



Full wwPDB EM Validation Report ⓘ

May 25, 2024 – 07:12 AM EDT

PDB ID : 7RIG
EMDB ID : EMD-24479
Title : Structure of ACLY-D1026A-substrates
Authors : Wei, X.; Marmorstein, R.
Deposited on : 2021-07-19
Resolution : 2.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

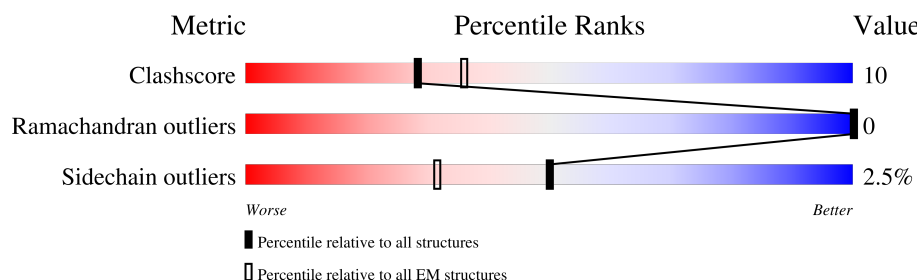
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1101	
1	B	1101	
1	C	1101	
1	D	1101	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32804 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ATP-citrate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1032	Total	C	N	O	S	1	0
			7978	5108	1353	1471	46		
1	B	1032	Total	C	N	O	S	1	0
			7978	5108	1353	1471	46		
1	C	1032	Total	C	N	O	S	1	0
			7978	5108	1353	1471	46		
1	D	1032	Total	C	N	O	S	1	0
			7978	5108	1353	1471	46		

There are 4 discrepancies between the modelled and reference sequences:

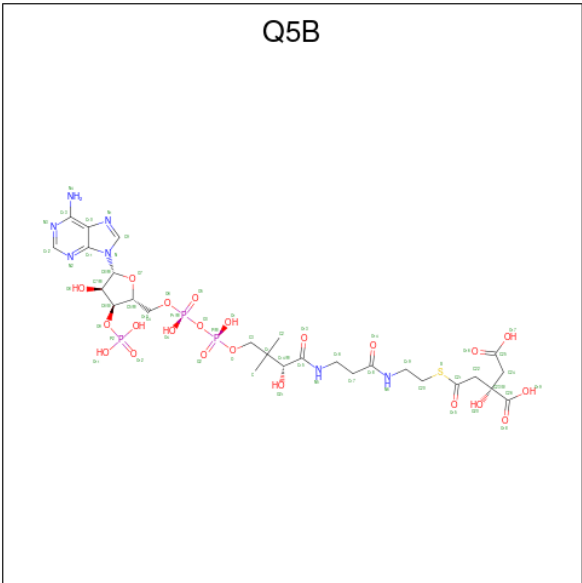
Chain	Residue	Modelled	Actual	Comment	Reference
A	1026	ALA	ASP	engineered mutation	UNP P53396
B	1026	ALA	ASP	engineered mutation	UNP P53396
C	1026	ALA	ASP	engineered mutation	UNP P53396
D	1026	ALA	ASP	engineered mutation	UNP P53396

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



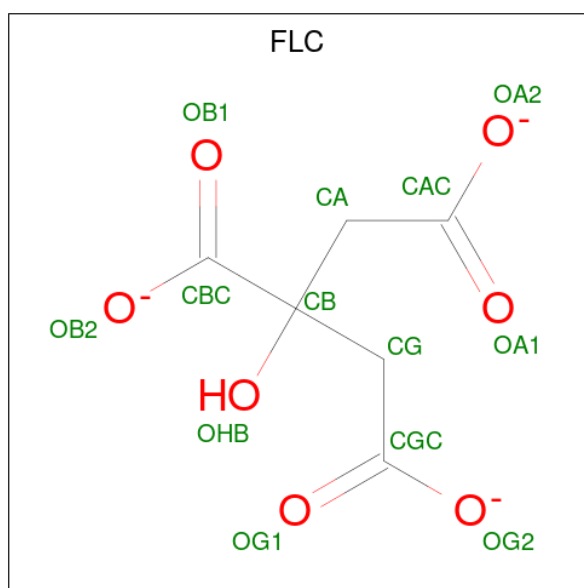
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is (3S)-citryl-Coenzyme A (three-letter code: Q5B) (formula: C₂₇H₄₂N₇O₂₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			60	27	7	22	3	1	
3	B	1	Total	C	N	O	P	S	0
			60	27	7	22	3	1	
3	C	1	Total	C	N	O	P	S	0
			60	27	7	22	3	1	
3	D	1	Total	C	N	O	P	S	0
			60	27	7	22	3	1	

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).

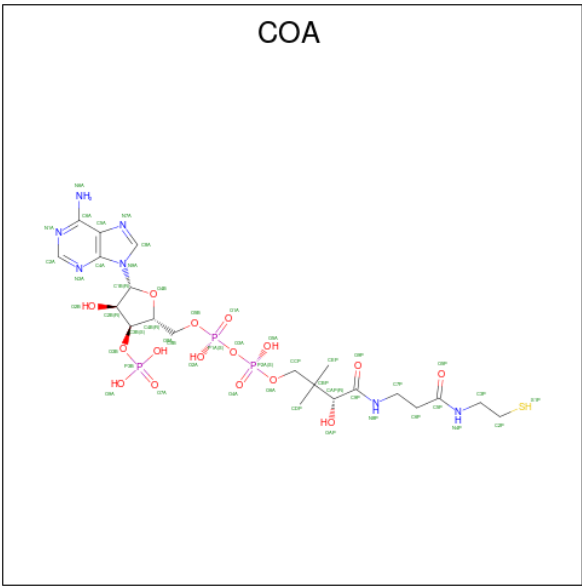


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			13	6	7	
4	B	1	Total	C	O	0
			13	6	7	
4	C	1	Total	C	O	0
			13	6	7	
4	D	1	Total	C	O	0
			13	6	7	

- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

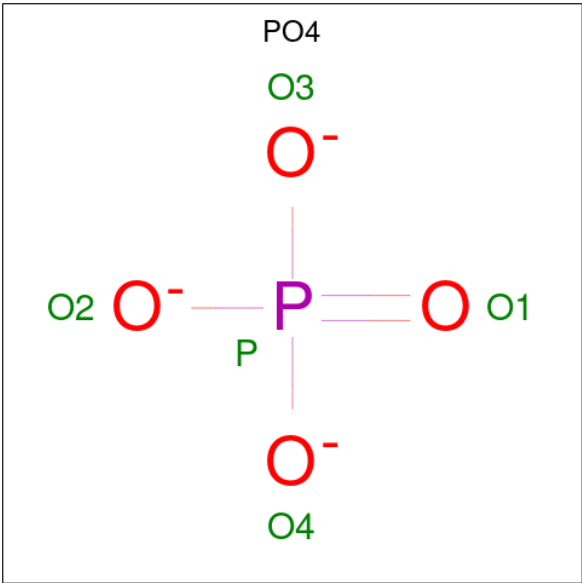
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	C	0
			1	1	
5	D	1	Total	C	0
			1	1	

- Molecule 6 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
6	B	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
6	C	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
6	D	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	O	P	0
			5	4	1	
7	B	1	Total	O	P	0
			5	4	1	
7	C	1	Total	O	P	0
			5	4	1	
7	D	1	Total	O	P	0
			5	4	1	

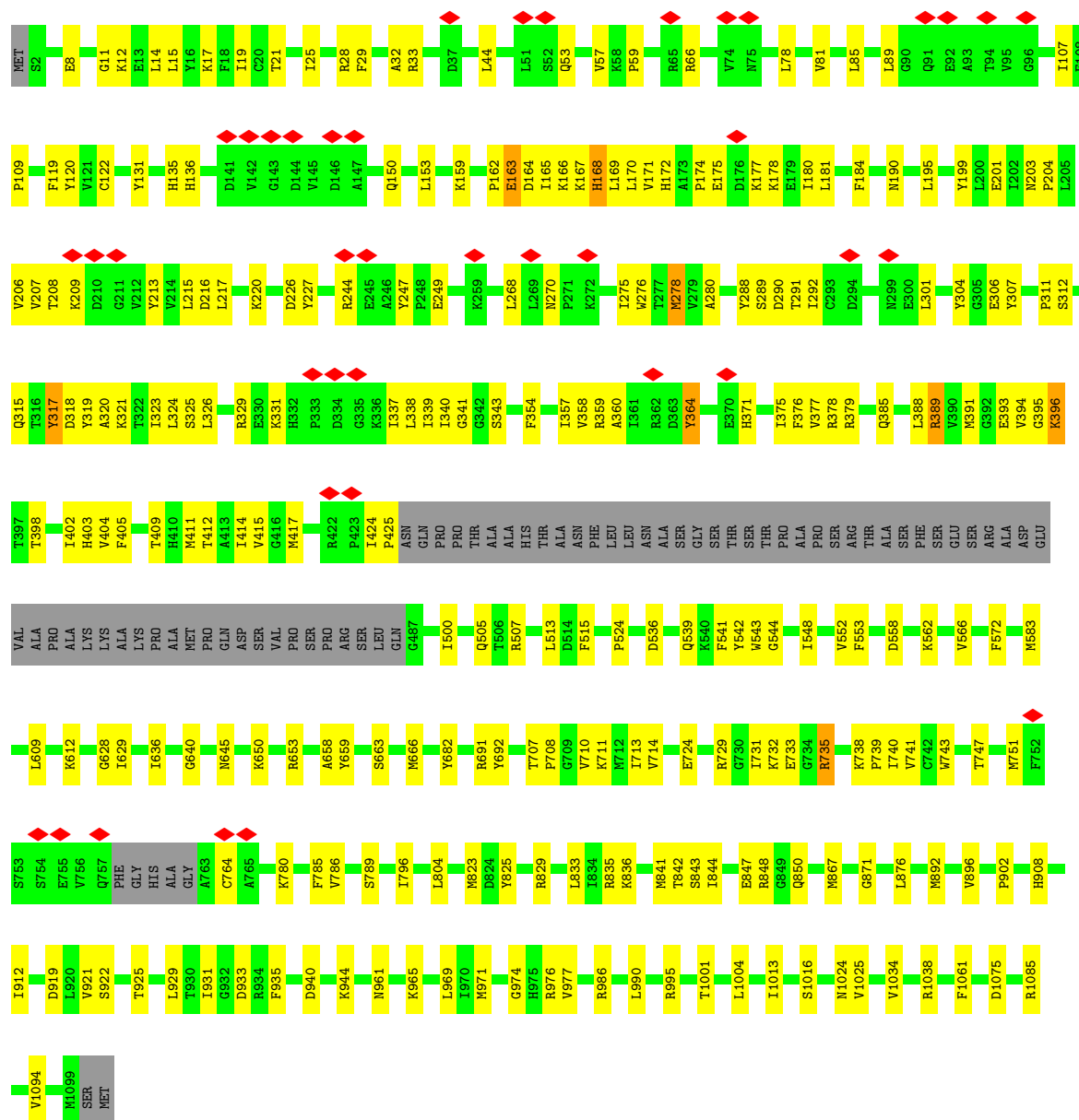
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	73	Total	O	0
			73	73	
8	B	68	Total	O	0
			68	68	
8	C	69	Total	O	0
			69	69	
8	D	68	Total	O	0
			68	68	



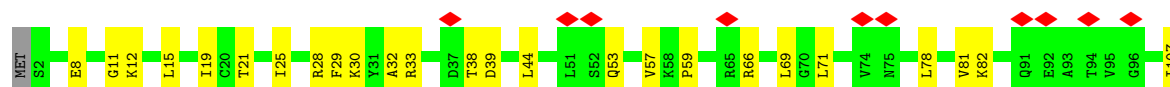
• Molecule 1: ATP-citrate synthase

Chain B: 71% 22% 6%



• Molecule 1: ATP-citrate synthase

Chain C: 70% 23% 6%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	378979	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.286	Depositor
Minimum map value	-1.373	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.165	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	182.59999, 182.59999, 182.59999	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, UNL, Q5B, FLC, ADP, PO4

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	0.32	0/8153	0.52	0/11036
1	B	0.31	0/8153	0.51	0/11036
1	C	0.31	0/8153	0.51	0/11036
1	D	0.31	0/8153	0.52	0/11036
All	All	0.31	0/32612	0.52	0/44144

There are no bond length outliers.

There are no bond angle outliers.

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	7978	0	8025	180	0
1	B	7978	0	8025	183	0
1	C	7978	0	8025	176	0
1	D	7978	0	8025	192	0
2	A	27	0	12	2	0
2	B	27	0	12	3	0
2	C	27	0	12	2	0
2	D	27	0	12	2	0
3	A	60	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	60	0	0	1	0
3	C	60	0	0	1	0
3	D	60	0	0	2	0
4	A	13	0	5	0	0
4	B	13	0	5	0	0
4	C	13	0	5	0	0
4	D	13	0	5	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	48	0	32	6	0
6	B	48	0	32	5	0
6	C	48	0	32	6	0
6	D	48	0	32	6	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
8	A	73	0	0	1	0
8	B	68	0	0	1	0
8	C	69	0	0	1	0
8	D	68	0	0	2	0
All	All	32804	0	32296	680	0

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 10.

All (680) 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:C:1085:ARG:HH11	6:D:2101:COA:H62A	1.11	0.99
6:C:2101:COA:H62A	1:D:1085:ARG:HH11	1.12	0.97
1:A:1085:ARG:HH11	6:B:1204:COA:H62A	1.12	0.95
6:A:1205:COA:H62A	1:B:1085:ARG:HH11	1.12	0.94
1:C:976:ARG:HD2	6:C:2101:COA:H2B	1.58	0.86
1:B:976:ARG:HD2	6:B:1204:COA:H2B	1.58	0.84
1:D:976:ARG:HD2	6:D:2101:COA:H2B	1.60	0.83
1:A:976:ARG:HD2	6:A:1205:COA:H2B	1.63	0.80
1:A:318:ASP:HA	1:A:321:LYS:HE3	1.70	0.74
1:C:206:VAL:HG23	1:C:213:TYR:HB2	1.70	0.74
1:C:663:SER:HB2	1:C:666:MET:HB2	1.69	0.73
1:A:663:SER:HB2	1:A:666:MET:HB2	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:ASP:HA	1:C:321:LYS:HE3	1.70	0.73
1:D:206:VAL:HG23	1:D:213:TYR:HB2	1.71	0.73
1:A:15:LEU:HD11	1:A:19:ILE:HD12	1.70	0.73
1:C:15:LEU:HD11	1:C:19:ILE:HD12	1.70	0.73
1:A:206:VAL:HG23	1:A:213:TYR:HB2	1.71	0.72
1:B:206:VAL:HG23	1:B:213:TYR:HB2	1.71	0.72
1:D:962:LYS:HA	1:D:965:LYS:HE2	1.71	0.72
1:D:15:LEU:HD11	1:D:19:ILE:HD12	1.71	0.71
1:D:318:ASP:HA	1:D:321:LYS:HE3	1.73	0.71
1:B:164:ASP:OD1	1:B:168:HIS:ND1	2.24	0.71
1:D:663:SER:HB2	1:D:666:MET:HB2	1.71	0.71
1:D:226:ASP:OD1	1:D:227:TYR:N	2.24	0.71
1:A:226:ASP:OD1	1:A:227:TYR:N	2.25	0.70
1:B:663:SER:HB2	1:B:666:MET:HB2	1.72	0.70
1:D:785:PHE:HB3	1:D:796:ILE:HD11	1.75	0.68
1:A:275:ILE:HB	1:A:301:LEU:HA	1.76	0.68
1:B:318:ASP:HA	1:B:321:LYS:HE3	1.75	0.67
1:B:388:LEU:HG	1:B:404:VAL:HG13	1.77	0.67
1:B:226:ASP:OD1	1:B:227:TYR:N	2.28	0.67
1:D:971:MET:HA	6:D:2101:COA:H62	1.77	0.67
1:B:974:GLY:O	1:B:1024:ASN:ND2	2.20	0.66
1:A:150:GLN:HE22	1:A:171:VAL:HB	1.60	0.66
1:D:163:GLU:HB2	1:D:167:LYS:HE2	1.77	0.66
1:C:150:GLN:HE22	1:C:171:VAL:HB	1.60	0.66
1:C:785:PHE:HB3	1:C:796:ILE:HD11	1.78	0.66
1:C:275:ILE:HB	1:C:301:LEU:HA	1.78	0.66
1:B:163:GLU:HB2	1:B:167:LYS:HE2	1.78	0.66
1:B:275:ILE:HB	1:B:301:LEU:HA	1.78	0.65
1:D:150:GLN:HE22	1:D:171:VAL:HB	1.60	0.65
1:B:513:LEU:HD22	1:B:524:PRO:HB3	1.77	0.65
1:C:583:MET:HE2	1:C:609:LEU:HD23	1.77	0.65
1:C:164:ASP:OD1	1:C:168:HIS:ND1	2.30	0.65
1:D:275:ILE:HB	1:D:301:LEU:HA	1.79	0.65
1:A:825:TYR:OH	1:A:829:ARG:NH1	2.29	0.65
1:A:867:MET:HB2	1:A:871:GLY:HA3	1.79	0.65
1:C:226:ASP:OD1	1:C:227:TYR:N	2.29	0.65
1:D:395:GLY:HA3	1:D:402:ILE:HG13	1.77	0.65
1:C:163:GLU:HB2	1:C:167:LYS:HE2	1.79	0.65
1:C:513:LEU:HD22	1:C:524:PRO:HB3	1.79	0.65
1:C:340:ILE:HG13	1:C:377:VAL:HG23	1.79	0.64
1:D:513:LEU:HD22	1:D:524:PRO:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:825:TYR:OH	1:D:829:ARG:NH1	2.30	0.64
1:B:867:MET:HB2	1:B:871:GLY:HA3	1.78	0.64
1:D:976:ARG:HG3	1:D:977:VAL:HG13	1.78	0.64
1:A:583:MET:HE2	1:A:609:LEU:HD23	1.79	0.64
1:A:976:ARG:HG3	1:A:977:VAL:HG13	1.78	0.64
1:A:163:GLU:HB2	1:A:167:LYS:HE2	1.81	0.63
1:D:867:MET:HB2	1:D:871:GLY:HA3	1.79	0.63
1:D:166:LYS:HA	1:D:170:LEU:HD12	1.81	0.63
1:B:933:ASP:OD1	1:B:933:ASP:N	2.30	0.63
1:B:150:GLN:HE22	1:B:171:VAL:HB	1.62	0.62
1:A:391:MET:HE2	1:A:402:ILE:HD12	1.82	0.62
1:A:164:ASP:OD1	1:A:168:HIS:ND1	2.31	0.62
1:C:201:GLU:O	1:C:217:LEU:HA	2.00	0.62
1:D:202:ILE:HG22	1:D:217:LEU:HB3	1.80	0.62
1:A:513:LEU:HD22	1:A:524:PRO:HB3	1.81	0.62
1:D:650:LYS:HD2	1:D:653:ARG:HH21	1.65	0.62
1:C:867:MET:HB2	1:C:871:GLY:HA3	1.81	0.61
1:A:933:ASP:OD1	1:A:933:ASP:N	2.31	0.61
1:B:583:MET:HE2	1:B:609:LEU:HD23	1.80	0.61
1:D:343:SER:O	1:D:379:ARG:NH1	2.32	0.61
1:A:1094:VAL:HG23	1:D:843:SER:HB3	1.81	0.61
1:A:785:PHE:HB3	1:A:796:ILE:HD11	1.81	0.61
1:B:785:PHE:HB3	1:B:796:ILE:HD11	1.82	0.61
1:C:731:ILE:HG22	1:C:736:LEU:HB2	1.81	0.61
1:C:971:MET:HA	6:C:2101:COA:H62	1.82	0.61
1:A:971:MET:HA	6:A:1205:COA:H62	1.82	0.61
1:A:843:SER:HB3	1:D:1094:VAL:HG23	1.82	0.61
1:B:825:TYR:OH	1:B:829:ARG:NH1	2.34	0.60
1:C:170:LEU:O	1:C:178:LYS:NZ	2.33	0.60
1:B:976:ARG:HG3	1:B:977:VAL:HG13	1.83	0.60
1:D:707:THR:O	1:D:738:LYS:NZ	2.35	0.60
1:A:167:LYS:HD3	1:A:167:LYS:N	2.16	0.60
1:A:343:SER:O	1:A:379:ARG:NH1	2.34	0.60
1:B:167:LYS:HD3	1:B:167:LYS:N	2.16	0.60
1:D:201:GLU:O	1:D:217:LEU:HA	2.02	0.60
1:C:167:LYS:HD3	1:C:167:LYS:N	2.17	0.60
1:C:933:ASP:OD1	1:C:933:ASP:N	2.31	0.60
1:A:395:GLY:HA3	1:A:402:ILE:HG13	1.84	0.59
1:C:339:ILE:HD13	1:C:376:PHE:HB2	1.84	0.59
1:B:15:LEU:HD11	1:B:19:ILE:HD12	1.84	0.59
1:D:731:ILE:HG22	1:D:736:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LEU:HG	1:A:404:VAL:HG13	1.85	0.59
1:B:244:ARG:NH1	1:B:268:LEU:O	2.35	0.59
1:C:244:ARG:NH1	1:C:268:LEU:O	2.36	0.59
1:A:888:GLN:O	1:A:892:MET:HG3	2.01	0.59
1:A:170:LEU:O	1:A:178:LYS:NZ	2.35	0.59
1:B:278:MET:HB2	1:B:319:TYR:HE2	1.68	0.59
1:B:14:LEU:HD22	1:B:195:LEU:HD21	1.84	0.59
1:B:892:MET:HG2	1:D:863:PHE:HE1	1.68	0.59
1:B:1094:VAL:HG23	1:C:843:SER:HB3	1.83	0.59
1:D:244:ARG:NH1	1:D:268:LEU:O	2.36	0.59
1:C:823:MET:HE1	1:C:833:LEU:HD12	1.85	0.59
1:A:201:GLU:O	1:A:217:LEU:HA	2.02	0.59
1:D:164:ASP:OD1	1:D:168:HIS:ND1	2.36	0.59
1:A:940:ASP:OD2	1:A:944:LYS:NZ	2.30	0.58
1:A:896:VAL:HG21	1:A:990:LEU:HD11	1.86	0.58
1:B:823:MET:HE1	1:B:833:LEU:HD12	1.85	0.58
1:D:933:ASP:N	1:D:933:ASP:OD1	2.31	0.58
1:A:539:GLN:HG2	1:A:541:PHE:CE2	2.39	0.58
1:B:539:GLN:HG2	1:B:541:PHE:CE2	2.38	0.58
1:B:843:SER:HB3	1:C:1094:VAL:HG23	1.85	0.58
1:A:244:ARG:NH1	1:A:268:LEU:O	2.36	0.58
1:B:896:VAL:HG21	1:B:990:LEU:HD11	1.86	0.58
1:B:902:PRO:HG3	1:D:842:THR:HG21	1.85	0.58
1:C:825:TYR:OH	1:C:829:ARG:NH1	2.35	0.58
1:D:53:GLN:HE21	1:D:109:PRO:HB3	1.69	0.58
1:A:823:MET:HE1	1:A:833:LEU:HD12	1.86	0.57
1:B:940:ASP:OD2	1:B:944:LYS:NZ	2.31	0.57
1:D:278:MET:HB2	1:D:319:TYR:HE2	1.69	0.57
1:A:339:ILE:HD13	1:A:376:PHE:HB2	1.86	0.57
1:A:931:ILE:HD12	1:A:1061:PHE:HE2	1.69	0.57
1:B:170:LEU:O	1:B:178:LYS:NZ	2.37	0.57
1:C:539:GLN:HG2	1:C:541:PHE:CE2	2.38	0.57
1:C:976:ARG:HG3	1:C:977:VAL:HG13	1.85	0.57
1:A:863:PHE:HE1	1:C:892:MET:HG2	1.69	0.57
1:B:44:LEU:HD11	1:B:78:LEU:HD11	1.87	0.57
1:D:167:LYS:HD3	1:D:167:LYS:N	2.19	0.57
1:B:340:ILE:O	1:B:377:VAL:HA	2.05	0.57
1:D:278:MET:O	1:D:278:MET:HG3	2.05	0.57
1:D:388:LEU:HG	1:D:404:VAL:HG13	1.86	0.57
1:A:707:THR:O	1:A:738:LYS:NZ	2.37	0.57
1:D:339:ILE:HD13	1:D:376:PHE:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:GLU:OE1	1:D:1085:ARG:NH1	2.38	0.56
1:A:53:GLN:HE21	1:A:109:PRO:HB3	1.70	0.56
1:D:931:ILE:HD12	1:D:1061:PHE:HE2	1.69	0.56
1:C:338:LEU:HB3	1:C:375:ILE:HG12	1.88	0.56
1:D:539:GLN:HG2	1:D:541:PHE:CE2	2.39	0.56
1:A:836:LYS:HE3	1:B:836:LYS:HE3	1.88	0.56
1:D:170:LEU:O	1:D:178:LYS:NZ	2.38	0.56
1:D:888:GLN:O	1:D:892:MET:HG3	2.05	0.56
1:A:14:LEU:HD22	1:A:195:LEU:HD21	1.86	0.56
1:B:338:LEU:HB3	1:B:375:ILE:HG12	1.87	0.56
1:B:707:THR:O	1:B:738:LYS:NZ	2.38	0.56
1:C:44:LEU:HD11	1:C:78:LEU:HD11	1.88	0.56
1:C:707:THR:O	1:C:738:LYS:NZ	2.38	0.56
1:B:204:PRO:HD2	1:B:215:LEU:HB2	1.88	0.56
1:C:1085:ARG:NH1	6:D:2101:COA:H62A	1.93	0.56
1:D:120:TYR:HB3	1:D:135:HIS:HB3	1.87	0.56
1:A:8:GLU:O	1:A:12:LYS:HG3	2.06	0.56
1:C:931:ILE:HD12	1:C:1061:PHE:HE2	1.70	0.56
1:C:650:LYS:HD2	1:C:653:ARG:HH21	1.71	0.55
1:C:896:VAL:HG21	1:C:990:LEU:HD11	1.87	0.55
1:D:389:ARG:NH1	1:D:393:GLU:OE1	2.39	0.55
1:C:216:ASP:OD1	1:C:217:LEU:N	2.39	0.55
1:C:166:LYS:HA	1:C:170:LEU:HD12	1.89	0.55
1:C:836:LYS:HE3	1:D:836:LYS:HE3	1.88	0.55
1:A:338:LEU:HB3	1:A:375:ILE:HG12	1.88	0.55
1:B:216:ASP:OD1	1:B:217:LEU:N	2.39	0.55
1:B:847:GLU:OE1	1:C:1085:ARG:NH1	2.39	0.55
1:B:971:MET:HA	6:B:1204:COA:H62	1.87	0.55
1:C:53:GLN:HE21	1:C:109:PRO:HB3	1.72	0.55
6:C:2101:COA:H62A	1:D:1085:ARG:NH1	1.94	0.55
1:A:842:THR:HG21	1:C:902:PRO:HG3	1.86	0.55
1:D:940:ASP:OD2	1:D:944:LYS:NZ	2.31	0.55
1:A:278:MET:HB3	1:A:340:ILE:HG22	1.89	0.55
1:C:32:ALA:HB3	1:C:107:ILE:HB	1.89	0.55
1:A:902:PRO:HG3	1:C:842:THR:HG21	1.89	0.55
1:C:343:SER:O	1:C:379:ARG:NH1	2.39	0.55
1:B:8:GLU:O	1:B:12:LYS:HG3	2.07	0.55
1:A:32:ALA:HB3	1:A:107:ILE:HB	1.89	0.54
1:B:278:MET:O	1:B:278:MET:HG3	2.07	0.54
1:D:14:LEU:HD22	1:D:195:LEU:HD21	1.89	0.54
1:A:44:LEU:HD11	1:A:78:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASP:OD1	1:A:217:LEU:N	2.41	0.54
1:A:974:GLY:O	1:A:1024:ASN:ND2	2.24	0.54
1:B:931:ILE:HD12	1:B:1061:PHE:HE2	1.73	0.54
1:C:940:ASP:OD2	1:C:944:LYS:NZ	2.32	0.54
1:D:162:PRO:O	1:D:166:LYS:HG2	2.08	0.54
1:B:53:GLN:HE21	1:B:109:PRO:HB3	1.73	0.54
1:B:11:GLY:HA3	1:B:217:LEU:HD11	1.90	0.54
1:B:650:LYS:HD2	1:B:653:ARG:HH21	1.72	0.54
1:C:417:MET:HG2	1:C:424:ILE:HA	1.90	0.54
1:D:896:VAL:HG21	1:D:990:LEU:HD11	1.88	0.54
1:C:8:GLU:O	1:C:12:LYS:HG3	2.07	0.53
1:C:11:GLY:HA3	1:C:217:LEU:HD11	1.90	0.53
1:D:32:ALA:HB3	1:D:107:ILE:HB	1.90	0.53
1:D:292:ILE:HD11	1:D:301:LEU:HD22	1.89	0.53
1:A:925:THR:HG23	1:C:925:THR:HG23	1.89	0.53
1:D:8:GLU:O	1:D:12:LYS:HG3	2.07	0.53
1:B:32:ALA:HB3	1:B:107:ILE:HB	1.90	0.53
1:D:823:MET:HE1	1:D:833:LEU:HD12	1.89	0.53
1:A:650:LYS:HD2	1:A:653:ARG:HH21	1.72	0.53
1:A:708:PRO:O	1:A:711:LYS:NZ	2.42	0.53
1:C:275:ILE:HG23	1:C:337:ILE:HD11	1.91	0.53
1:C:202:ILE:HD12	1:C:205:LEU:HD13	1.91	0.53
1:C:292:ILE:HD11	1:C:301:LEU:HD22	1.90	0.53
1:A:1085:ARG:NH1	1:D:847:GLU:OE1	2.37	0.53
1:B:908:HIS:O	1:B:912:ILE:HG12	2.09	0.53
1:C:908:HIS:O	1:C:912:ILE:HG12	2.09	0.53
1:D:275:ILE:HG23	1:D:337:ILE:HD11	1.90	0.53
1:B:925:THR:HG23	1:D:925:THR:HG23	1.90	0.52
1:D:216:ASP:OD1	1:D:217:LEU:N	2.42	0.52
1:B:842:THR:HG21	1:D:902:PRO:HG3	1.89	0.52
1:C:500:ILE:HG13	1:C:566:VAL:HG11	1.91	0.52
1:B:339:ILE:HD13	1:B:376:PHE:HB2	1.92	0.52
1:B:731:ILE:HD11	1:B:740:ILE:HD12	1.90	0.52
1:D:908:HIS:O	1:D:912:ILE:HG12	2.10	0.52
1:A:500:ILE:HG13	1:A:566:VAL:HG11	1.91	0.52
1:A:908:HIS:O	1:A:912:ILE:HG12	2.10	0.52
1:A:292:ILE:HD11	1:A:301:LEU:HD22	1.91	0.52
1:D:500:ILE:HG13	1:D:566:VAL:HG11	1.92	0.52
1:A:204:PRO:HD2	1:A:215:LEU:HB2	1.92	0.52
1:D:204:PRO:HD2	1:D:215:LEU:HB2	1.92	0.52
1:B:275:ILE:HG23	1:B:337:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1085:ARG:NH1	1:C:847:GLU:OE1	2.38	0.51
1:C:78:LEU:O	1:C:81:VAL:HG22	2.10	0.51
1:A:389:ARG:NH1	1:A:393:GLU:OE1	2.43	0.51
1:B:162:PRO:O	1:B:166:LYS:HG2	2.11	0.51
1:D:78:LEU:O	1:D:81:VAL:HG22	2.10	0.51
1:A:78:LEU:O	1:A:81:VAL:HG22	2.10	0.51
1:C:21:THR:HG21	1:C:184:PHE:HA	1.92	0.51
1:D:338:LEU:HB3	1:D:375:ILE:HG12	1.91	0.51
1:A:166:LYS:HA	1:A:170:LEU:HD12	1.92	0.51
1:A:1085:ARG:NH1	6:B:1204:COA:H62A	1.94	0.51
1:B:199:TYR:HB3	1:B:220:LYS:HB2	1.92	0.51
1:B:292:ILE:HD11	1:B:301:LEU:HD22	1.92	0.51
1:B:500:ILE:HG13	1:B:566:VAL:HG11	1.93	0.51
1:C:208:THR:HG22	1:C:209:LYS:H	1.76	0.51
1:B:343:SER:O	1:B:379:ARG:NH1	2.43	0.51
1:C:131:TYR:CE1	1:C:153:LEU:HD12	2.46	0.51
1:D:21:THR:HG21	1:D:184:PHE:HA	1.92	0.51
1:A:21:THR:HG21	1:A:184:PHE:HA	1.92	0.51
1:D:208:THR:HG22	1:D:209:LYS:H	1.76	0.51
1:B:708:PRO:O	1:B:711:LYS:NZ	2.44	0.50
6:A:1205:COA:H62A	1:B:1085:ARG:NH1	1.94	0.50
1:B:289:SER:O	1:B:292:ILE:HG13	2.12	0.50
1:B:122:CYS:SG	1:B:201:GLU:HB3	2.51	0.50
1:D:391:MET:HE2	1:D:402:ILE:HD12	1.94	0.50
1:B:208:THR:HG22	1:B:209:LYS:H	1.76	0.50
1:C:708:PRO:O	1:C:711:LYS:NZ	2.44	0.49
1:A:919:ASP:HB3	1:A:922:SER:HB2	1.94	0.49
1:D:340:ILE:O	1:D:377:VAL:HA	2.11	0.49
1:B:892:MET:HG2	1:D:863:PHE:CE1	2.46	0.49
1:A:11:GLY:HA3	1:A:217:LEU:HD11	1.94	0.49
1:B:320:ALA:HB2	1:B:357:ILE:HG22	1.94	0.49
1:B:395:GLY:HA3	1:B:402:ILE:HG13	1.94	0.49
1:B:919:ASP:HB3	1:B:922:SER:HB2	1.94	0.49
1:C:289:SER:O	1:C:292:ILE:HG13	2.12	0.49
1:A:244:ARG:HD2	1:A:247:TYR:HE1	1.77	0.49
1:A:358:VAL:HG13	1:A:394:VAL:HG11	1.95	0.49
1:B:244:ARG:HD2	1:B:247:TYR:HE1	1.77	0.49
1:B:843:SER:OG	1:D:1075:ASP:OD1	2.31	0.49
1:D:244:ARG:HD2	1:D:247:TYR:HE1	1.77	0.49
1:A:199:TYR:HB3	1:A:220:LYS:HB2	1.95	0.49
1:A:208:THR:HG22	1:A:209:LYS:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:MET:HG2	1:A:424:ILE:HA	1.94	0.49
1:A:863:PHE:CE1	1:C:892:MET:HG2	2.48	0.49
1:C:377:VAL:HG11	1:C:391:MET:HE1	1.94	0.49
1:C:396:LYS:NZ	1:C:402:ILE:O	2.46	0.49
1:C:919:ASP:HB3	1:C:922:SER:HB2	1.95	0.49
1:B:741:VAL:HG22	1:B:785:PHE:HB2	1.94	0.49
1:D:136:HIS:CE1	1:D:174:PRO:HD3	2.48	0.49
1:D:277:THR:HG22	1:D:339:ILE:HB	1.94	0.49
1:A:131:TYR:CE1	1:A:153:LEU:HD12	2.47	0.49
1:A:394:VAL:O	1:A:398:THR:HG22	2.13	0.49
1:A:1075:ASP:OD1	1:C:843:SER:OG	2.31	0.49
1:D:175:GLU:HA	1:D:178:LYS:HD3	1.95	0.49
1:D:289:SER:O	1:D:292:ILE:HG13	2.13	0.49
1:D:394:VAL:O	1:D:398:THR:HG22	2.13	0.49
1:A:289:SER:O	1:A:292:ILE:HG13	2.13	0.48
1:A:317:TYR:CZ	1:A:360:ALA:HA	2.48	0.48
1:D:417:MET:HE3	1:D:425:PRO:HD2	1.95	0.48
1:C:175:GLU:HA	1:C:178:LYS:HD3	1.95	0.48
1:D:199:TYR:HB3	1:D:220:LYS:HB2	1.95	0.48
1:B:131:TYR:HE1	1:B:153:LEU:HB2	1.78	0.48
1:C:215:LEU:HD13	2:C:2102:ADP:C4	2.49	0.48
1:A:317:TYR:HE2	1:A:359:ARG:HG2	1.78	0.48
1:B:21:THR:HG21	1:B:184:PHE:HA	1.95	0.48
1:D:44:LEU:HD11	1:D:78:LEU:HD11	1.94	0.48
1:B:166:LYS:HA	1:B:170:LEU:HD12	1.94	0.48
1:C:244:ARG:HD2	1:C:247:TYR:HE1	1.78	0.48
1:D:417:MET:HG2	1:D:424:ILE:HA	1.95	0.48
1:A:120:TYR:HB3	1:A:135:HIS:HB3	1.95	0.48
1:A:278:MET:HE1	1:A:357:ILE:HG21	1.94	0.48
1:A:1034:VAL:O	1:A:1038:ARG:HG2	2.13	0.48
1:B:417:MET:HB3	1:B:424:ILE:HG13	1.96	0.48
1:B:1034:VAL:O	1:B:1038:ARG:HG2	2.13	0.48
1:C:136:HIS:CE1	1:C:174:PRO:HD3	2.49	0.48
1:A:275:ILE:HG23	1:A:337:ILE:HD11	1.94	0.48
1:A:378:ARG:HB2	1:A:414:ILE:HG21	1.96	0.48
1:C:553:PHE:HE1	1:C:562:LYS:HE2	1.79	0.48
1:A:417:MET:HE3	1:A:425:PRO:HD2	1.96	0.48
1:A:843:SER:OG	1:C:1075:ASP:OD1	2.32	0.48
1:D:974:GLY:O	6:D:2101:COA:H133	2.14	0.48
1:A:136:HIS:CE1	1:A:174:PRO:HD3	2.49	0.48
1:A:553:PHE:HE1	1:A:562:LYS:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ILE:HA	1:B:169:LEU:HB2	1.96	0.48
1:B:331:LYS:HD2	1:B:371:HIS:CD2	2.49	0.48
1:D:919:ASP:HB3	1:D:922:SER:HB2	1.96	0.48
1:D:57:VAL:HB	1:D:107:ILE:HD13	1.96	0.47
1:A:165:ILE:HA	1:A:169:LEU:HB2	1.96	0.47
1:B:131:TYR:CE1	1:B:153:LEU:HB2	2.49	0.47
1:B:136:HIS:CE1	1:B:174:PRO:HD3	2.49	0.47
1:B:320:ALA:O	1:B:324:LEU:HG	2.14	0.47
1:D:128:GLU:HG3	1:D:153:LEU:HD11	1.96	0.47
1:D:553:PHE:HE1	1:D:562:LYS:HE2	1.79	0.47
1:D:583:MET:SD	1:D:609:LEU:HD23	2.54	0.47
1:D:682:TYR:CD1	1:D:710:VAL:HG12	2.50	0.47
1:B:59:PRO:O	1:B:66:ARG:NH1	2.47	0.47
1:C:962:LYS:HA	1:C:965:LYS:HE2	1.97	0.47
1:D:1034:VAL:O	1:D:1038:ARG:HG2	2.14	0.47
1:B:215:LEU:HD13	2:B:1201:ADP:C4	2.49	0.47
1:B:291:THR:HG22	1:B:415:VAL:HG11	1.96	0.47
1:C:542:TYR:CZ	1:D:835:ARG:HG2	2.50	0.47
1:A:175:GLU:HA	1:A:178:LYS:HD3	1.96	0.47
1:D:378:ARG:HB2	1:D:414:ILE:HG21	1.95	0.47
1:D:780:LYS:HD3	1:D:786:VAL:HB	1.96	0.47
1:A:320:ALA:O	1:A:323:ILE:HG22	2.15	0.47
1:A:969:LEU:HD22	3:C:2103:Q5B:C10	2.45	0.47
3:A:1202:Q5B:C10	1:C:969:LEU:HD22	2.44	0.47
1:B:120:TYR:HB3	1:B:135:HIS:HB3	1.96	0.47
1:C:291:THR:HG22	1:C:415:VAL:HG11	1.97	0.47
1:C:1034:VAL:O	1:C:1038:ARG:HG2	2.14	0.47
1:D:30:LYS:HE2	1:D:30:LYS:HB2	1.81	0.47
1:D:312:SER:OG	1:D:315:GLN:OE1	2.28	0.47
1:D:320:ALA:HB2	1:D:357:ILE:HG22	1.97	0.47
1:D:331:LYS:HD2	1:D:371:HIS:CD2	2.50	0.47
1:A:312:SER:OG	1:A:315:GLN:OE1	2.29	0.47
1:A:976:ARG:HD2	6:A:1205:COA:C2B	2.41	0.47
1:B:1075:ASP:OD1	1:D:843:SER:OG	2.33	0.47
1:C:165:ILE:HA	1:C:169:LEU:HB2	1.96	0.47
1:C:835:ARG:HG2	1:D:542:TYR:CZ	2.50	0.47
1:A:8:GLU:HG2	1:A:12:LYS:HE3	1.97	0.47
1:A:268:LEU:HD21	1:A:326:LEU:HD21	1.97	0.47
1:A:542:TYR:CZ	1:B:835:ARG:HG2	2.50	0.47
1:A:835:ARG:HG2	1:B:542:TYR:CZ	2.50	0.47
1:B:175:GLU:HA	1:B:178:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:TYR:CZ	1:C:360:ALA:HA	2.50	0.47
1:C:320:ALA:O	1:C:323:ILE:HG22	2.15	0.47
1:A:215:LEU:HD13	2:A:1201:ADP:C4	2.50	0.46
1:C:780:LYS:HD3	1:C:786:VAL:HB	1.97	0.46
1:D:558:ASP:N	1:D:558:ASP:OD1	2.47	0.46
1:A:823:MET:O	1:B:835:ARG:N	2.48	0.46
1:B:378:ARG:HB2	1:B:414:ILE:HG21	1.97	0.46
1:C:727:ILE:O	1:C:731:ILE:HG23	2.16	0.46
1:D:215:LEU:HD13	2:D:2103:ADP:C4	2.51	0.46
1:D:320:ALA:O	1:D:324:LEU:HG	2.15	0.46
1:C:331:LYS:HD2	1:C:371:HIS:CD2	2.51	0.46
1:C:682:TYR:CD1	1:C:710:VAL:HG12	2.50	0.46
1:D:741:VAL:HG22	1:D:785:PHE:HB2	1.97	0.46
1:B:8:GLU:HG2	1:B:12:LYS:HE3	1.98	0.46
1:C:325:SER:HA	1:C:364:TYR:OH	2.15	0.46
1:C:30:LYS:HE2	1:C:30:LYS:HB2	1.81	0.46
1:C:57:VAL:HB	1:C:107:ILE:HD13	1.98	0.46
1:C:354:PHE:HE2	1:C:388:LEU:HD23	1.80	0.46
1:D:170:LEU:HD11	1:D:182:ALA:HB2	1.98	0.46
1:D:974:GLY:O	1:D:1024:ASN:ND2	2.25	0.46
1:A:57:VAL:HB	1:A:107:ILE:HD13	1.98	0.46
1:D:291:THR:HG22	1:D:415:VAL:HG11	1.98	0.46
1:B:57:VAL:HB	1:B:107:ILE:HD13	1.97	0.46
1:B:204:PRO:HD3	2:B:1201:ADP:O1A	2.16	0.46
3:B:1202:Q5B:C10	1:D:969:LEU:HD22	2.46	0.46
1:D:8:GLU:HG2	1:D:12:LYS:HE3	1.97	0.46
1:A:691:ARG:HD2	1:A:692:TYR:CE1	2.51	0.46
1:B:682:TYR:CD1	1:B:710:VAL:HG12	2.50	0.46
1:C:974:GLY:O	1:C:1024:ASN:ND2	2.24	0.46
1:C:8:GLU:HG2	1:C:12:LYS:HE3	1.97	0.46
1:D:59:PRO:O	1:D:66:ARG:NH1	2.49	0.46
1:D:131:TYR:CE1	1:D:153:LEU:HD12	2.51	0.46
1:A:128:GLU:HG3	1:A:153:LEU:HD11	1.98	0.46
1:B:691:ARG:HD2	1:B:692:TYR:CE1	2.51	0.46
1:A:320:ALA:O	1:A:324:LEU:HG	2.16	0.45
1:A:325:SER:HA	1:A:364:TYR:OH	2.16	0.45
1:A:682:TYR:CD1	1:A:710:VAL:HG12	2.51	0.45
1:B:340:ILE:HD12	1:B:341:GLY:N	2.31	0.45
1:B:986:ARG:CZ	1:B:1025:VAL:HG21	2.47	0.45
1:C:280:ALA:HB2	1:C:307:TYR:CZ	2.52	0.45
1:D:276:TRP:CD2	1:D:327:MET:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:ALA:O	1:D:323:ILE:HG22	2.17	0.45
1:D:659:TYR:HA	1:D:714:VAL:O	2.16	0.45
1:D:691:ARG:HD2	1:D:692:TYR:CE1	2.51	0.45
1:B:325:SER:HA	1:B:364:TYR:OH	2.17	0.45
1:B:417:MET:HG2	1:B:424:ILE:HA	1.97	0.45
1:B:659:TYR:HA	1:B:714:VAL:O	2.16	0.45
1:A:202:ILE:HG22	1:A:217:LEU:HB3	1.98	0.45
1:A:507:ARG:NH2	8:A:1309:HOH:O	2.49	0.45
1:A:986:ARG:CZ	1:A:1025:VAL:HG21	2.47	0.45
1:D:268:LEU:HD21	1:D:326:LEU:HD21	1.97	0.45
1:A:278:MET:HG3	1:A:319:TYR:HE2	1.82	0.45
1:A:659:TYR:HA	1:A:714:VAL:O	2.16	0.45
1:B:848:ARG:NH1	8:B:1310:HOH:O	2.49	0.45
1:B:969:LEU:HD22	3:D:2104:Q5B:C10	2.47	0.45
1:A:291:THR:HG22	1:A:415:VAL:HG11	1.98	0.45
1:A:728:CYS:HA	1:A:731:ILE:HG22	1.98	0.45
1:B:340:ILE:HG23	1:B:377:VAL:HG23	1.97	0.45
1:C:128:GLU:HG3	1:C:153:LEU:HD11	1.99	0.45
1:D:6:ILE:HG21	1:D:236:ILE:HD11	1.97	0.45
1:D:986:ARG:CZ	1:D:1025:VAL:HG21	2.47	0.45
1:A:316:THR:HG21	1:A:353:THR:O	2.17	0.45
1:C:986:ARG:CZ	1:C:1025:VAL:HG21	2.46	0.45
1:A:280:ALA:HB2	1:A:307:TYR:CZ	2.51	0.45
1:A:331:LYS:HD2	1:A:371:HIS:CD2	2.51	0.45
1:A:835:ARG:N	1:B:823:MET:O	2.50	0.45
1:B:85:LEU:O	1:B:89:LEU:N	2.33	0.45
1:B:163:GLU:H	1:B:163:GLU:CD	2.19	0.45
1:C:741:VAL:HG22	1:C:785:PHE:HB2	1.99	0.45
1:D:325:SER:HA	1:D:364:TYR:OH	2.16	0.45
1:B:505:GLN:HG3	1:B:572:PHE:CG	2.52	0.45
1:D:724:GLU:OE1	1:D:724:GLU:N	2.49	0.45
1:B:190:ASN:HD22	1:B:190:ASN:H	1.64	0.44
1:C:691:ARG:HD2	1:C:692:TYR:CE1	2.52	0.44
1:C:739:PRO:HG2	1:C:804:LEU:HD11	1.99	0.44
1:B:268:LEU:HD21	1:B:326:LEU:HD21	2.00	0.44
1:B:317:TYR:HE2	1:B:359:ARG:HE	1.63	0.44
1:C:163:GLU:CD	1:C:163:GLU:H	2.19	0.44
1:D:181:LEU:HD11	1:D:205:LEU:HD21	1.99	0.44
1:D:270:ASN:O	1:D:270:ASN:ND2	2.51	0.44
1:A:1001:THR:HB	1:A:1004:LEU:HB3	1.99	0.44
1:C:164:ASP:HA	1:C:168:HIS:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ALA:O	1:C:324:LEU:HG	2.16	0.44
1:C:543:TRP:HB2	1:C:548:ILE:HD13	1.99	0.44
1:C:659:TYR:HA	1:C:714:VAL:O	2.17	0.44
1:C:724:GLU:OE1	1:C:724:GLU:N	2.49	0.44
1:D:580:ASP:OD1	8:D:2201:HOH:O	2.21	0.44
1:B:14:LEU:HD22	1:B:195:LEU:CD2	2.48	0.44
1:B:270:ASN:ND2	1:B:270:ASN:O	2.51	0.44
1:C:270:ASN:O	1:C:270:ASN:ND2	2.51	0.44
1:C:505:GLN:HG3	1:C:572:PHE:CG	2.52	0.44
1:D:317:TYR:CZ	1:D:360:ALA:HA	2.53	0.44
1:D:1001:THR:HB	1:D:1004:LEU:HB3	1.99	0.44
1:B:340:ILE:HD12	1:B:341:GLY:H	1.81	0.44
1:B:583:MET:SD	1:B:612:LYS:HD3	2.58	0.44
1:A:215:LEU:HD13	2:A:1201:ADP:C5	2.52	0.44
1:A:290:ASP:OD1	1:A:747:THR:OG1	2.26	0.44
1:B:780:LYS:HD3	1:B:786:VAL:HB	2.00	0.44
1:C:120:TYR:HB3	1:C:135:HIS:HB3	1.99	0.44
1:A:270:ASN:O	1:A:270:ASN:ND2	2.51	0.44
1:A:276:TRP:CD2	1:A:327:MET:HG3	2.52	0.44
1:A:780:LYS:HD3	1:A:786:VAL:HB	2.00	0.44
1:B:249:GLU:OE2	1:B:325:SER:OG	2.27	0.44
1:C:394:VAL:O	1:C:398:THR:HG22	2.18	0.44
1:D:69:LEU:HB3	1:D:71:LEU:HD23	1.98	0.44
1:B:215:LEU:HD13	2:B:1201:ADP:C5	2.52	0.44
1:D:658:ALA:O	1:D:713:ILE:HA	2.18	0.44
1:B:317:TYR:CZ	1:B:360:ALA:HA	2.53	0.44
1:B:377:VAL:HG11	1:B:391:MET:HE1	1.99	0.44
1:A:925:THR:CG2	1:C:925:THR:HG23	2.49	0.43
1:B:1001:THR:HB	1:B:1004:LEU:HB3	2.00	0.43
1:C:317:TYR:HE2	1:C:359:ARG:HG2	1.82	0.43
1:C:395:GLY:HA3	1:C:402:ILE:HG13	1.99	0.43
1:D:316:THR:HG21	1:D:353:THR:O	2.18	0.43
1:A:898:ALA:HA	1:A:1064:GLY:O	2.18	0.43
1:C:268:LEU:HD21	1:C:326:LEU:HD21	1.98	0.43
1:D:389:ARG:HD2	1:D:393:GLU:OE1	2.19	0.43
1:D:640:GLY:O	1:D:645:ASN:ND2	2.43	0.43
1:A:6:ILE:HG21	1:A:236:ILE:HD11	2.00	0.43
1:A:340:ILE:O	1:A:377:VAL:HA	2.18	0.43
1:C:126:THR:OG1	1:C:129:GLY:O	2.32	0.43
1:C:558:ASP:OD1	1:C:558:ASP:N	2.51	0.43
1:D:17:LYS:HB2	1:D:17:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:844:ILE:HD12	1:B:876:LEU:HD22	2.00	0.43
1:D:165:ILE:HA	1:D:169:LEU:HB2	2.00	0.43
1:D:215:LEU:HD13	2:D:2103:ADP:C5	2.54	0.43
1:A:18:PHE:CZ	1:A:232:LYS:HG2	2.53	0.43
1:A:558:ASP:OD1	1:A:558:ASP:N	2.51	0.43
1:A:640:GLY:O	1:A:645:ASN:ND2	2.41	0.43
1:B:78:LEU:O	1:B:81:VAL:HG22	2.19	0.43
1:B:312:SER:OG	1:B:315:GLN:OE1	2.28	0.43
1:B:320:ALA:O	1:B:323:ILE:HG22	2.18	0.43
1:B:394:VAL:O	1:B:398:THR:HG22	2.18	0.43
1:B:417:MET:HE3	1:B:425:PRO:HD2	2.01	0.43
1:B:735:ARG:HD2	1:B:735:ARG:HA	1.70	0.43
1:C:199:TYR:HB3	1:C:220:LYS:HB2	2.00	0.43
1:D:164:ASP:HA	1:D:168:HIS:HD1	1.84	0.43
1:D:543:TRP:HB2	1:D:548:ILE:HD13	2.00	0.43
1:D:898:ALA:HA	1:D:1064:GLY:O	2.18	0.43
1:A:974:GLY:O	6:A:1205:COA:H133	2.18	0.43
1:C:320:ALA:HB2	1:C:357:ILE:HG22	2.01	0.43
1:C:340:ILE:O	1:C:377:VAL:HA	2.18	0.43
1:C:974:GLY:O	6:C:2101:COA:H133	2.19	0.43
1:D:276:TRP:CH2	1:D:326:LEU:HG	2.53	0.43
1:D:403:HIS:CE1	1:D:424:ILE:HG21	2.53	0.43
1:D:574:SER:OG	3:D:2104:Q5B:O12	2.23	0.43
1:A:976:ARG:HG3	1:A:977:VAL:N	2.34	0.43
1:C:1001:THR:HB	1:C:1004:LEU:HB3	2.00	0.43
1:D:163:GLU:H	1:D:163:GLU:CD	2.21	0.43
1:D:203:ASN:HA	1:D:204:PRO:HA	1.63	0.43
1:A:290:ASP:OD1	1:A:747:THR:N	2.52	0.43
1:A:505:GLN:HG3	1:A:572:PHE:CG	2.54	0.43
1:A:515:PHE:CE1	1:A:629:ILE:HD11	2.54	0.43
1:C:743:TRP:CH2	1:C:789:SER:HA	2.54	0.43
1:C:848:ARG:NH1	8:C:2210:HOH:O	2.50	0.43
1:A:320:ALA:HB2	1:A:357:ILE:HG22	2.01	0.43
1:A:516:ASP:OD2	1:A:525:SER:OG	2.27	0.43
1:B:201:GLU:O	1:B:217:LEU:HA	2.19	0.43
1:C:202:ILE:HG22	1:C:217:LEU:HB3	1.99	0.43
1:C:571:ASN:HD21	1:C:581:SER:HB2	1.84	0.43
1:D:750:THR:OG1	1:D:751:MET:SD	2.76	0.43
1:B:122:CYS:HA	1:B:201:GLU:HA	2.01	0.42
1:B:280:ALA:HB2	1:B:307:TYR:CZ	2.54	0.42
1:B:543:TRP:HB2	1:B:548:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:PRO:HG2	1:B:804:LEU:HD11	2.01	0.42
1:B:925:THR:CG2	1:D:925:THR:HG23	2.50	0.42
1:C:25:ILE:HG23	1:C:28:ARG:HD3	2.01	0.42
1:C:377:VAL:HG12	1:C:403:HIS:O	2.18	0.42
1:D:11:GLY:HA3	1:D:217:LEU:HD11	2.00	0.42
1:D:134:PHE:HD1	1:D:135:HIS:N	2.17	0.42
1:D:358:VAL:HG13	1:D:394:VAL:HG11	2.01	0.42
1:D:659:TYR:CZ	1:D:684:GLY:HA3	2.54	0.42
1:A:835:ARG:HD2	1:B:544:GLY:O	2.20	0.42
1:A:925:THR:HG23	1:C:925:THR:CG2	2.49	0.42
1:B:119:PHE:CD2	1:B:181:LEU:HD11	2.54	0.42
1:B:391:MET:HE2	1:B:402:ILE:HG23	2.01	0.42
1:B:396:LYS:HA	1:B:396:LYS:HD3	1.86	0.42
1:D:804:LEU:HB3	1:D:810:ILE:HD12	2.01	0.42
1:A:536:ASP:HA	1:A:552:VAL:O	2.18	0.42
1:A:543:TRP:HB2	1:A:548:ILE:HD13	2.01	0.42
1:A:741:VAL:HG22	1:A:785:PHE:HB2	2.01	0.42
1:B:159:LYS:HB3	1:B:159:LYS:HE3	1.86	0.42
1:B:203:ASN:HA	1:B:204:PRO:HA	1.80	0.42
1:B:389:ARG:NH1	1:B:393:GLU:OE1	2.52	0.42
1:B:925:THR:HG23	1:D:925:THR:CG2	2.49	0.42
1:D:290:ASP:OD1	1:D:747:THR:N	2.51	0.42
1:A:931:ILE:HB	1:C:921:VAL:HG21	2.02	0.42
1:B:841:MET:HB3	1:D:1079:LEU:HD13	2.01	0.42
1:B:976:ARG:HG3	1:B:977:VAL:N	2.35	0.42
1:C:38:THR:HG23	1:C:39:ASP:O	2.20	0.42
1:C:358:VAL:HG13	1:C:394:VAL:HG11	2.01	0.42
1:C:388:LEU:HD23	1:C:388:LEU:HA	1.91	0.42
1:C:976:ARG:HG3	1:C:977:VAL:N	2.34	0.42
1:D:708:PRO:O	1:D:711:LYS:NZ	2.51	0.42
1:A:25:ILE:HG23	1:A:28:ARG:HD3	2.01	0.42
1:B:290:ASP:OD1	1:B:747:THR:N	2.52	0.42
1:B:377:VAL:HG12	1:B:403:HIS:O	2.19	0.42
1:D:918:LYS:HD2	1:D:918:LYS:HA	1.78	0.42
1:A:159:LYS:HB3	1:A:159:LYS:HE3	1.86	0.42
1:C:918:LYS:HD2	1:C:918:LYS:HA	1.79	0.42
1:D:536:ASP:HA	1:D:552:VAL:O	2.18	0.42
1:A:733:GLU:HG2	1:A:734:GLY:H	1.83	0.42
1:B:290:ASP:OD1	1:B:747:THR:OG1	2.28	0.42
1:B:658:ALA:O	1:B:713:ILE:HA	2.19	0.42
1:B:743:TRP:CH2	1:B:789:SER:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:976:ARG:HD2	6:B:1204:COA:C2B	2.39	0.42
1:C:121:VAL:HB	1:C:202:ILE:HG12	2.00	0.42
1:C:290:ASP:OD1	1:C:747:THR:N	2.52	0.42
1:C:976:ARG:HD2	6:C:2101:COA:C2B	2.40	0.42
1:A:583:MET:SD	1:A:612:LYS:HD3	2.60	0.42
1:A:921:VAL:HG21	1:C:931:ILE:HB	2.02	0.42
1:B:288:TYR:OH	1:B:411:MET:O	2.27	0.42
1:B:931:ILE:HB	1:D:921:VAL:HG21	2.02	0.42
1:C:59:PRO:O	1:C:66:ARG:NH1	2.52	0.42
1:C:69:LEU:HB3	1:C:71:LEU:HD23	2.01	0.42
1:C:378:ARG:HB2	1:C:414:ILE:HG21	2.02	0.42
1:C:544:GLY:O	1:D:835:ARG:HD2	2.19	0.42
1:C:844:ILE:HD12	1:C:876:LEU:HD22	2.00	0.42
1:D:792:GLU:O	1:D:796:ILE:HG22	2.19	0.42
1:D:976:ARG:HG3	1:D:977:VAL:N	2.35	0.42
1:A:331:LYS:HB3	1:A:331:LYS:HE3	1.83	0.42
1:A:739:PRO:HG2	1:A:804:LEU:HD11	2.02	0.42
1:B:921:VAL:HG21	1:D:931:ILE:HB	2.02	0.42
1:C:931:ILE:HD13	1:C:935:PHE:CE2	2.55	0.42
1:A:69:LEU:HB3	1:A:71:LEU:HD23	2.00	0.42
1:B:291:THR:HG21	1:B:412:THR:HB	2.02	0.42
1:B:396:LYS:NZ	1:B:402:ILE:O	2.53	0.42
1:D:358:VAL:CG1	1:D:394:VAL:HG21	2.50	0.42
1:D:891:GLU:O	1:D:895:MET:HG3	2.20	0.42
1:A:521:ARG:HD2	1:A:633:CYS:O	2.20	0.41
1:B:724:GLU:OE1	1:B:724:GLU:N	2.50	0.41
1:C:378:ARG:HD2	1:C:411:MET:HA	2.02	0.41
1:C:396:LYS:HA	1:C:396:LYS:HD3	1.87	0.41
1:C:536:ASP:HA	1:C:552:VAL:O	2.19	0.41
1:C:929:LEU:HD13	1:D:925:THR:HG22	2.02	0.41
1:B:15:LEU:CD1	1:B:19:ILE:HD12	2.50	0.41
1:B:331:LYS:HB3	1:B:331:LYS:HE3	1.83	0.41
1:C:215:LEU:HD13	2:C:2102:ADP:C5	2.56	0.41
1:C:316:THR:HG21	1:C:353:THR:O	2.21	0.41
1:D:38:THR:HG23	1:D:39:ASP:O	2.21	0.41
1:D:291:THR:HG21	1:D:412:THR:HB	2.02	0.41
1:A:17:LYS:HB2	1:A:17:LYS:NZ	2.36	0.41
1:A:59:PRO:O	1:A:66:ARG:NH1	2.54	0.41
1:B:177:LYS:HD2	1:B:207:VAL:HG13	2.02	0.41
1:B:358:VAL:HG13	1:B:394:VAL:HG11	2.02	0.41
1:B:405:PHE:CD2	1:B:409:THR:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:LEU:HD12	1:C:181:LEU:HA	1.84	0.41
1:C:823:MET:O	1:D:835:ARG:N	2.50	0.41
1:D:507:ARG:NH2	8:D:2211:HOH:O	2.52	0.41
1:A:119:PHE:CD2	1:A:181:LEU:HD11	2.54	0.41
1:A:658:ALA:O	1:A:713:ILE:HA	2.20	0.41
1:B:553:PHE:HE1	1:B:562:LYS:HE2	1.86	0.41
1:C:312:SER:OG	1:C:315:GLN:OE1	2.30	0.41
1:C:583:MET:CE	1:C:609:LEU:HD23	2.48	0.41
1:C:835:ARG:N	1:D:823:MET:O	2.48	0.41
1:D:280:ALA:HB2	1:D:307:TYR:CZ	2.55	0.41
1:D:290:ASP:OD1	1:D:747:THR:OG1	2.26	0.41
1:A:339:ILE:HD11	1:A:418:ALA:HB2	2.02	0.41
1:A:389:ARG:HD2	1:A:393:GLU:OE1	2.20	0.41
1:B:25:ILE:HG23	1:B:28:ARG:HD3	2.02	0.41
1:B:536:ASP:HA	1:B:552:VAL:O	2.19	0.41
1:D:515:PHE:CE1	1:D:629:ILE:HD11	2.55	0.41
1:D:743:TRP:CH2	1:D:789:SER:HA	2.56	0.41
1:D:931:ILE:HD13	1:D:935:PHE:CE2	2.56	0.41
1:A:743:TRP:CH2	1:A:789:SER:HA	2.56	0.41
1:B:181:LEU:HD23	1:B:181:LEU:HA	1.83	0.41
1:B:515:PHE:CE1	1:B:629:ILE:HD11	2.55	0.41
1:D:505:GLN:HG3	1:D:572:PHE:CG	2.55	0.41
1:D:516:ASP:OD2	1:D:525:SER:OG	2.27	0.41
1:A:724:GLU:OE1	1:A:724:GLU:N	2.51	0.41
1:C:516:ASP:OD2	1:C:525:SER:OG	2.26	0.41
1:D:683:GLU:OE2	1:D:703:ARG:NH2	2.52	0.41
1:A:571:ASN:HD21	1:A:581:SER:HB2	1.85	0.41
1:B:850:GLN:O	1:D:978:LYS:HE3	2.21	0.41
1:C:987:VAL:HG13	1:C:1028:LEU:HD22	2.01	0.41
1:D:571:ASN:HD21	1:D:581:SER:HB2	1.86	0.41
1:A:15:LEU:HD12	1:A:19:ILE:HB	2.02	0.41
1:A:277:THR:HG22	1:A:339:ILE:HB	2.02	0.41
1:A:288:TYR:OH	1:A:411:MET:O	2.25	0.41
1:A:403:HIS:CE1	1:A:424:ILE:HG21	2.56	0.41
1:A:659:TYR:CZ	1:A:684:GLY:HA3	2.56	0.41
1:B:276:TRP:CH2	1:B:326:LEU:HG	2.56	0.41
1:B:307:TYR:HD2	1:B:311:PRO:HG3	1.85	0.41
1:B:640:GLY:O	1:B:645:ASN:ND2	2.45	0.41
1:B:1013:ILE:O	1:B:1016:SER:OG	2.23	0.41
1:C:177:LYS:HD2	1:C:207:VAL:HG13	2.03	0.41
1:C:490:THR:HA	1:C:703:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:ALA:O	1:C:713:ILE:HA	2.21	0.41
1:C:888:GLN:HB3	1:C:993:TYR:OH	2.21	0.41
1:D:78:LEU:O	1:D:82:LYS:HG3	2.20	0.41
1:D:787:PRO:HB3	1:D:796:ILE:HG21	2.03	0.41
1:B:628:GLY:H	1:B:636:ILE:HB	1.85	0.41
1:C:276:TRP:CH2	1:C:326:LEU:HG	2.55	0.41
1:A:180:ILE:HG13	1:A:181:LEU:N	2.36	0.40
1:A:345:ALA:O	1:A:382:PRO:HD3	2.21	0.40
1:A:358:VAL:CG1	1:A:394:VAL:HG21	2.51	0.40
1:A:929:LEU:HD13	1:B:925:THR:HG22	2.02	0.40
1:B:931:ILE:HD13	1:B:935:PHE:CE2	2.56	0.40
1:C:82:LYS:HE3	1:C:82:LYS:HB3	1.89	0.40
1:D:976:ARG:HD2	6:D:2101:COA:C2B	2.41	0.40
1:A:13:GLU:HB2	1:A:31:TYR:OH	2.21	0.40
1:A:78:LEU:O	1:A:82:LYS:HG3	2.21	0.40
1:A:405:PHE:CD2	1:A:409:THR:HG21	2.57	0.40
1:A:925:THR:HG22	1:B:929:LEU:HD13	2.02	0.40
1:A:978:LYS:HE3	1:C:850:GLN:O	2.21	0.40
1:B:17:LYS:NZ	1:B:17:LYS:HB2	2.36	0.40
1:B:729:ARG:O	1:B:733:GLU:HG3	2.21	0.40
1:C:180:ILE:HG13	1:C:181:LEU:N	2.37	0.40
1:C:339:ILE:HD11	1:C:418:ALA:HB2	2.03	0.40
1:C:583:MET:SD	1:C:612:LYS:HD3	2.62	0.40
1:D:82:LYS:HE3	1:D:82:LYS:HB3	1.89	0.40
1:D:331:LYS:HE3	1:D:331:LYS:HB3	1.83	0.40
1:D:573:ALA:O	1:D:598:ALA:HB2	2.22	0.40
1:D:980:ILE:HD13	1:D:1015:THR:HB	2.03	0.40
1:D:1024:ASN:HD22	1:D:1024:ASN:HA	1.73	0.40
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.84	0.40
1:A:850:GLN:O	1:C:978:LYS:HE3	2.22	0.40
1:B:180:ILE:HG13	1:B:181:LEU:N	2.36	0.40
1:B:203:ASN:O	1:B:216:ASP:HB3	2.21	0.40
1:B:403:HIS:CE1	1:B:424:ILE:HG21	2.56	0.40
1:D:307:TYR:HD2	1:D:311:PRO:HG3	1.85	0.40
1:D:384:TYR:O	1:D:388:LEU:HB2	2.21	0.40
1:D:534:THR:HG21	1:D:537:HIS:HE1	1.87	0.40
1:D:628:GLY:H	1:D:636:ILE:HB	1.85	0.40
1:A:856:GLY:H	1:D:1095:LEU:HD23	1.87	0.40
1:A:931:ILE:HD13	1:A:935:PHE:CE2	2.56	0.40
1:C:78:LEU:O	1:C:82:LYS:HG3	2.20	0.40
1:C:405:PHE:CD2	1:C:409:THR:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:683:GLU:OE2	1:C:703:ARG:NH2	2.52	0.40
1:D:249:GLU:OE1	1:D:326:LEU:HB2	2.22	0.40
1:D:521:ARG:HD2	1:D:633:CYS:O	2.22	0.40
1:D:698:MET:SD	1:D:727:ILE:HD13	2.62	0.40
1:A:38:THR:HG23	1:A:39:ASP:O	2.21	0.40
1:A:291:THR:HG21	1:A:412:THR:HB	2.04	0.40
1:B:961:ASN:O	1:B:965:LYS:HD3	2.22	0.40
1:C:521:ARG:HD2	1:C:633:CYS:O	2.22	0.40
1:C:673:ILE:O	1:C:677:THR:HG23	2.22	0.40
1:C:788:ARG:HH11	1:C:788:ARG:HG2	1.87	0.40
1:C:792:GLU:HA	1:C:795:GLU:OE1	2.22	0.40
1:C:925:THR:HG22	1:D:929:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1027/1101 (93%)	999 (97%)	28 (3%)	0	100	100
1	B	1027/1101 (93%)	995 (97%)	32 (3%)	0	100	100
1	C	1027/1101 (93%)	997 (97%)	30 (3%)	0	100	100
1	D	1027/1101 (93%)	993 (97%)	34 (3%)	0	100	100
All	All	4108/4404 (93%)	3984 (97%)	124 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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	849/908 (94%)	829 (98%)	20 (2%)	49	62
1	B	849/908 (94%)	827 (97%)	22 (3%)	46	58
1	C	849/908 (94%)	829 (98%)	20 (2%)	49	62
1	D	849/908 (94%)	827 (97%)	22 (3%)	46	58
All	All	3396/3632 (94%)	3312 (98%)	84 (2%)	50	60

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	134	PHE
1	A	166	LYS
1	A	172	HIS
1	A	203	ASN
1	A	274	ARG
1	A	304	TYR
1	A	317	TYR
1	A	329	ARG
1	A	364	TYR
1	A	384	TYR
1	A	385	GLN
1	A	389	ARG
1	A	391	MET
1	A	396	LYS
1	A	556	MET
1	A	558	ASP
1	A	751	MET
1	A	764	CYS
1	A	995	ARG
1	B	29	PHE
1	B	33	ARG
1	B	163	GLU
1	B	168	HIS
1	B	172	HIS
1	B	278	MET
1	B	304	TYR
1	B	306	GLU

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Mol	Chain	Res	Type
1	B	317	TYR
1	B	329	ARG
1	B	354	PHE
1	B	364	TYR
1	B	385	GLN
1	B	389	ARG
1	B	396	LYS
1	B	507	ARG
1	B	558	ASP
1	B	732	LYS
1	B	735	ARG
1	B	751	MET
1	B	764	CYS
1	B	995	ARG
1	C	29	PHE
1	C	33	ARG
1	C	134	PHE
1	C	163	GLU
1	C	166	LYS
1	C	278	MET
1	C	304	TYR
1	C	306	GLU
1	C	317	TYR
1	C	329	ARG
1	C	336	LYS
1	C	354	PHE
1	C	364	TYR
1	C	385	GLN
1	C	396	LYS
1	C	558	ASP
1	C	735	ARG
1	C	751	MET
1	C	764	CYS
1	C	995	ARG
1	D	29	PHE
1	D	33	ARG
1	D	134	PHE
1	D	172	HIS
1	D	203	ASN
1	D	270	ASN
1	D	278	MET
1	D	304	TYR

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Mol	Chain	Res	Type
1	D	317	TYR
1	D	327	MET
1	D	329	ARG
1	D	364	TYR
1	D	384	TYR
1	D	385	GLN
1	D	389	ARG
1	D	391	MET
1	D	396	LYS
1	D	556	MET
1	D	558	ASP
1	D	751	MET
1	D	764	CYS
1	D	995	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 2 are unknown - leaving 20 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
4	FLC	A	1203	-	12,12,12	1.11	0	17,17,17	1.44	1 (5%)
3	Q5B	D	2104	-	54,62,62	2.58	15 (27%)	70,93,93	1.61	14 (20%)
3	Q5B	A	1202	-	54,62,62	2.56	15 (27%)	70,93,93	1.59	13 (18%)
6	COA	A	1205	-	41,50,50	0.86	1 (2%)	52,75,75	1.24	6 (11%)
6	COA	D	2101	-	41,50,50	0.87	1 (2%)	52,75,75	1.25	6 (11%)
7	PO4	D	2106	-	4,4,4	0.97	0	6,6,6	0.43	0
2	ADP	D	2103	-	24,29,29	0.95	1 (4%)	29,45,45	1.51	4 (13%)
3	Q5B	C	2103	-	54,62,62	2.56	15 (27%)	70,93,93	1.60	12 (17%)
2	ADP	B	1201	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)
3	Q5B	B	1202	-	54,62,62	2.56	15 (27%)	70,93,93	1.58	13 (18%)
4	FLC	B	1203	-	12,12,12	1.10	0	17,17,17	1.47	1 (5%)
2	ADP	A	1201	-	24,29,29	0.95	1 (4%)	29,45,45	1.52	4 (13%)
7	PO4	A	1206	-	4,4,4	0.99	0	6,6,6	0.43	0
7	PO4	C	2105	-	4,4,4	0.97	0	6,6,6	0.44	0
6	COA	C	2101	-	41,50,50	0.87	1 (2%)	52,75,75	1.25	6 (11%)
4	FLC	C	2104	-	12,12,12	1.11	0	17,17,17	1.57	1 (5%)
4	FLC	D	2105	-	12,12,12	1.11	0	17,17,17	1.45	1 (5%)
2	ADP	C	2102	-	24,29,29	0.95	1 (4%)	29,45,45	1.51	4 (13%)
6	COA	B	1204	-	41,50,50	0.87	1 (2%)	52,75,75	1.25	5 (9%)
7	PO4	B	1205	-	4,4,4	0.99	0	6,6,6	0.43	0

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
6	COA	D	2101	-	-	14/44/64/64	0/3/3/3
2	ADP	D	2103	-	-	2/12/32/32	0/3/3/3
3	Q5B	C	2103	-	-	22/62/83/83	0/3/3/3
4	FLC	A	1203	-	-	10/16/16/16	-
4	FLC	C	2104	-	-	8/16/16/16	-
6	COA	C	2101	-	-	16/44/64/64	0/3/3/3
3	Q5B	D	2104	-	-	18/62/83/83	0/3/3/3
2	ADP	C	2102	-	-	5/12/32/32	0/3/3/3
4	FLC	D	2105	-	-	10/16/16/16	-
6	COA	B	1204	-	-	18/44/64/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	1201	-	-	5/12/32/32	0/3/3/3
4	FLC	B	1203	-	-	5/16/16/16	-
3	Q5B	B	1202	-	-	22/62/83/83	0/3/3/3
2	ADP	A	1201	-	-	2/12/32/32	0/3/3/3
3	Q5B	A	1202	-	-	21/62/83/83	0/3/3/3
6	COA	A	1205	-	-	9/44/64/64	0/3/3/3

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2104	Q5B	C6-C5	-7.69	1.32	1.52
3	A	1202	Q5B	C6-C5	-7.63	1.32	1.52
3	C	2103	Q5B	C18-N6	7.62	1.50	1.33
3	C	2103	Q5B	C6-C5	-7.62	1.32	1.52
3	D	2104	Q5B	C18-N6	7.59	1.50	1.33
3	B	1202	Q5B	C6-C5	-7.58	1.32	1.52
3	B	1202	Q5B	C18-N6	7.58	1.50	1.33
3	A	1202	Q5B	C18-N6	7.56	1.50	1.33
3	D	2104	Q5B	C15-N5	7.12	1.49	1.33
3	D	2104	Q5B	C7-C6	7.06	1.68	1.52
3	B	1202	Q5B	C7-C6	7.04	1.68	1.52
3	A	1202	Q5B	C15-N5	7.04	1.49	1.33
3	C	2103	Q5B	C15-N5	7.03	1.49	1.33
3	B	1202	Q5B	C15-N5	7.03	1.48	1.33
3	C	2103	Q5B	C7-C6	7.01	1.68	1.52
3	A	1202	Q5B	C7-C6	7.00	1.68	1.52
3	B	1202	Q5B	O7-C5	3.98	1.53	1.45
3	D	2104	Q5B	O7-C5	3.98	1.53	1.45
3	A	1202	Q5B	O7-C5	3.96	1.53	1.45
3	C	2103	Q5B	O7-C5	3.94	1.53	1.45
3	D	2104	Q5B	C21-S	3.67	1.85	1.76
3	C	2103	Q5B	C21-S	3.65	1.85	1.76
3	A	1202	Q5B	C21-S	3.64	1.85	1.76
3	B	1202	Q5B	C21-S	3.63	1.84	1.76
3	D	2104	Q5B	O20-C23	-3.21	1.37	1.43
3	A	1202	Q5B	O20-C23	-3.21	1.37	1.43
3	C	2103	Q5B	O20-C23	-3.17	1.37	1.43
3	B	1202	Q5B	O20-C23	-3.15	1.37	1.43
3	D	2104	Q5B	C22-C23	3.04	1.57	1.53
3	B	1202	Q5B	C22-C23	2.97	1.57	1.53
3	A	1202	Q5B	C22-C23	2.96	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2103	Q5B	C22-C23	2.95	1.57	1.53
3	B	1202	Q5B	P2-O9	2.85	1.64	1.59
3	C	2103	Q5B	P2-O9	2.84	1.64	1.59
3	D	2104	Q5B	P2-O9	2.84	1.64	1.59
3	A	1202	Q5B	P2-O9	2.82	1.64	1.59
3	C	2103	Q5B	O14-C18	-2.66	1.17	1.23
3	A	1202	Q5B	O14-C18	-2.66	1.17	1.23
3	B	1202	Q5B	O14-C18	-2.63	1.17	1.23
3	D	2104	Q5B	O14-C18	-2.61	1.18	1.23
3	D	2104	Q5B	O13-C15	-2.57	1.18	1.23
3	A	1202	Q5B	O13-C15	-2.56	1.18	1.23
3	B	1202	Q5B	O13-C15	-2.52	1.18	1.23
3	C	2103	Q5B	O13-C15	-2.51	1.18	1.23
2	D	2103	ADP	C5-C4	2.49	1.47	1.40
2	A	1201	ADP	C5-C4	2.48	1.47	1.40
2	B	1201	ADP	C5-C4	2.47	1.47	1.40
2	C	2102	ADP	C5-C4	2.47	1.47	1.40
3	D	2104	Q5B	C23-C26	-2.46	1.50	1.53
3	B	1202	Q5B	C23-C26	-2.43	1.50	1.53
3	A	1202	Q5B	C23-C26	-2.40	1.50	1.53
3	C	2103	Q5B	C23-C26	-2.39	1.50	1.53
3	B	1202	Q5B	C22-C21	2.32	1.56	1.51
3	C	2103	Q5B	C22-C21	2.28	1.56	1.51
3	D	2104	Q5B	C2-C1	2.28	1.58	1.53
6	C	2101	COA	C5A-C4A	2.27	1.46	1.40
6	B	1204	COA	C5A-C4A	2.27	1.46	1.40
3	D	2104	Q5B	C22-C21	2.27	1.56	1.51
6	D	2101	COA	C5A-C4A	2.27	1.46	1.40
3	B	1202	Q5B	C2-C1	2.26	1.58	1.53
3	A	1202	Q5B	C2-C1	2.26	1.58	1.53
3	C	2103	Q5B	C2-C1	2.25	1.58	1.53
6	A	1205	COA	C5A-C4A	2.24	1.46	1.40
3	A	1202	Q5B	C22-C21	2.22	1.56	1.51
3	D	2104	Q5B	P1-O6	2.04	1.67	1.59
3	A	1202	Q5B	P1-O6	2.03	1.67	1.59
3	B	1202	Q5B	P1-O6	2.03	1.67	1.59
3	C	2103	Q5B	P1-O6	2.02	1.67	1.59

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2104	Q5B	C22-C21-S	5.44	120.36	113.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1202	Q5B	C22-C21-S	5.35	120.25	113.63
3	C	2103	Q5B	C22-C21-S	5.34	120.23	113.63
3	A	1202	Q5B	C22-C21-S	5.26	120.14	113.63
3	D	2104	Q5B	N2-C12-N3	-5.13	120.66	128.68
3	C	2103	Q5B	N2-C12-N3	-5.13	120.66	128.68
3	B	1202	Q5B	N2-C12-N3	-5.11	120.70	128.68
3	A	1202	Q5B	N2-C12-N3	-5.08	120.73	128.68
4	C	2104	FLC	OB2-CBC-CB	4.33	120.56	113.05
3	D	2104	Q5B	C16-C17-C18	4.32	119.54	112.36
2	C	2102	ADP	PA-O3A-PB	-4.19	118.45	132.83
2	B	1201	ADP	PA-O3A-PB	-4.15	118.57	132.83
3	A	1202	Q5B	C16-C17-C18	4.12	119.22	112.36
3	C	2103	Q5B	C16-C17-C18	4.10	119.19	112.36
3	B	1202	Q5B	C16-C17-C18	4.09	119.16	112.36
4	D	2105	FLC	OB2-CBC-CB	4.05	120.09	113.05
4	A	1203	FLC	OB2-CBC-CB	4.03	120.05	113.05
3	C	2103	Q5B	O19-C26-C23	4.02	120.02	113.05
4	B	1203	FLC	OB2-CBC-CB	3.99	119.97	113.05
3	A	1202	Q5B	O19-C26-C23	3.97	119.94	113.05
3	B	1202	Q5B	O19-C26-C23	3.95	119.91	113.05
3	D	2104	Q5B	O19-C26-C23	3.93	119.87	113.05
2	A	1201	ADP	C3'-C2'-C1'	3.79	106.69	100.98
2	D	2103	ADP	C3'-C2'-C1'	3.77	106.66	100.98
6	A	1205	COA	N3A-C2A-N1A	-3.56	123.12	128.68
2	D	2103	ADP	PA-O3A-PB	-3.55	120.63	132.83
2	A	1201	ADP	PA-O3A-PB	-3.55	120.64	132.83
6	B	1204	COA	N3A-C2A-N1A	-3.49	123.22	128.68
6	D	2101	COA	N3A-C2A-N1A	-3.47	123.26	128.68
6	C	2101	COA	N3A-C2A-N1A	-3.46	123.27	128.68
6	C	2101	COA	C4A-C5A-N7A	-3.32	105.94	109.40
6	B	1204	COA	C4A-C5A-N7A	-3.32	105.94	109.40
2	B	1201	ADP	C3'-C2'-C1'	3.28	105.92	100.98
6	D	2101	COA	C4A-C5A-N7A	-3.27	105.99	109.40
2	C	2102	ADP	C3'-C2'-C1'	3.26	105.88	100.98
6	A	1205	COA	C4A-C5A-N7A	-3.19	106.08	109.40
2	B	1201	ADP	N3-C2-N1	-3.13	123.79	128.68
2	C	2102	ADP	N3-C2-N1	-3.12	123.80	128.68
2	A	1201	ADP	N3-C2-N1	-3.06	123.89	128.68
2	D	2103	ADP	N3-C2-N1	-3.04	123.93	128.68
2	C	2102	ADP	C4-C5-N7	-3.00	106.28	109.40
2	B	1201	ADP	C4-C5-N7	-2.95	106.32	109.40
2	A	1201	ADP	C4-C5-N7	-2.92	106.36	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2103	ADP	C4-C5-N7	-2.89	106.39	109.40
6	A	1205	COA	P2A-O3A-P1A	-2.79	123.24	132.83
6	B	1204	COA	P2A-O3A-P1A	-2.74	123.43	132.83
6	D	2101	COA	P2A-O3A-P1A	-2.71	123.52	132.83
6	C	2101	COA	P2A-O3A-P1A	-2.66	123.69	132.83
3	A	1202	Q5B	C17-C18-N6	2.59	120.79	116.42
3	D	2104	Q5B	C17-C18-N6	2.59	120.78	116.42
3	B	1202	Q5B	C17-C18-N6	2.53	120.68	116.42
6	D	2101	COA	C7P-C6P-C5P	-2.53	108.15	112.36
3	C	2103	Q5B	C17-C18-N6	2.52	120.67	116.42
3	D	2104	Q5B	C14-C15-N5	2.52	121.59	116.58
6	A	1205	COA	C7P-C6P-C5P	-2.52	108.17	112.36
6	B	1204	COA	C7P-C6P-C5P	-2.47	108.25	112.36
6	C	2101	COA	C7P-C6P-C5P	-2.45	108.28	112.36
3	C	2103	Q5B	C-C1-C14	2.43	113.04	108.82
3	A	1202	Q5B	C14-C15-N5	2.41	121.39	116.58
3	C	2103	Q5B	O15-C21-C22	-2.41	119.78	123.64
3	D	2104	Q5B	O15-C21-C22	-2.40	119.80	123.64
3	B	1202	Q5B	O15-C21-C22	-2.38	119.83	123.64
3	D	2104	Q5B	P1-O3-P	-2.37	124.69	132.83
3	C	2103	Q5B	P1-O3-P	-2.37	124.70	132.83
3	D	2104	Q5B	C20-S-C21	2.35	109.19	101.87
3	A	1202	Q5B	O15-C21-C22	-2.34	119.90	123.64
3	B	1202	Q5B	C14-C15-N5	2.33	121.22	116.58
3	B	1202	Q5B	C-C1-C14	2.32	112.84	108.82
3	C	2103	Q5B	C14-C15-N5	2.30	121.15	116.58
3	A	1202	Q5B	C20-S-C21	2.27	108.95	101.87
3	D	2104	Q5B	O13-C15-N5	-2.27	118.12	122.99
3	A	1202	Q5B	C-C1-C14	2.26	112.75	108.82
3	A	1202	Q5B	P1-O3-P	-2.25	125.09	132.83
3	B	1202	Q5B	C20-S-C21	2.25	108.89	101.87
3	B	1202	Q5B	P1-O3-P	-2.24	125.13	132.83
3	D	2104	Q5B	O7-C8-C7	-2.23	103.67	106.93
3	C	2103	Q5B	C20-S-C21	2.22	108.78	101.87
3	A	1202	Q5B	O13-C15-N5	-2.19	118.28	122.99
3	D	2104	Q5B	C-C1-C14	2.19	112.62	108.82
3	A	1202	Q5B	O7-C8-C7	-2.17	103.75	106.93
3	B	1202	Q5B	O13-C15-N5	-2.17	118.33	122.99
3	C	2103	Q5B	O13-C15-N5	-2.17	118.33	122.99
6	D	2101	COA	O6A-CCP-CBP	-2.14	107.10	110.55
3	D	2104	Q5B	O15-C21-S	-2.14	119.84	122.61
6	B	1204	COA	C2A-N1A-C6A	2.11	122.37	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1205	COA	C2A-N1A-C6A	2.08	122.32	118.75
6	A	1205	COA	O6A-CCP-CBP	-2.08	107.20	110.55
3	B	1202	Q5B	O15-C21-S	-2.08	119.92	122.61
6	C	2101	COA	C2A-N1A-C6A	2.07	122.29	118.75
6	C	2101	COA	O6A-CCP-CBP	-2.07	107.22	110.55
3	B	1202	Q5B	O7-C8-C7	-2.04	103.94	106.93
3	A	1202	Q5B	O15-C21-S	-2.04	119.96	122.61
3	D	2104	Q5B	C11-C10-N1	-2.04	107.28	109.40
3	C	2103	Q5B	O15-C21-S	-2.02	119.98	122.61
6	D	2101	COA	C2A-N1A-C6A	2.00	122.18	118.75

There are no chirality outliers.

All (187) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ADP	C5'-O5'-PA-O3A
2	B	1201	ADP	C5'-O5'-PA-O1A
2	B	1201	ADP	C5'-O5'-PA-O3A
2	C	2102	ADP	C5'-O5'-PA-O3A
2	D	2103	ADP	C5'-O5'-PA-O3A
3	A	1202	Q5B	C3-O-P-O1
3	A	1202	Q5B	C3-O-P-O3
3	A	1202	Q5B	C-C1-C14-C15
3	A	1202	Q5B	C-C1-C14-O21
3	A	1202	Q5B	C2-C1-C14-C15
3	A	1202	Q5B	C2-C1-C14-O21
3	A	1202	Q5B	C3-C1-C14-C15
3	A	1202	Q5B	C3-C1-C14-O21
3	A	1202	Q5B	C14-C15-N5-C16
3	A	1202	Q5B	P-O3-P1-O6
3	A	1202	Q5B	C6-O9-P2-O10
3	B	1202	Q5B	C3-O-P-O1
3	B	1202	Q5B	C3-O-P-O3
3	B	1202	Q5B	C-C1-C14-C15
3	B	1202	Q5B	C-C1-C14-O21
3	B	1202	Q5B	C2-C1-C14-C15
3	B	1202	Q5B	C2-C1-C14-O21
3	B	1202	Q5B	C3-C1-C14-C15
3	B	1202	Q5B	C3-C1-C14-O21
3	B	1202	Q5B	C14-C15-N5-C16
3	B	1202	Q5B	P-O3-P1-O6
3	B	1202	Q5B	C6-O9-P2-O10

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Mol	Chain	Res	Type	Atoms
3	C	2103	Q5B	C3-O-P-O1
3	C	2103	Q5B	C3-O-P-O3
3	C	2103	Q5B	C-C1-C14-C15
3	C	2103	Q5B	C-C1-C14-O21
3	C	2103	Q5B	C2-C1-C14-C15
3	C	2103	Q5B	C2-C1-C14-O21
3	C	2103	Q5B	C3-C1-C14-C15
3	C	2103	Q5B	C3-C1-C14-O21
3	C	2103	Q5B	C14-C15-N5-C16
3	C	2103	Q5B	O6-C4-C5-O7
3	C	2103	Q5B	P-O3-P1-O6
3	C	2103	Q5B	C6-O9-P2-O10
3	D	2104	Q5B	C3-O-P-O1
3	D	2104	Q5B	C-C1-C14-C15
3	D	2104	Q5B	C-C1-C14-O21
3	D	2104	Q5B	C2-C1-C14-C15
3	D	2104	Q5B	C2-C1-C14-O21
3	D	2104	Q5B	C3-C1-C14-C15
3	D	2104	Q5B	C3-C1-C14-O21
3	D	2104	Q5B	C14-C15-N5-C16
3	D	2104	Q5B	P-O3-P1-O6
3	D	2104	Q5B	C6-O9-P2-O10
4	A	1203	FLC	CA-CB-CBC-OB1
4	A	1203	FLC	CA-CB-CBC-OB2
4	A	1203	FLC	OHB-CB-CBC-OB1
4	A	1203	FLC	OHB-CB-CBC-OB2
4	B	1203	FLC	CG-CB-CBC-OB1
4	B	1203	FLC	CG-CB-CBC-OB2
4	B	1203	FLC	OHB-CB-CBC-OB1
4	B	1203	FLC	OHB-CB-CBC-OB2
4	C	2104	FLC	CA-CB-CBC-OB1
4	C	2104	FLC	CA-CB-CBC-OB2
4	C	2104	FLC	OHB-CB-CBC-OB1
4	C	2104	FLC	OHB-CB-CBC-OB2
4	D	2105	FLC	CA-CB-CBC-OB1
4	D	2105	FLC	CA-CB-CBC-OB2
4	D	2105	FLC	OHB-CB-CBC-OB1
4	D	2105	FLC	OHB-CB-CBC-OB2
6	A	1205	COA	S1P-C2P-C3P-N4P
6	B	1204	COA	O4B-C4B-C5B-O5B
6	B	1204	COA	C5B-O5B-P1A-O1A
6	B	1204	COA	C5B-O5B-P1A-O2A

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Mol	Chain	Res	Type	Atoms
6	B	1204	COA	C5B-O5B-P1A-O3A
6	B	1204	COA	CCP-O6A-P2A-O5A
6	B	1204	COA	S1P-C2P-C3P-N4P
6	C	2101	COA	O4B-C4B-C5B-O5B
6	C	2101	COA	C5B-O5B-P1A-O2A
6	C	2101	COA	C5B-O5B-P1A-O3A
6	C	2101	COA	S1P-C2P-C3P-N4P
6	D	2101	COA	O4B-C4B-C5B-O5B
6	D	2101	COA	C5B-O5B-P1A-O1A
6	D	2101	COA	C5B-O5B-P1A-O2A
6	D	2101	COA	C5B-O5B-P1A-O3A
6	D	2101	COA	S1P-C2P-C3P-N4P
3	A	1202	Q5B	O13-C15-N5-C16
3	B	1202	Q5B	O13-C15-N5-C16
3	C	2103	Q5B	O13-C15-N5-C16
3	D	2104	Q5B	O13-C15-N5-C16
2	B	1201	ADP	O4'-C4'-C5'-O5'
3	A	1202	Q5B	O6-C4-C5-O7
3	B	1202	Q5B	O6-C4-C5-O7
3	D	2104	Q5B	O6-C4-C5-O7
6	B	1204	COA	C3B-C4B-C5B-O5B
6	C	2101	COA	C3B-C4B-C5B-O5B
6	D	2101	COA	C3B-C4B-C5B-O5B
2	B	1201	ADP	C3'-C4'-C5'-O5'
6	B	1204	COA	CEP-CBP-CCP-O6A
6	C	2101	COA	CEP-CBP-CCP-O6A
4	B	1203	FLC	CAC-CA-CB-OHB
6	A	1205	COA	CDP-CBP-CCP-O6A
6	A	1205	COA	CEP-CBP-CCP-O6A
6	B	1204	COA	CDP-CBP-CCP-O6A
6	C	2101	COA	CDP-CBP-CCP-O6A
6	D	2101	COA	CDP-CBP-CCP-O6A
6	D	2101	COA	CEP-CBP-CCP-O6A
4	C	2104	FLC	CAC-CA-CB-OHB
4	D	2105	FLC	CBC-CB-CG-CGC
4	A	1203	FLC	CG-CB-CBC-OB1
4	A	1203	FLC	CG-CB-CBC-OB2
4	D	2105	FLC	CG-CB-CBC-OB1
4	D	2105	FLC	CG-CB-CBC-OB2
4	A	1203	FLC	CA-CB-CG-CGC
4	A	1203	FLC	CBC-CB-CG-CGC
4	C	2104	FLC	CBC-CB-CG-CGC

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Mol	Chain	Res	Type	Atoms
4	D	2105	FLC	CA-CB-CG-CGC
3	A	1202	Q5B	O15-C21-S-C20
3	B	1202	Q5B	O15-C21-S-C20
3	C	2103	Q5B	O15-C21-S-C20
3	D	2104	Q5B	O15-C21-S-C20
6	A	1205	COA	P1A-O3A-P2A-O6A
6	B	1204	COA	P1A-O3A-P2A-O6A
6	C	2101	COA	P1A-O3A-P2A-O6A
6	D	2101	COA	P1A-O3A-P2A-O6A
3	A	1202	Q5B	O6-C4-C5-C6
3	D	2104	Q5B	O6-C4-C5-C6
3	A	1202	Q5B	C22-C21-S-C20
3	B	1202	Q5B	C22-C21-S-C20
3	C	2103	Q5B	C22-C21-S-C20
3	D	2104	Q5B	C22-C21-S-C20
4	A	1203	FLC	OHB-CB-CG-CGC
4	D	2105	FLC	OHB-CB-CG-CGC
3	D	2104	Q5B	C3-O-P-O3
6	B	1204	COA	C3B-O3B-P3B-O8A
6	C	2101	COA	C3B-O3B-P3B-O8A
6	D	2101	COA	C3B-O3B-P3B-O8A
2	C	2102	ADP	O4'-C4'-C5'-O5'
6	B	1204	COA	P2A-O3A-P1A-O2A
6	C	2101	COA	P2A-O3A-P1A-O2A
6	D	2101	COA	P2A-O3A-P1A-O2A
2	A	1201	ADP	C5'-O5'-PA-O1A
2	B	1201	ADP	C5'-O5'-PA-O2A
2	C	2102	ADP	C5'-O5'-PA-O1A
2	C	2102	ADP	C5'-O5'-PA-O2A
2	D	2103	ADP	C5'-O5'-PA-O1A
3	A	1202	Q5B	C3-O-P-O2
3	B	1202	Q5B	C3-O-P-O2
3	C	2103	Q5B	C3-O-P-O2
3	D	2104	Q5B	C3-O-P-O2
6	C	2101	COA	C5B-O5B-P1A-O1A
6	B	1204	COA	C4B-C3B-O3B-P3B
6	C	2101	COA	C4B-C3B-O3B-P3B
6	D	2101	COA	C4B-C3B-O3B-P3B
3	B	1202	Q5B	O6-C4-C5-C6
6	B	1204	COA	CAP-CBP-CCP-O6A
6	C	2101	COA	CAP-CBP-CCP-O6A
3	C	2103	Q5B	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	B	1202	Q5B	C-C1-C3-O
3	B	1202	Q5B	C2-C1-C3-O
3	C	2103	Q5B	C2-C1-C3-O
6	B	1204	COA	C2B-C3B-O3B-P3B
6	C	2101	COA	C2B-C3B-O3B-P3B
6	D	2101	COA	C2B-C3B-O3B-P3B
4	C	2104	FLC	CA-CB-CG-CGC
4	C	2104	FLC	OHB-CB-CG-CGC
4	D	2105	FLC	CAC-CA-CB-OHB
4	A	1203	FLC	CAC-CA-CB-OHB
6	A	1205	COA	C4B-C3B-O3B-P3B
3	A	1202	Q5B	C2-C1-C3-O
3	C	2103	Q5B	C-C1-C3-O
3	A	1202	Q5B	C19-C20-S-C21
3	B	1202	Q5B	C19-C20-S-C21
3	C	2103	Q5B	C19-C20-S-C21
3	D	2104	Q5B	C19-C20-S-C21
6	A	1205	COA	C2B-C3B-O3B-P3B
3	A	1202	Q5B	C16-C17-C18-O14
3	B	1202	Q5B	C16-C17-C18-O14
3	C	2103	Q5B	C16-C17-C18-O14
3	A	1202	Q5B	C16-C17-C18-N6
6	A	1205	COA	C3B-O3B-P3B-O8A
6	B	1204	COA	CCP-O6A-P2A-O3A
6	C	2101	COA	CCP-O6A-P2A-O3A
2	C	2102	ADP	C3'-C4'-C5'-O5'
6	A	1205	COA	P2A-O3A-P1A-O1A
6	A	1205	COA	P2A-O3A-P1A-O2A
6	B	1204	COA	P2A-O3A-P1A-O1A
6	D	2101	COA	P2A-O3A-P1A-O1A
6	B	1204	COA	CCP-O6A-P2A-O4A
6	C	2101	COA	CCP-O6A-P2A-O4A
3	B	1202	Q5B	C16-C17-C18-N6
3	C	2103	Q5B	C16-C17-C18-N6

There are no ring outliers.

12 monomers are involved in 37 short contacts:

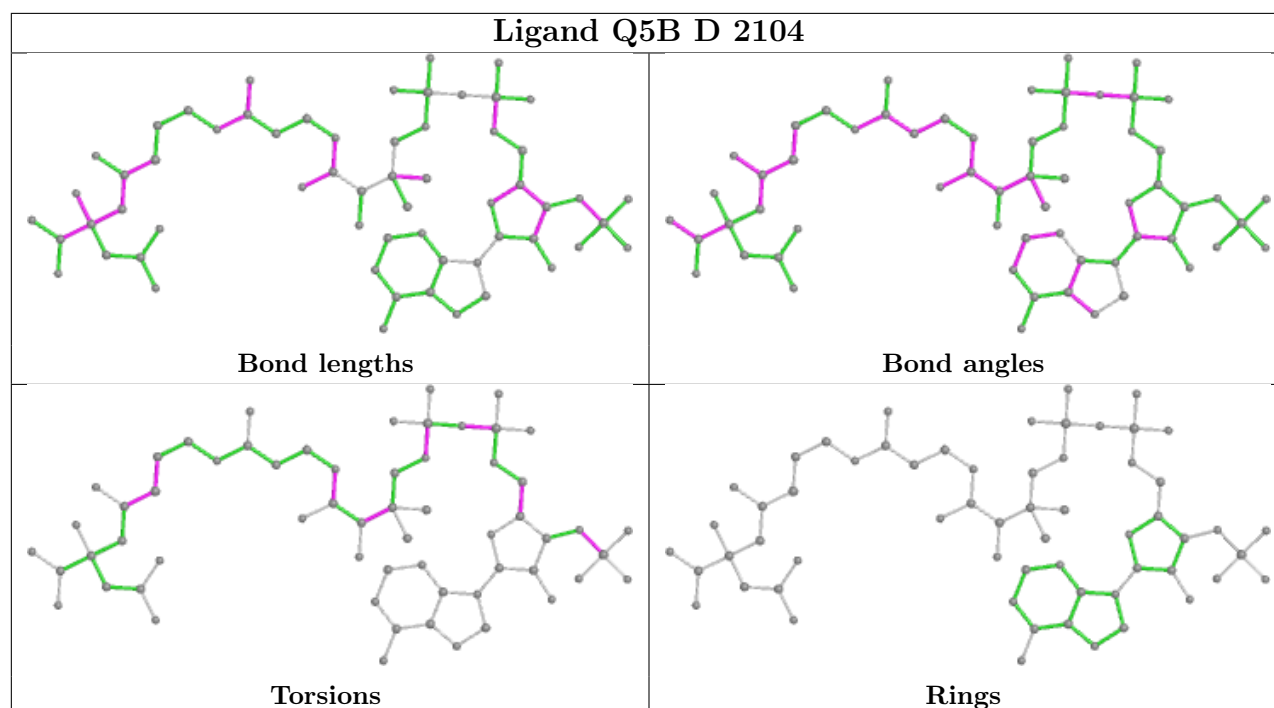
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2104	Q5B	2	0
3	A	1202	Q5B	1	0
6	A	1205	COA	6	0

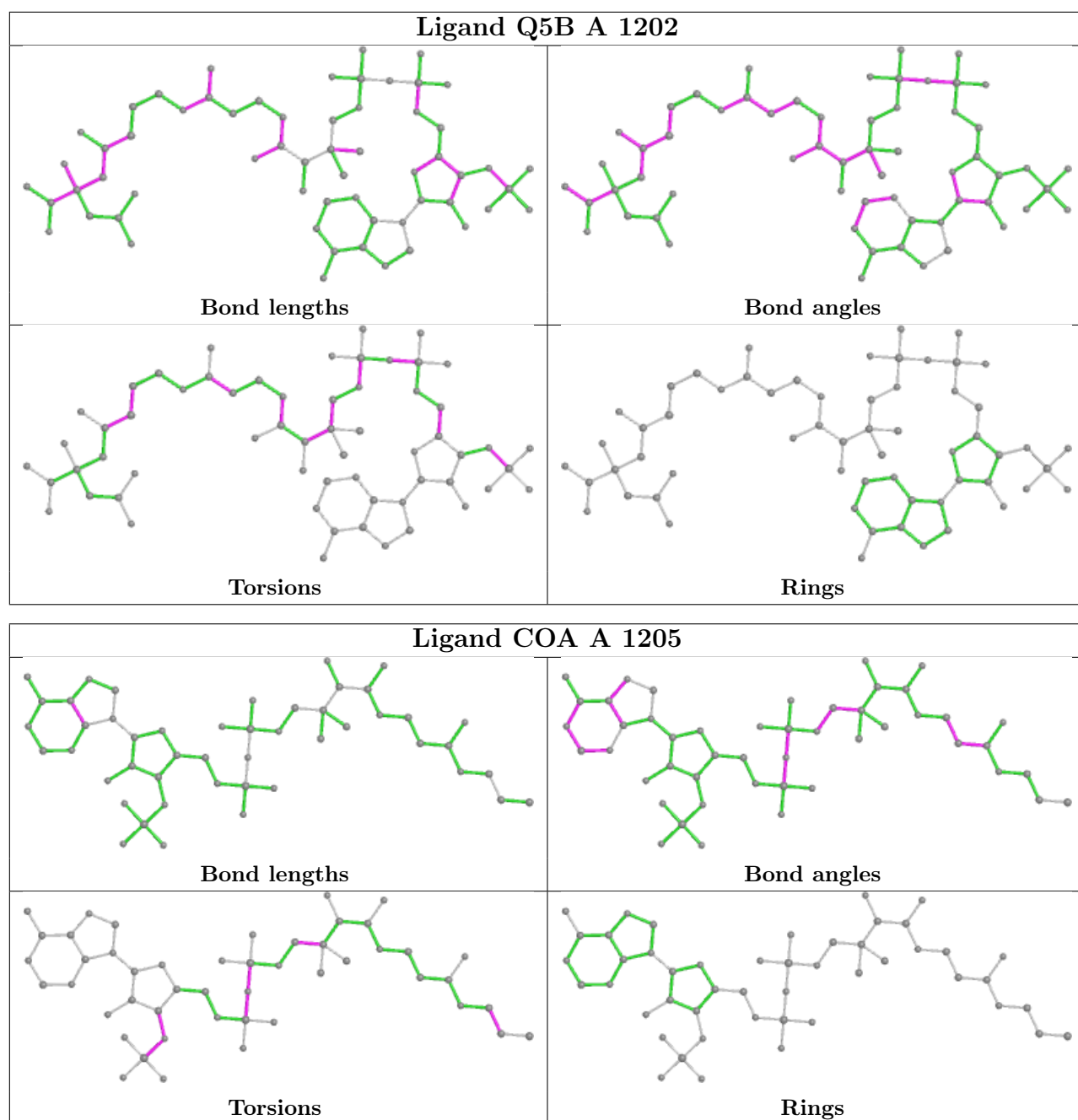
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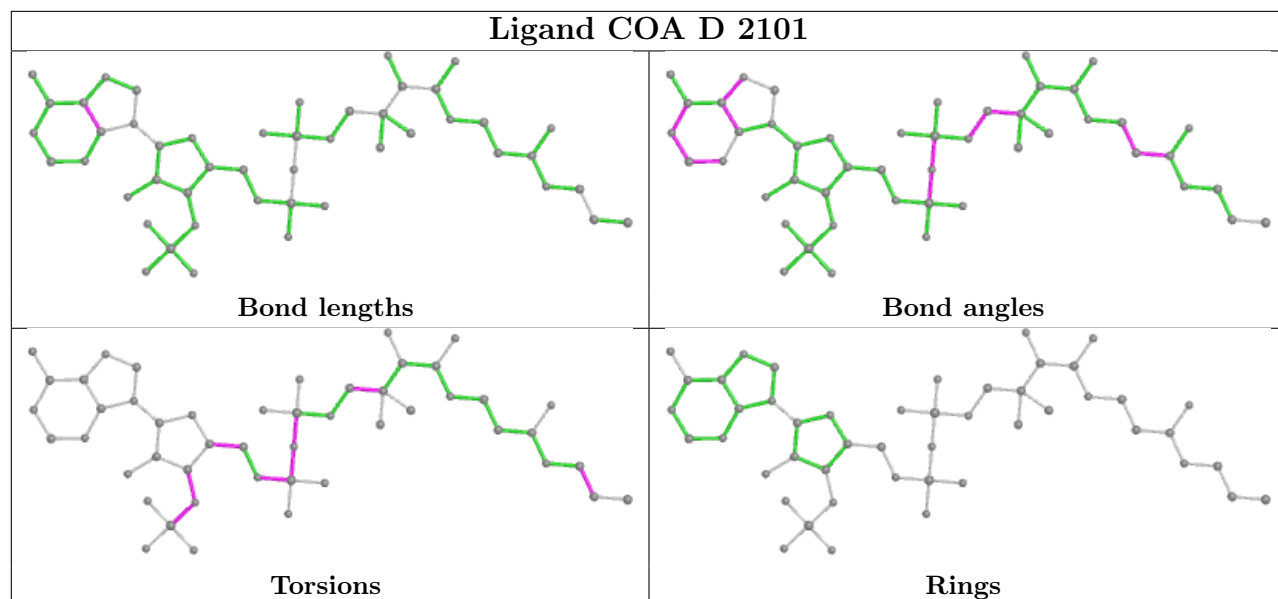
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	2101	COA	6	0
2	D	2103	ADP	2	0
3	C	2103	Q5B	1	0
2	B	1201	ADP	3	0
3	B	1202	Q5B	1	0
2	A	1201	ADP	2	0
6	C	2101	COA	6	0
2	C	2102	ADP	2	0
6	B	1204	COA	5	0

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 than 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.

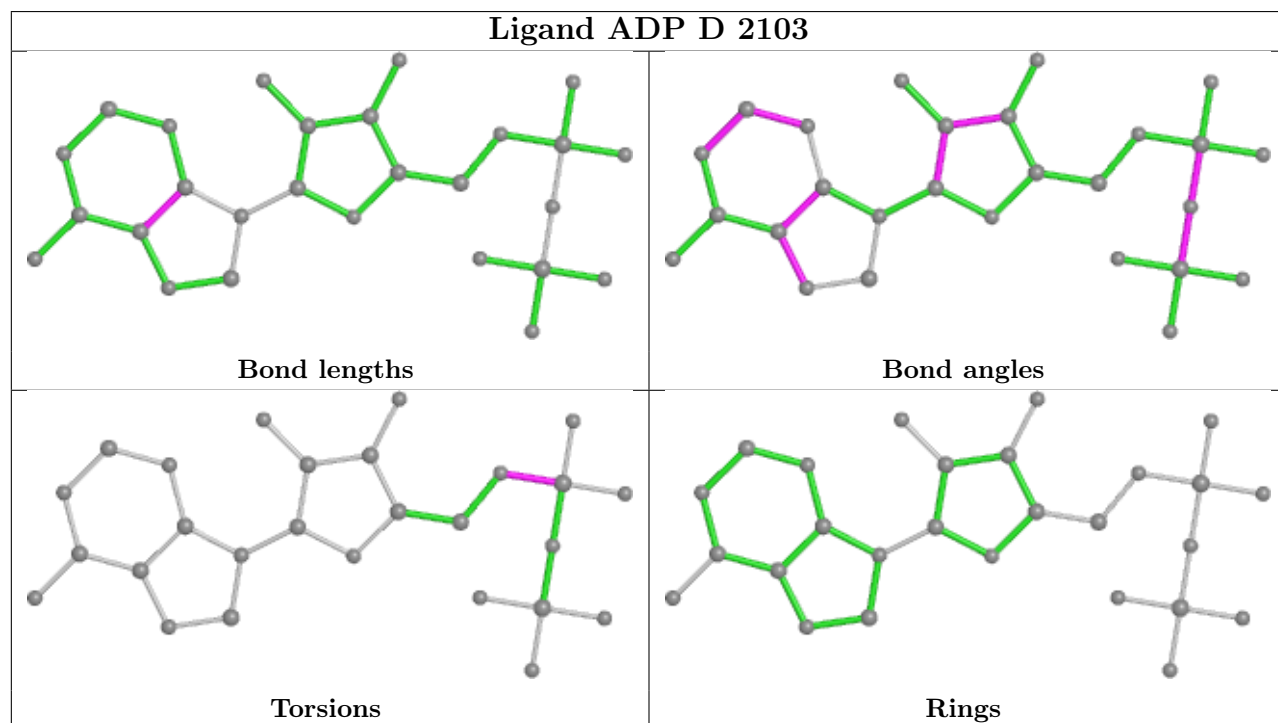




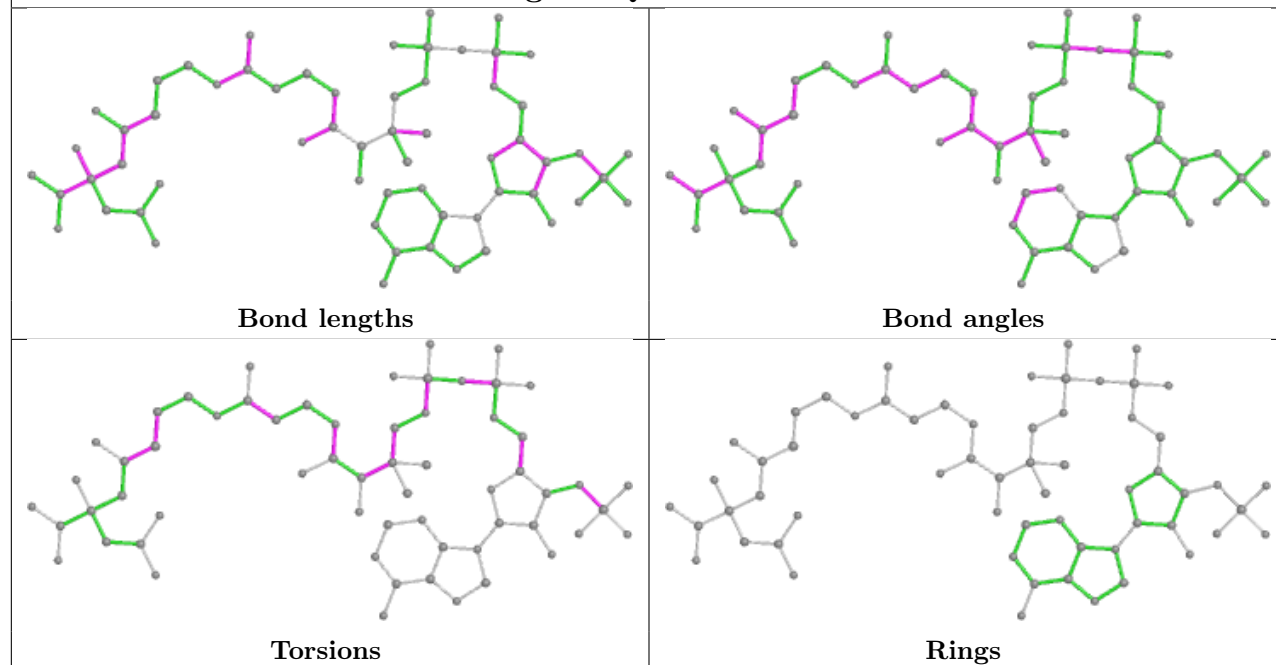
Ligand COA D 2101



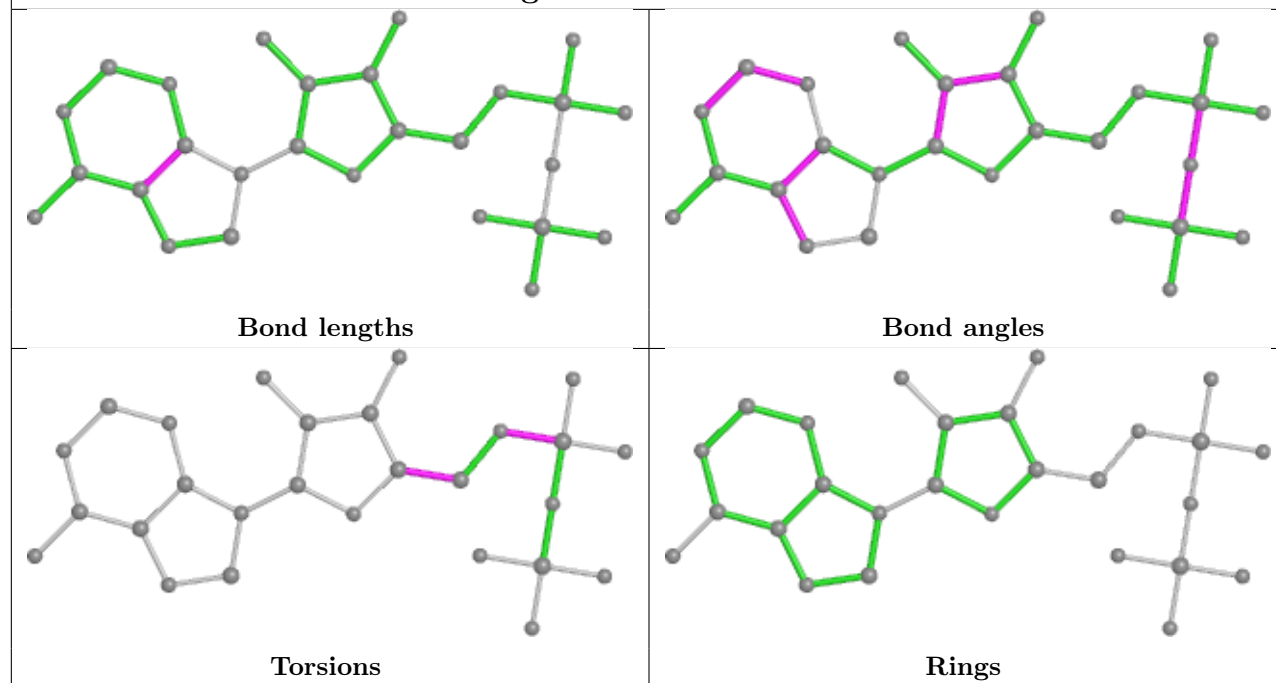
Ligand ADP D 2103



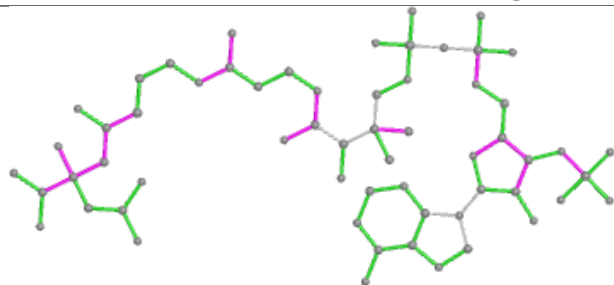
Ligand Q5B C 2103



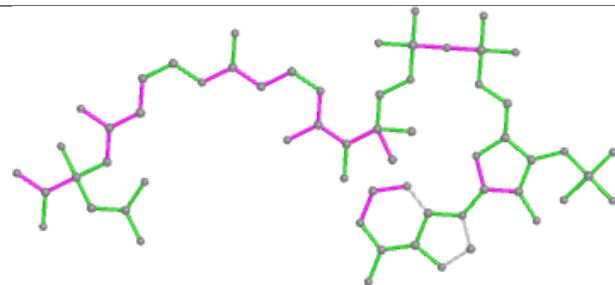
Ligand ADP B 1201



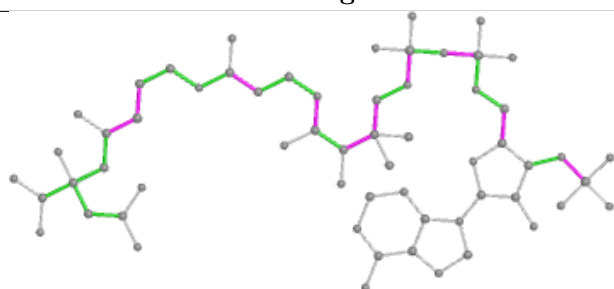
Ligand Q5B B 1202



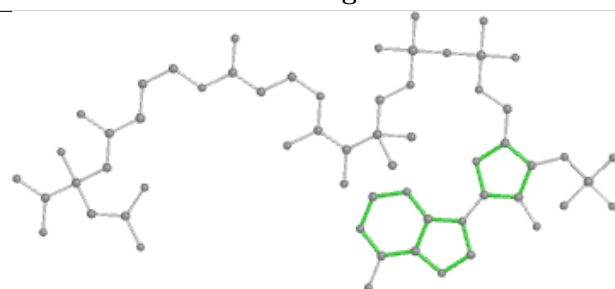
Bond lengths



Bond angles

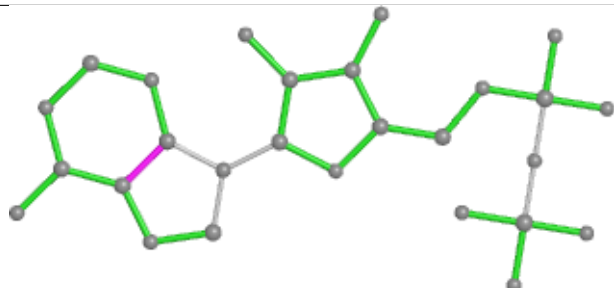


Torsions

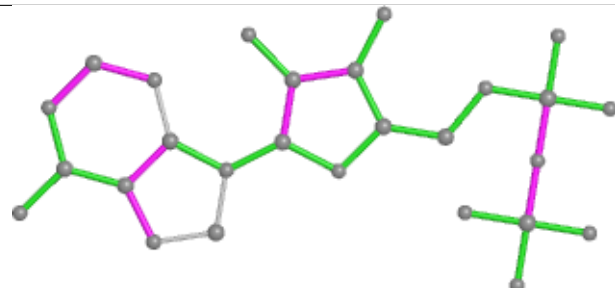


Rings

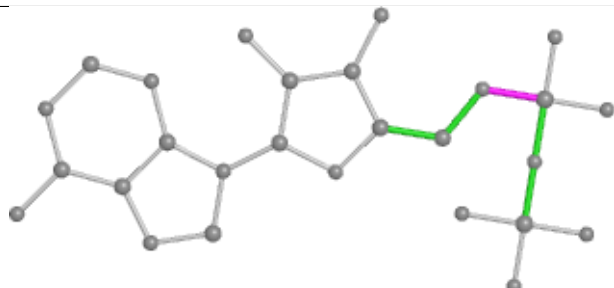
Ligand ADP A 1201



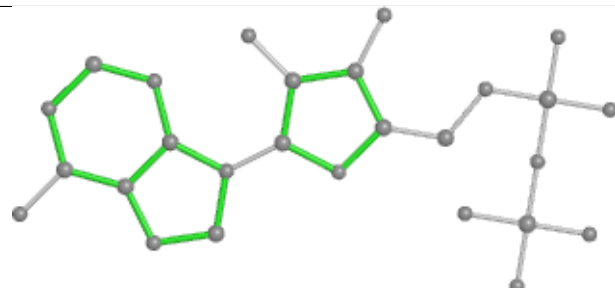
Bond lengths



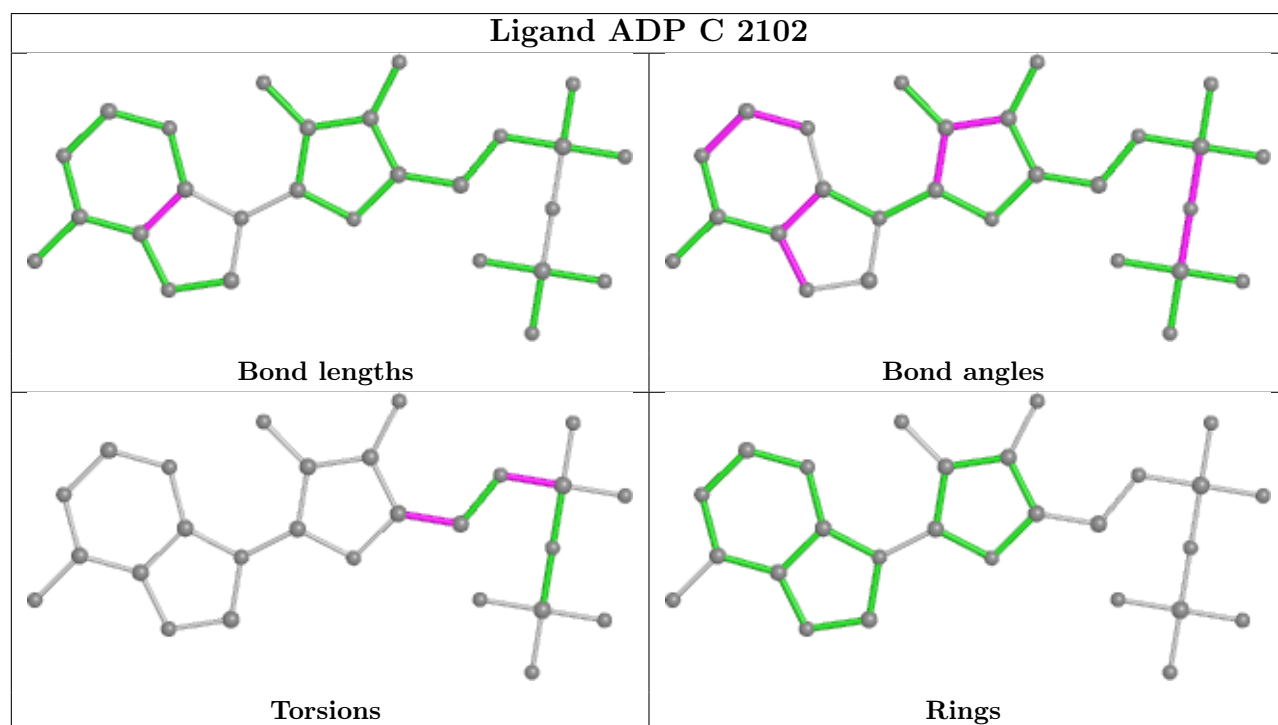
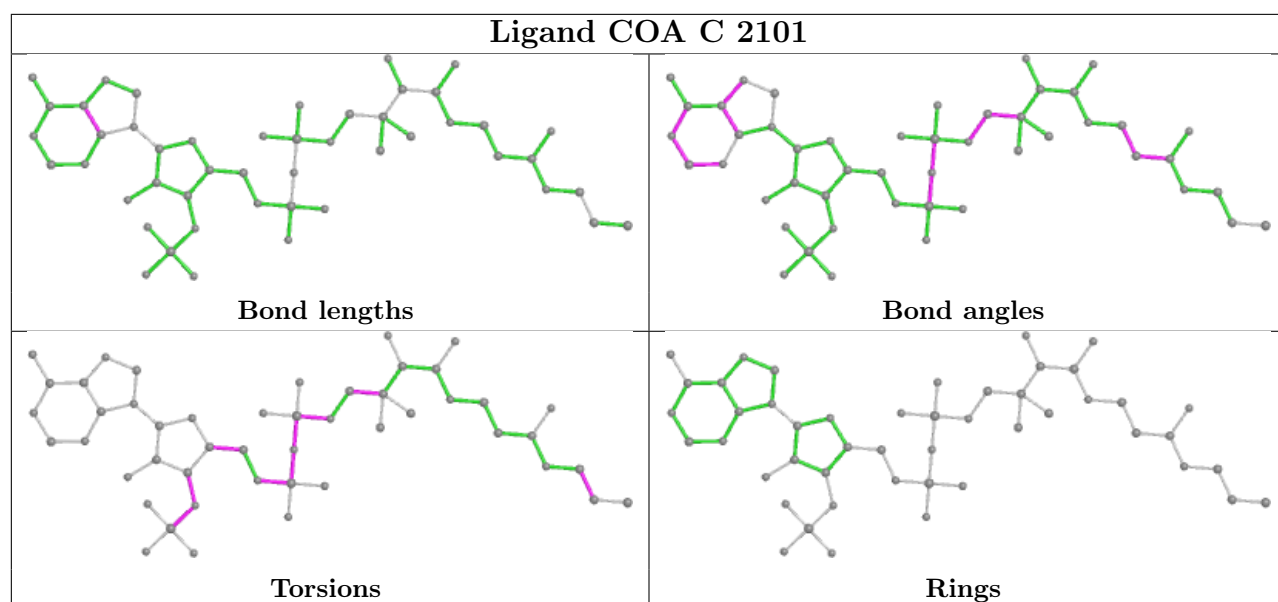
Bond angles

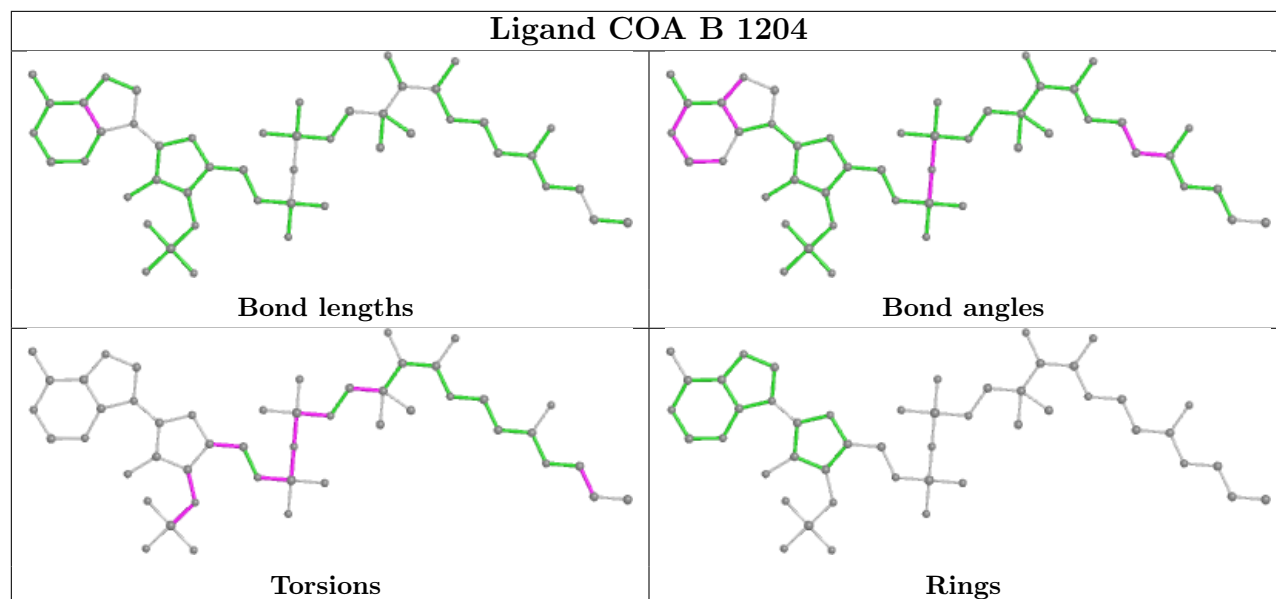


Torsions



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.

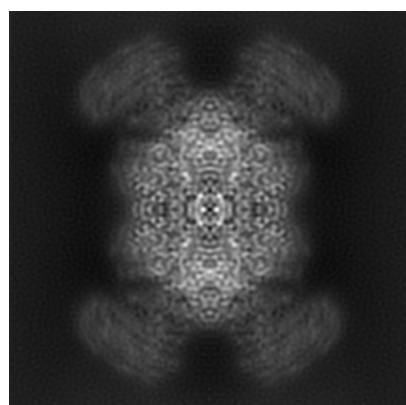
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24479. These allow visual inspection of the internal detail of the map and identification of artifacts.

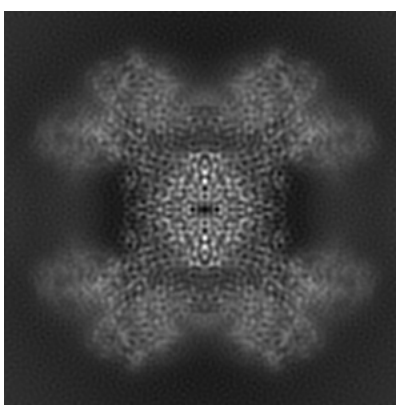
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

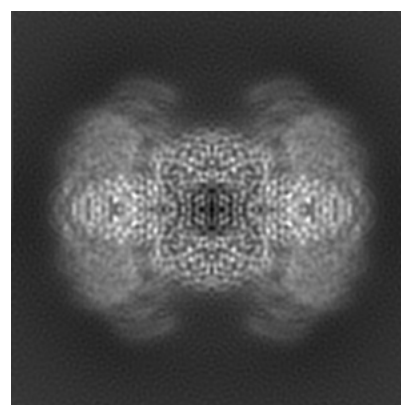
6.1.1 Primary map



X



Y

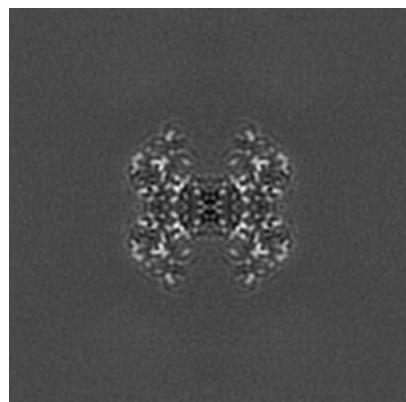


Z

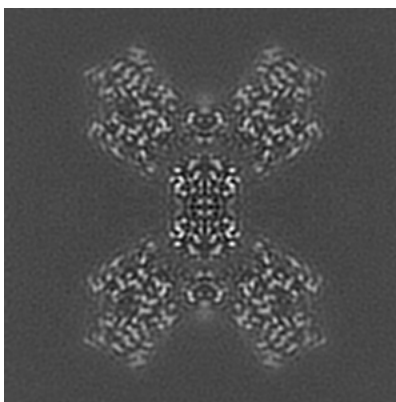
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

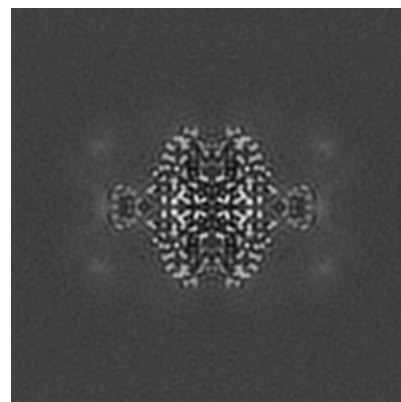
6.2.1 Primary map



X Index: 110



Y Index: 110

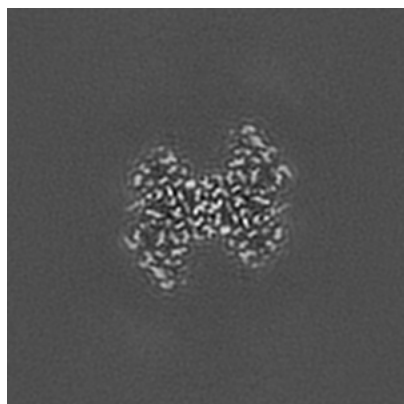


Z Index: 110

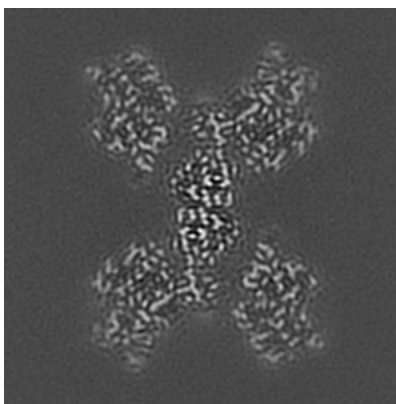
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

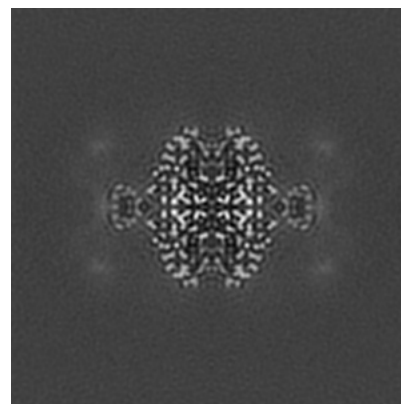
6.3.1 Primary map



X Index: 118



Y Index: 106

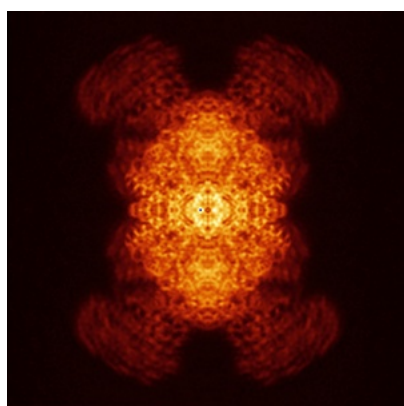


Z Index: 110

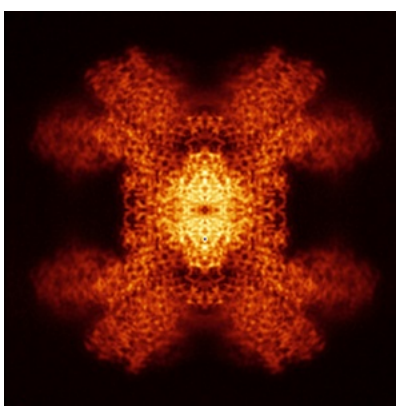
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

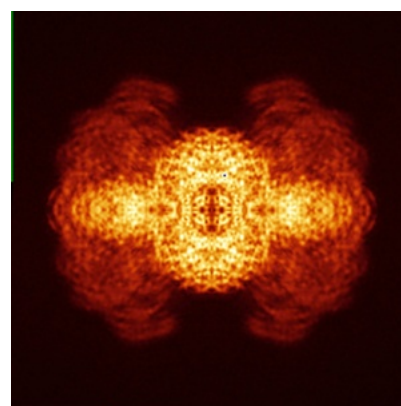
6.4.1 Primary map



X



Y

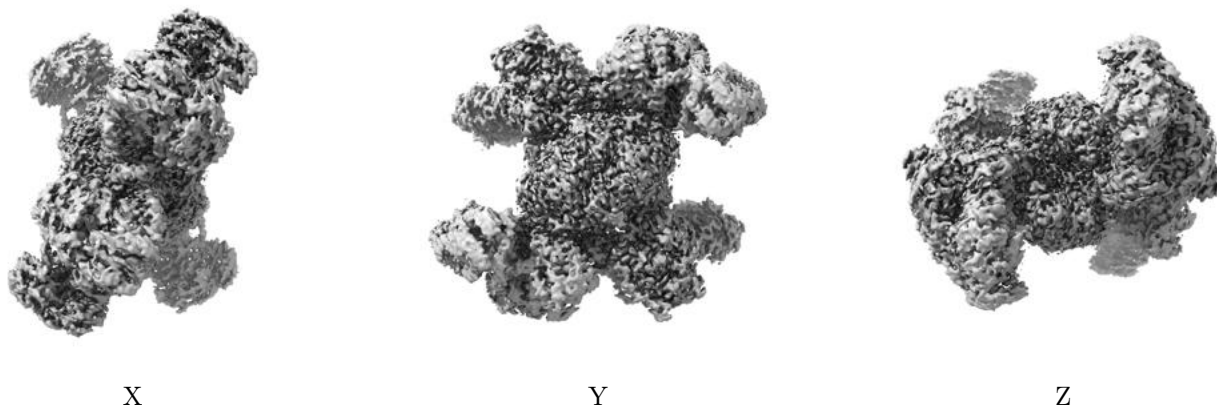


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

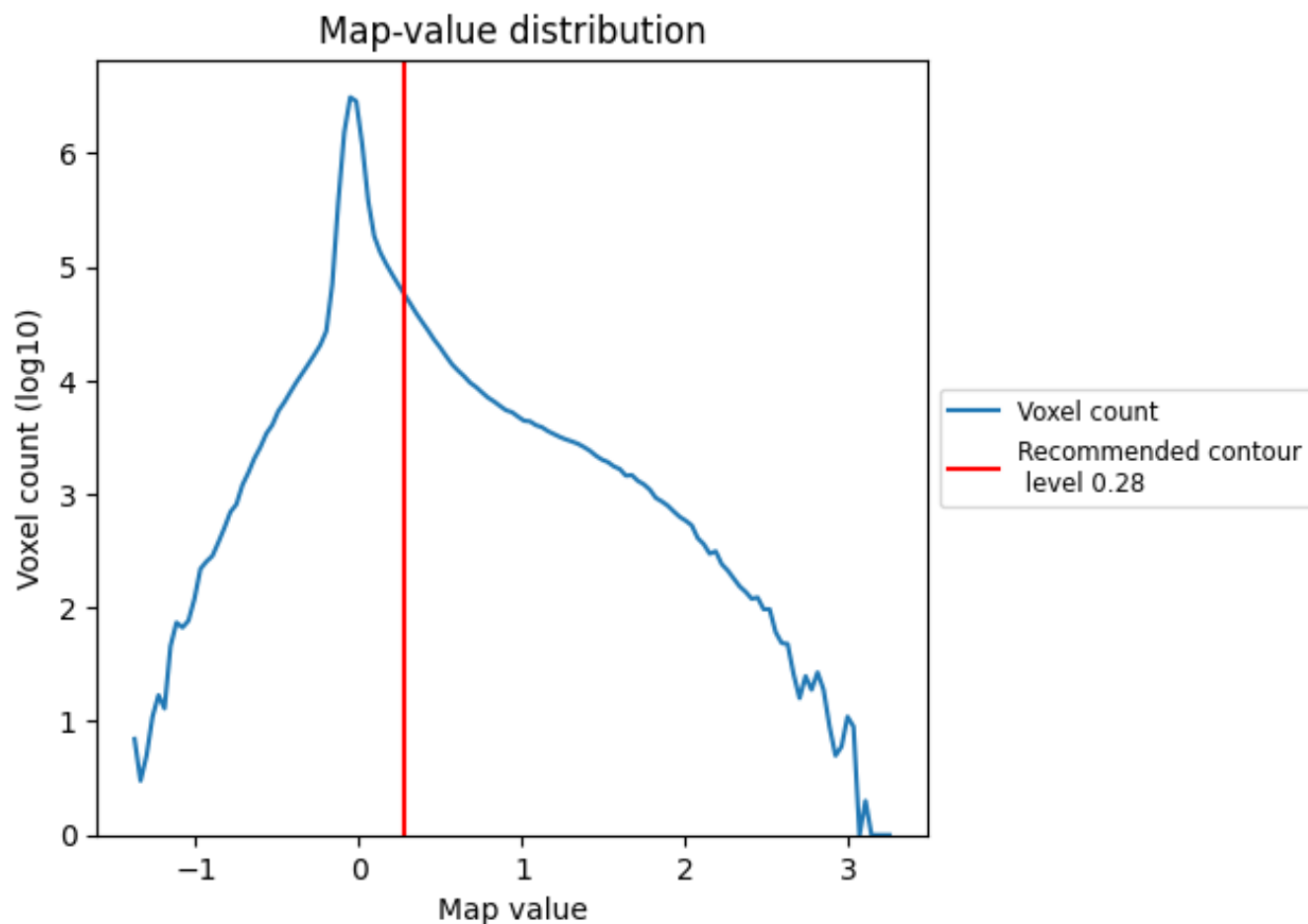
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

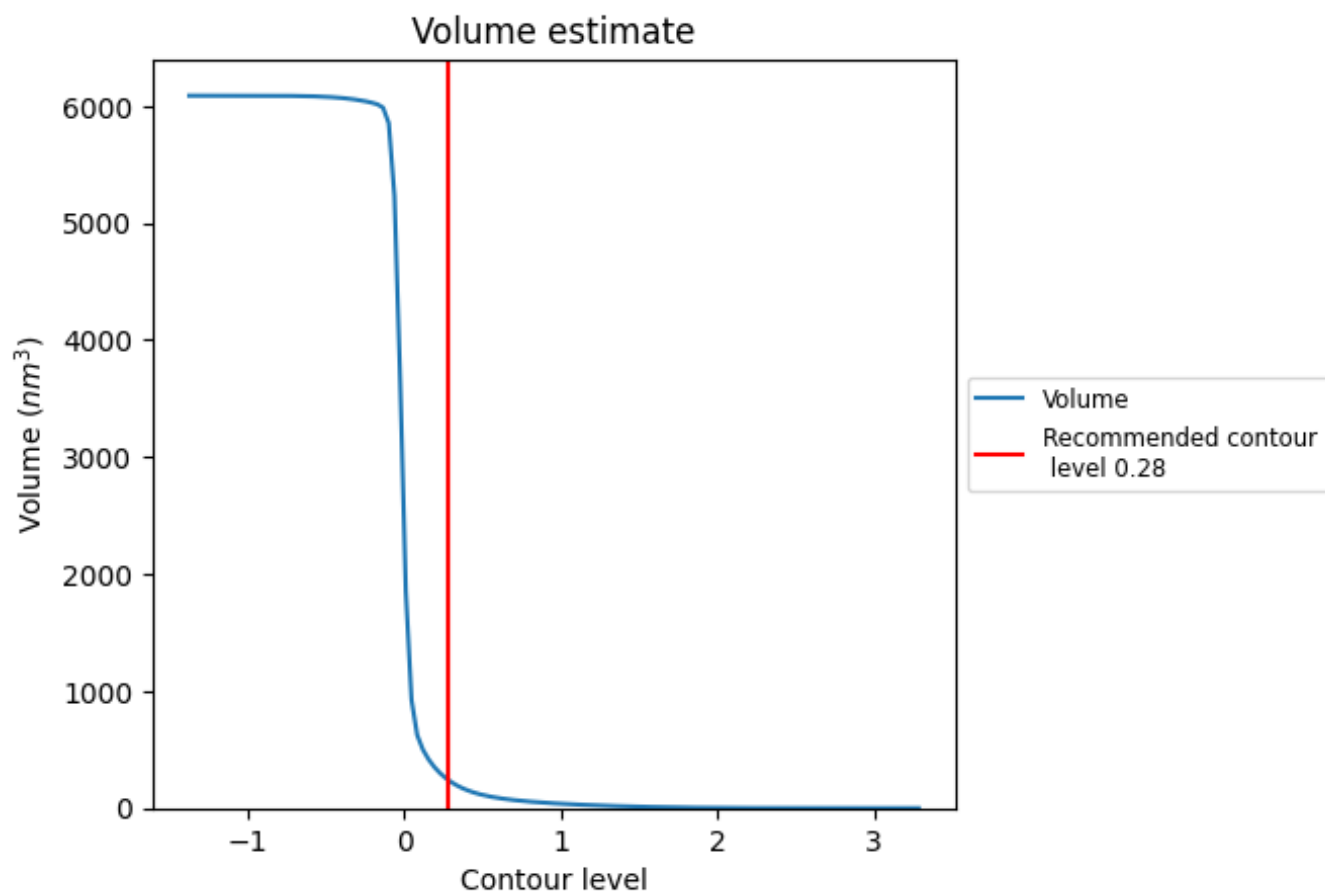
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

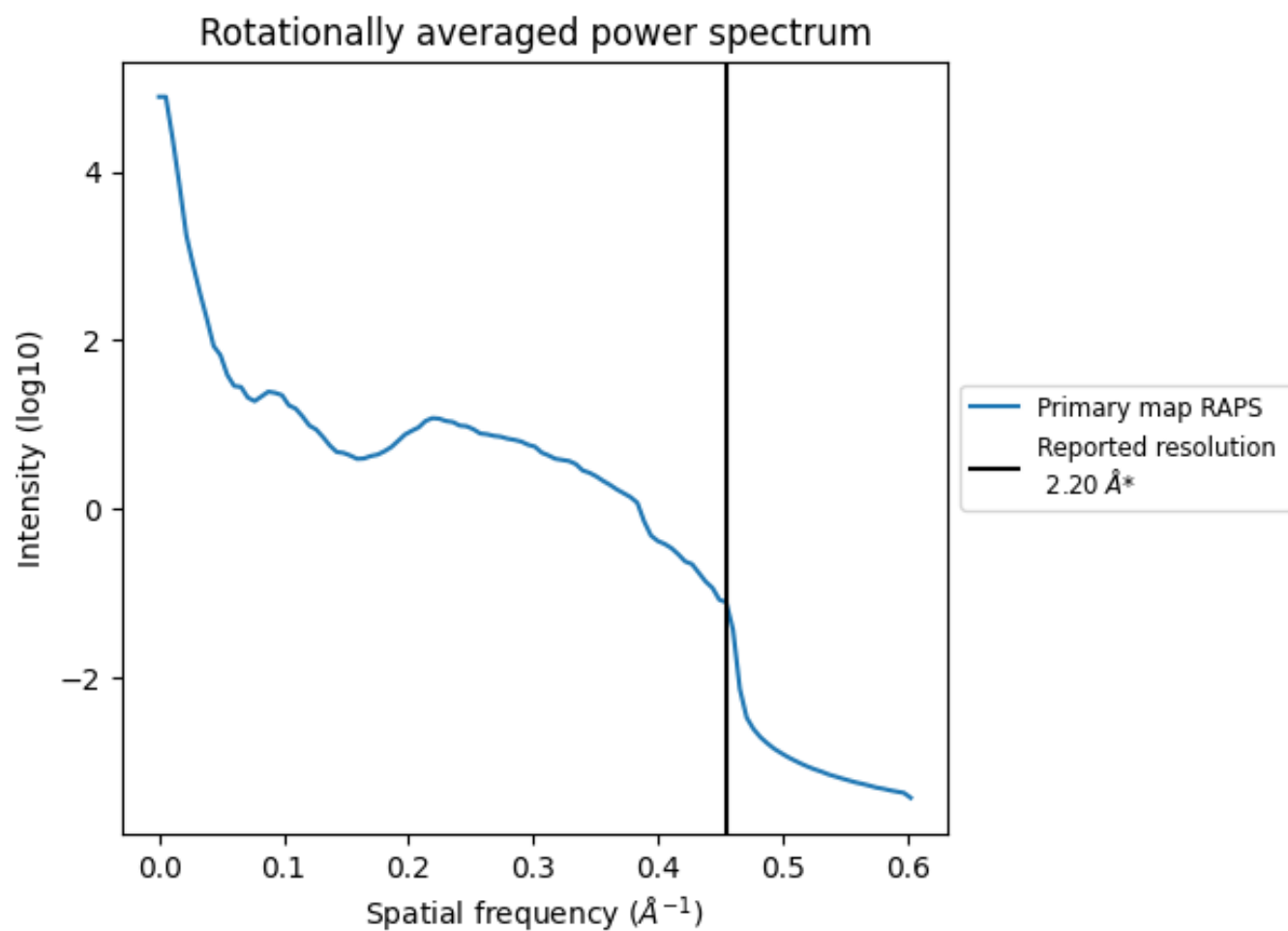
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 nm^3 ; this corresponds to an approximate mass of 219 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

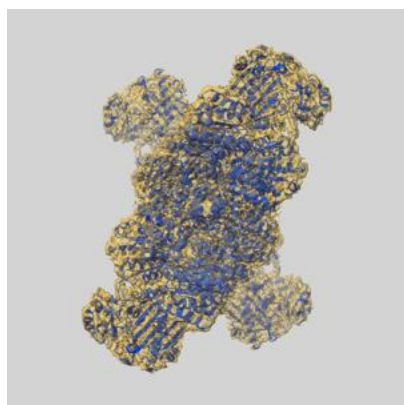
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

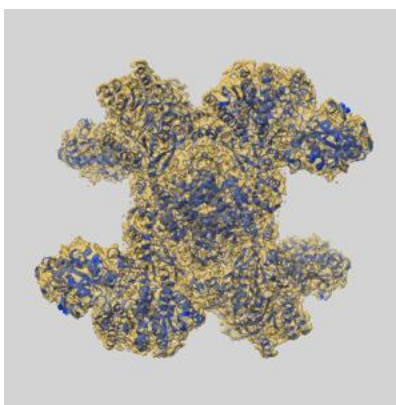
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24479 and PDB model 7RIG. Per-residue inclusion information can be found in section [3](#) on page [8](#).

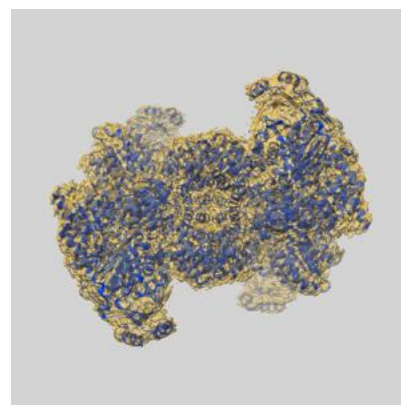
9.1 Map-model overlay [i](#)



X



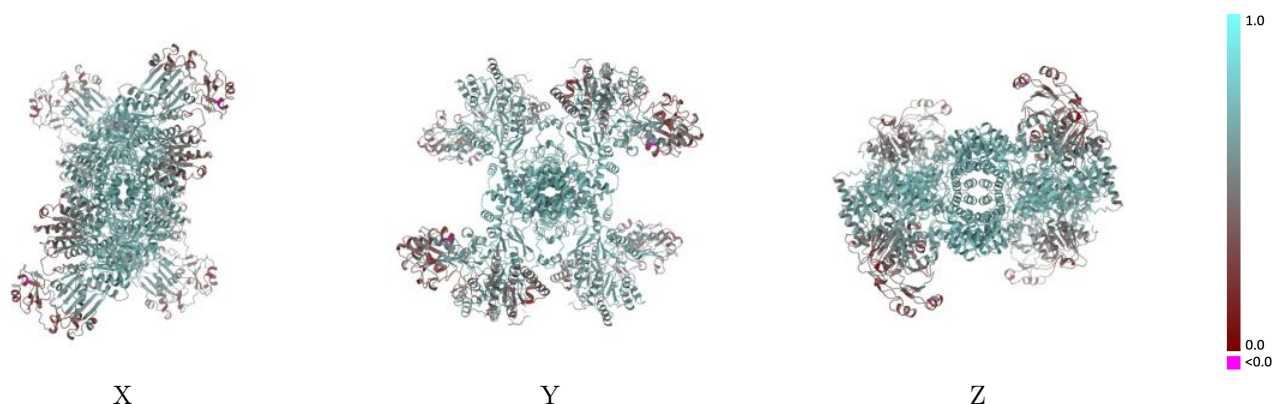
Y



Z

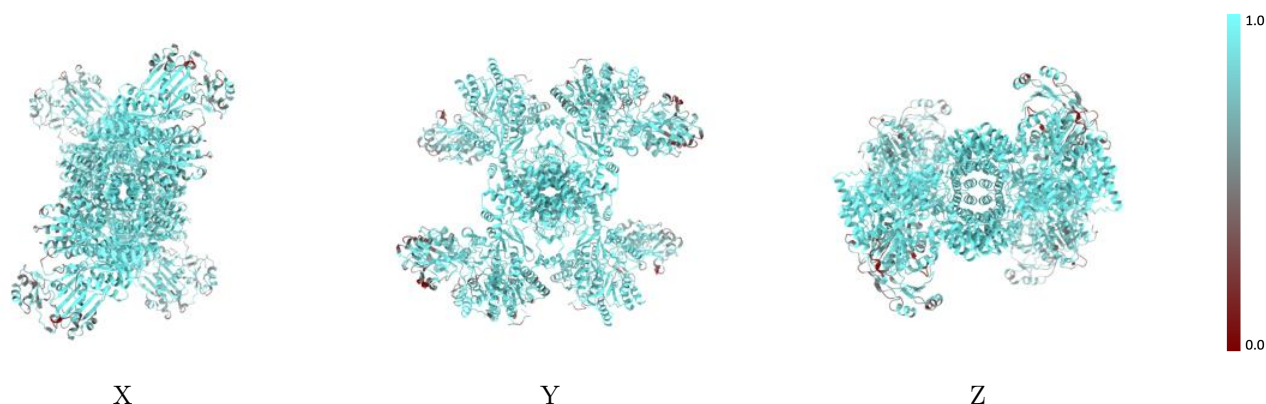
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



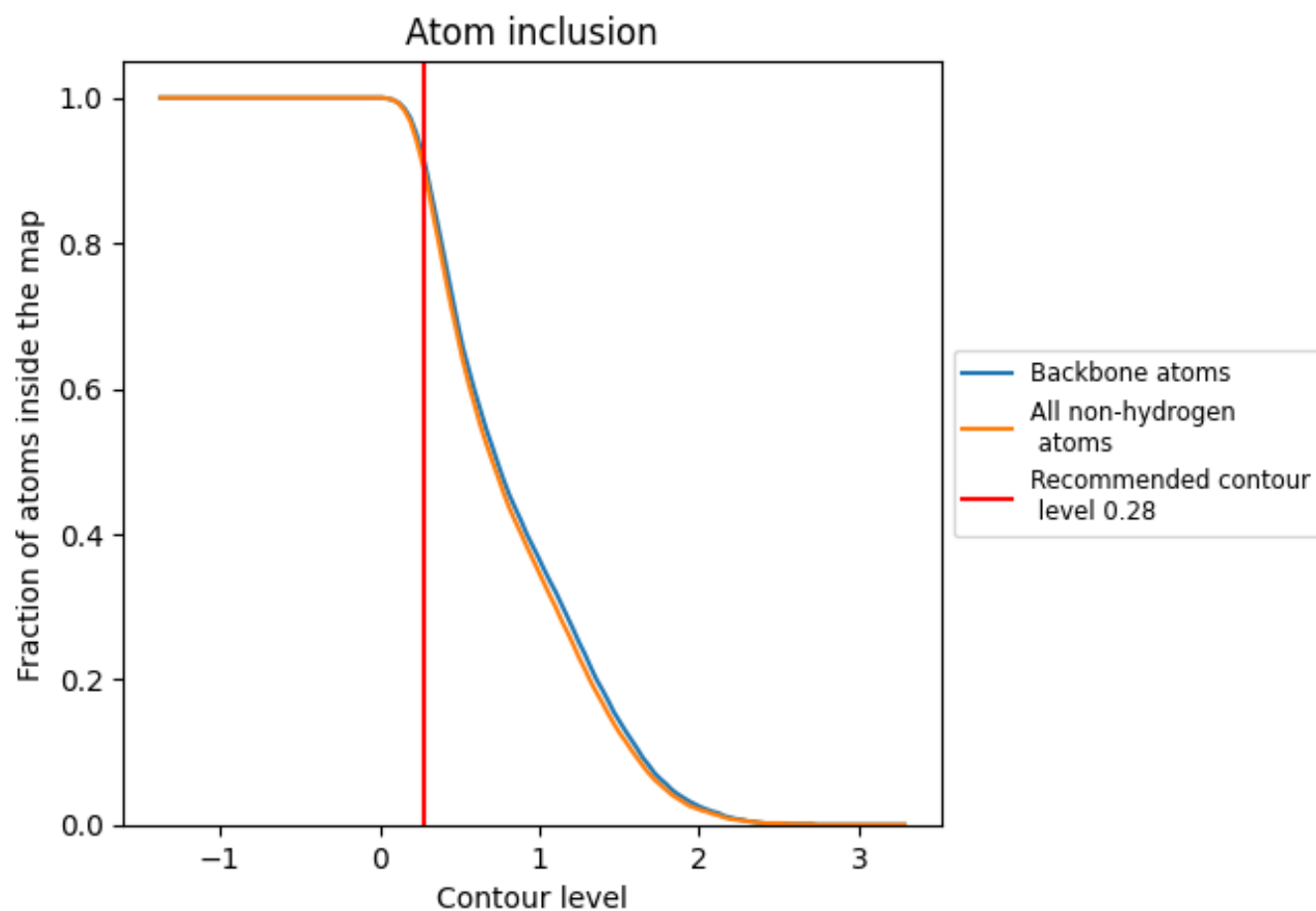
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.28).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8990	<div></div> 0.5880
A	<div></div> 0.9020	<div></div> 0.5880
B	<div></div> 0.8980	<div></div> 0.5870
C	<div></div> 0.9010	<div></div> 0.5890
D	<div></div> 0.8990	<div></div> 0.5880

