	C	1179	ALA	2.2
1	A	33	ASN	2.2
1	E	2304	ILE	2.1
1	D	1403	ARG	2.1
1	C	1318	LEU	2.1
1	C	1368	PHE	2.1
1	E	2017	THR	2.1
1	E	2215	LYS	2.1
1	D	1763	GLU	2.1
1	D	1561	GLY	2.1
1	B	572	ALA	2.1
1	B	789	ILE	2.1
1	E	2345	PRO	2.1
1	C	1351	VAL	2.1
1	A	307	VAL	2.0
1	D	1428	ILE	2.0
1	C	1251	VAL	2.0
1	E	2211	PHE	2.0
1	E	2368	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

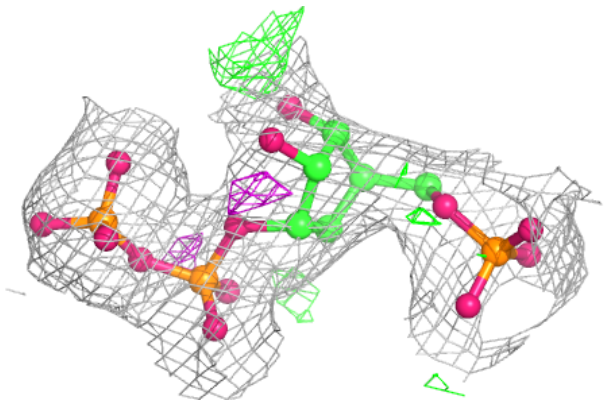
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

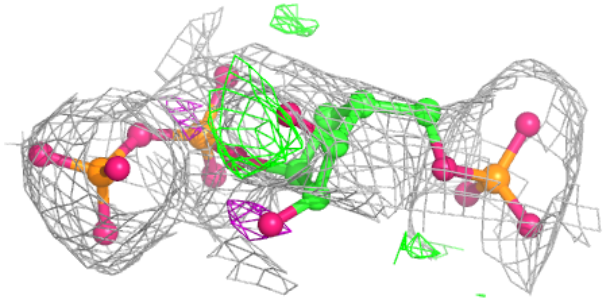
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PCP	A	392	22/22	0.73	0.26	103,109,112,112	0
3	PCP	C	1392	22/22	0.74	0.29	104,110,112,113	0
3	PCP	E	2392	22/22	0.75	0.27	103,109,112,112	0
3	PCP	D	1792	22/22	0.80	0.26	102,109,112,113	0
3	PCP	F	2792	22/22	0.80	0.30	103,109,112,112	0
3	PCP	B	792	22/22	0.82	0.28	103,109,112,112	0
2	ZN	B	793	1/1	0.86	0.09	85,85,85,85	0
2	ZN	D	1793	1/1	0.92	0.12	84,84,84,84	0
2	ZN	A	393	1/1	0.94	0.09	76,76,76,76	0
2	ZN	C	1393	1/1	0.95	0.09	85,85,85,85	0
2	ZN	E	2391	1/1	0.96	0.05	82,82,82,82	0
2	ZN	E	2393	1/1	0.96	0.09	77,77,77,77	0
2	ZN	B	791	1/1	0.96	0.08	78,78,78,78	0
2	ZN	C	1391	1/1	0.96	0.11	62,62,62,62	0
2	ZN	F	2791	1/1	0.97	0.08	83,83,83,83	0
2	ZN	A	391	1/1	0.98	0.11	57,57,57,57	0
2	ZN	D	1791	1/1	0.98	0.08	77,77,77,77	0
2	ZN	F	2793	1/1	0.99	0.09	77,77,77,77	0

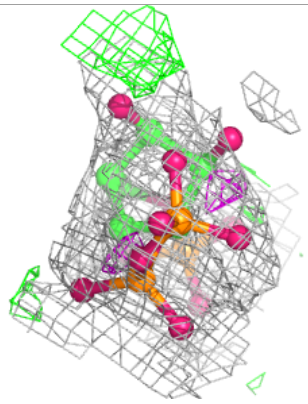
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PCP A 392:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

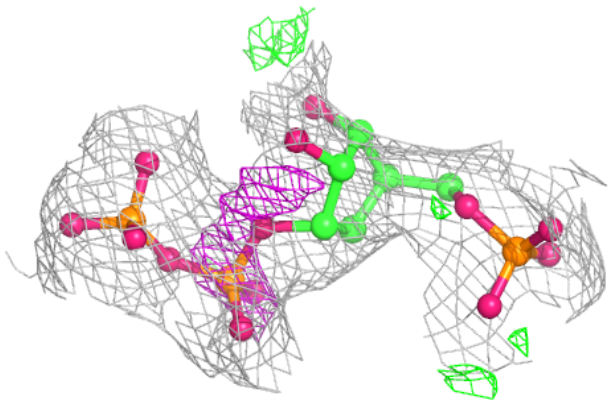


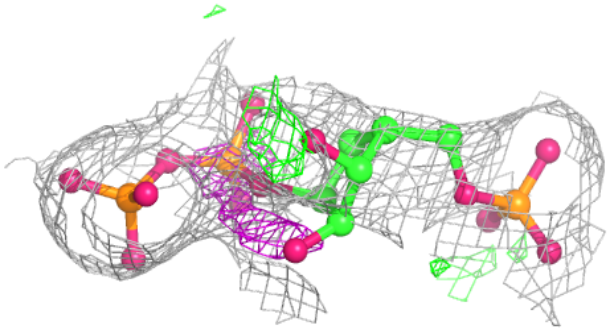


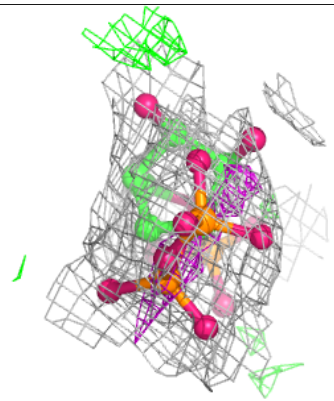


Electron density around PCP C 1392:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

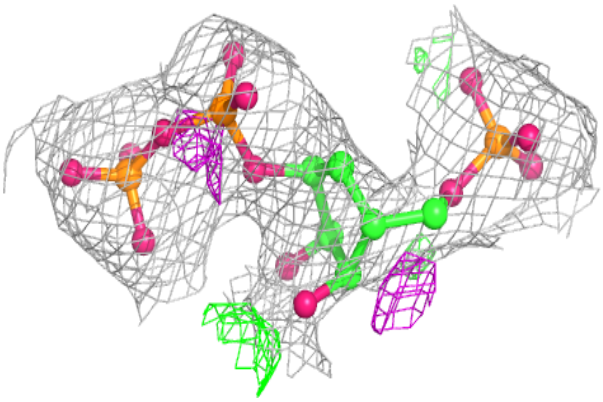


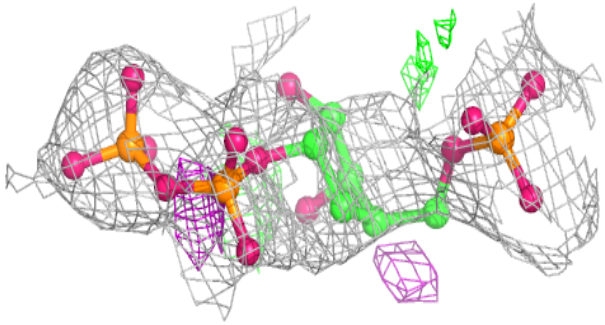




Electron density around PCP E 2392:

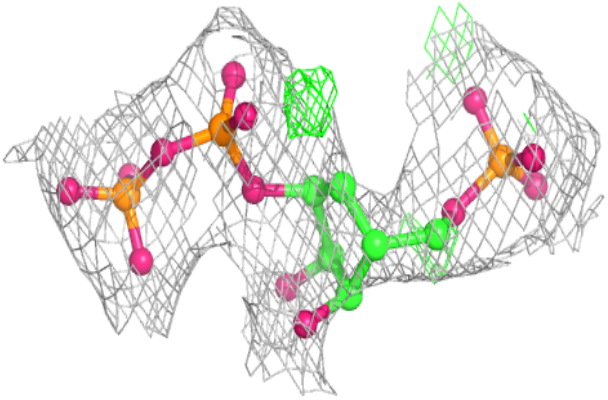
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

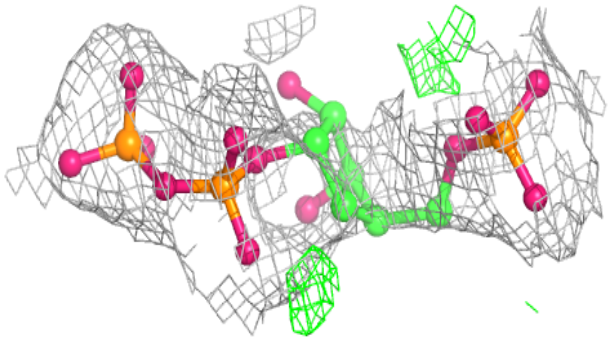


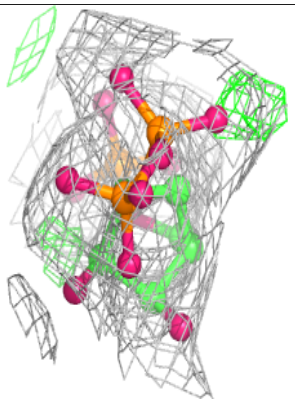


Electron density around PCP D 1792:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

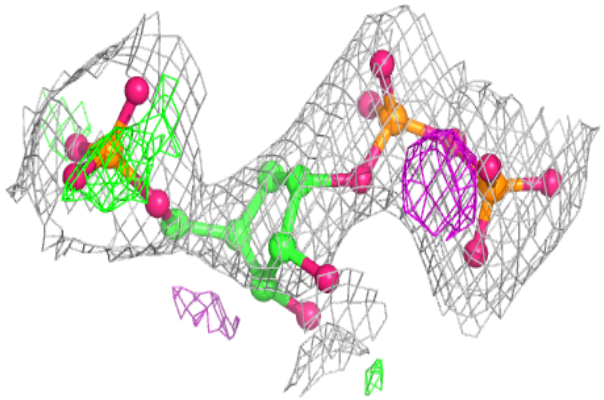


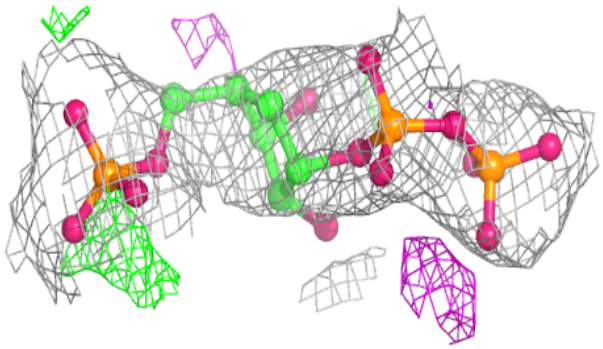


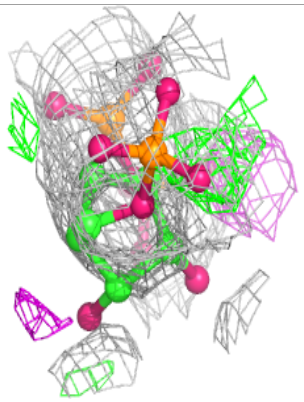


Electron density around PCP F 2792:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

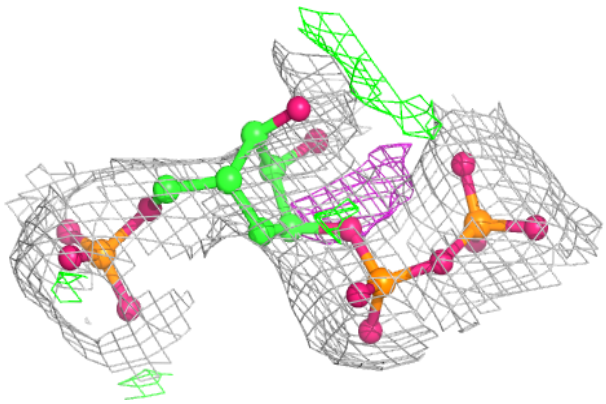


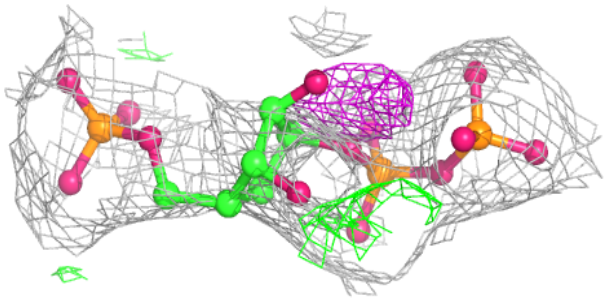


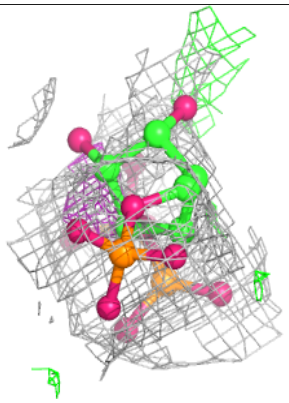


Electron density around PCP B 792:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.