Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 03:27 PM EDT

PDB ID	:	5XN7
Title	:	Crystal structure of the effector domain RID of Vibrio vulnificus MARTX toxin
Authors	:	Yin, L.; Zhu, Y.
Deposited on	:	2017-05-18
Resolution	:	2.70 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:

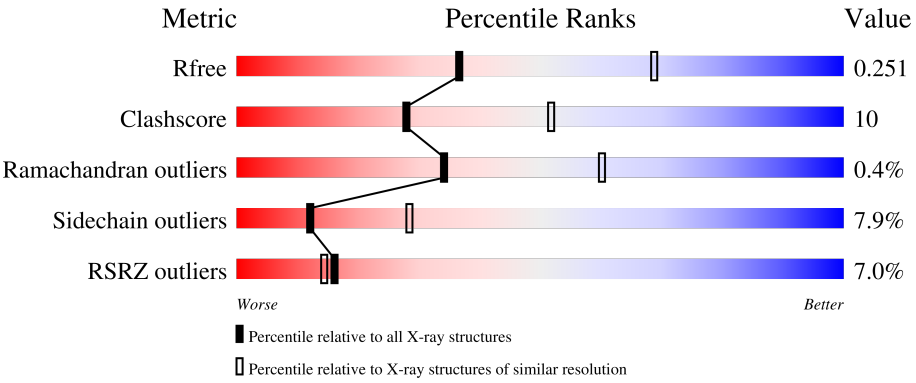
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	616	7% 66% 20% · 12%
1	B	616	5% 69% 19% · 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CL	A	2906	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8384 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.

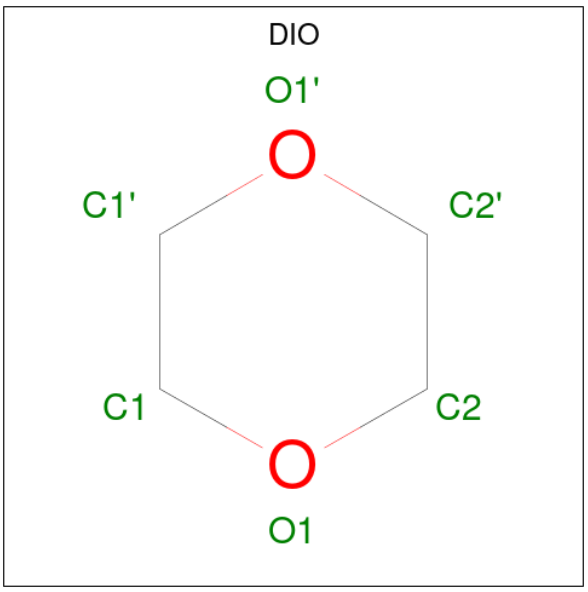
- Molecule 1 is a protein called Putative RTX-toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	Se	0	0	0
			4105	2576	726	794	9			
1	B	551	Total	C	N	O	Se	0	0	0
			4143	2597	731	807	8			

There are 6 discrepancies between the modelled and reference sequences:

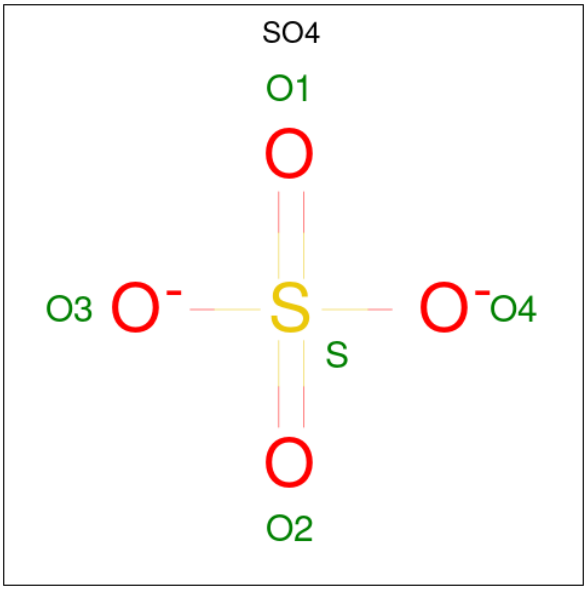
Chain	Residue	Modelled	Actual	Comment	Reference
A	2361	ARG	GLN	conflict	UNP F1CLG1
A	2541	ASP	GLY	conflict	UNP F1CLG1
A	2835	ALA	CYS	engineered mutation	UNP F1CLG1
B	2361	ARG	GLN	conflict	UNP F1CLG1
B	2541	ASP	GLY	conflict	UNP F1CLG1
B	2835	ALA	CYS	engineered mutation	UNP F1CLG1

- Molecule 2 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



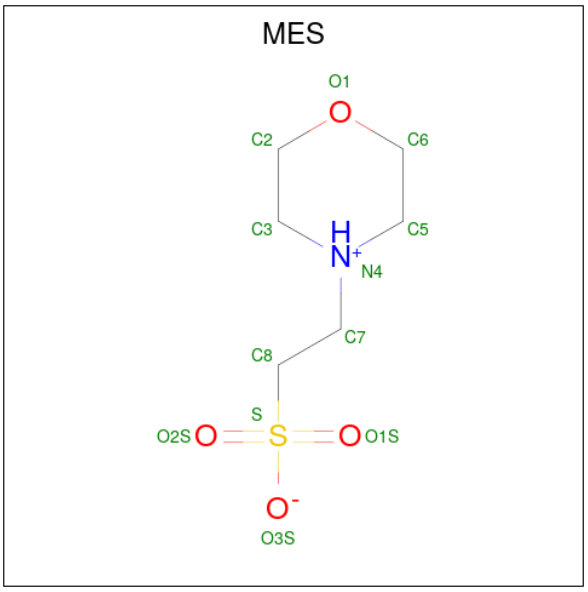
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 4 2	0	0
2	A	1	Total C O 6 4 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



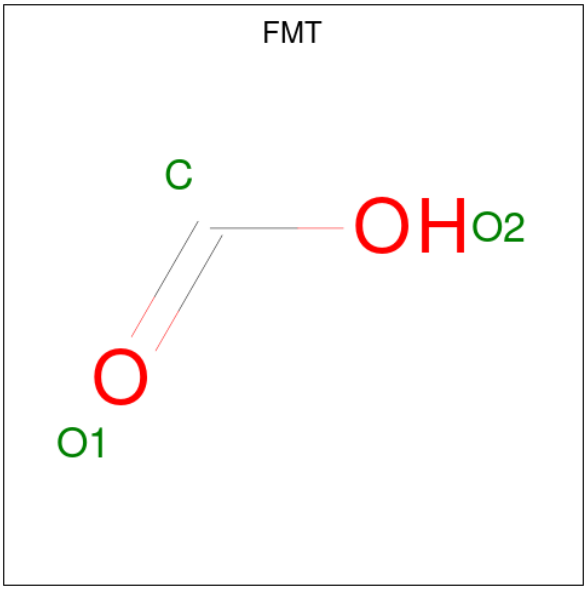
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			3	1	2			

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Cl 2 2	0	0
6	B	1	Total Cl 1 1	0	0

- Molecule 7 is water.

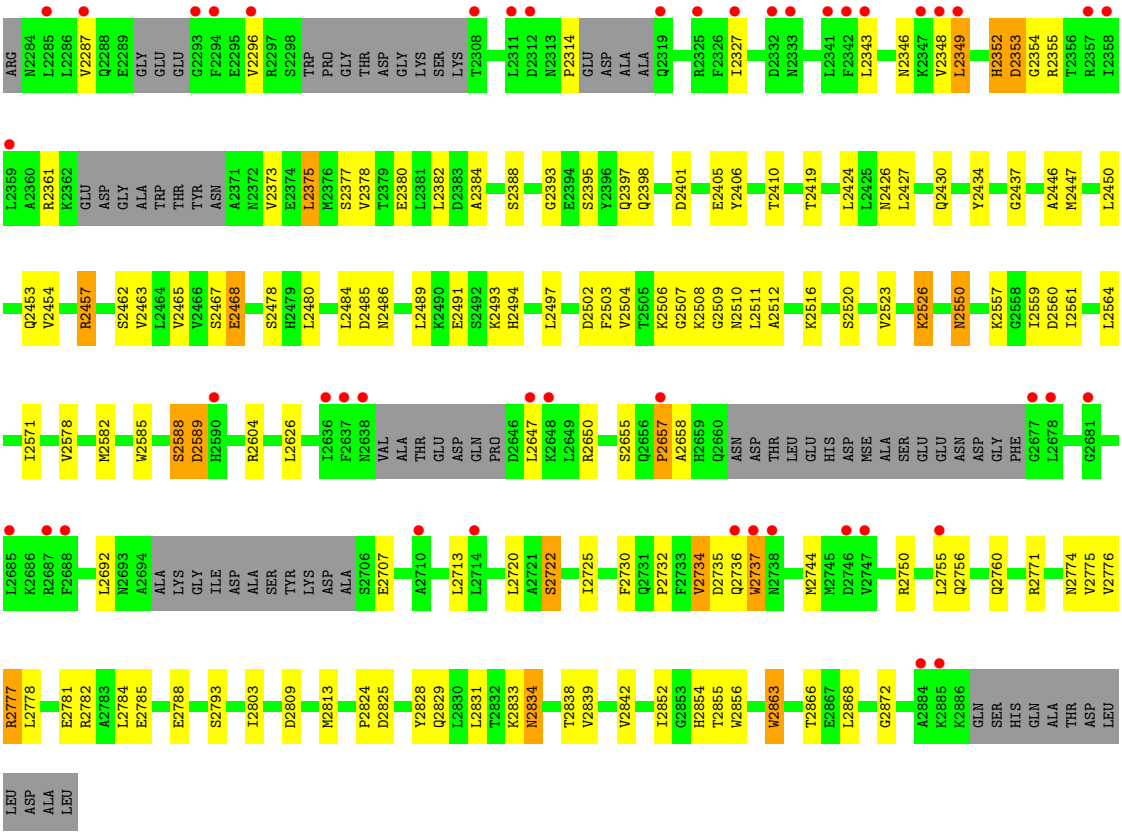
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	60	Total O 60 60	0	0
7	B	29	Total O 29 29	0	0

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.

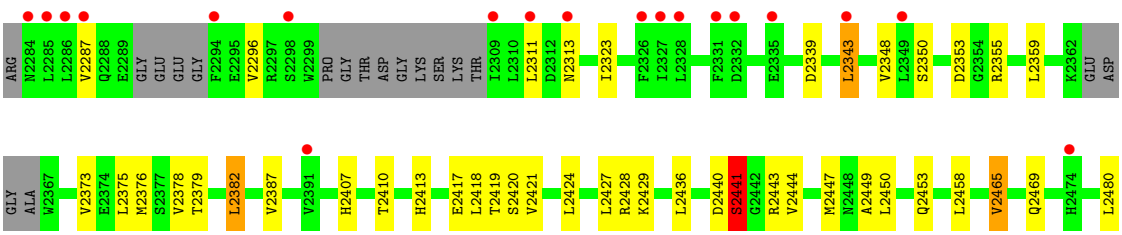
• Molecule 1: Putative RTX-toxin

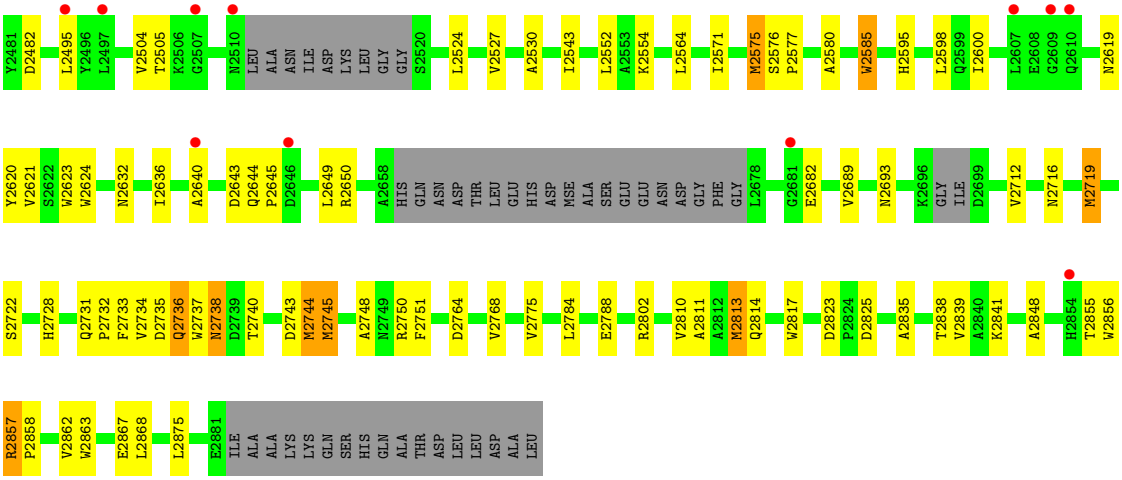
Chain A:



• Molecule 1: Putative RTX-toxin

Chain B:




Y2481 D2482 L2495 Y2496 L2497 V2504 T2505 K2506 G2507 N2510 LEU ALA ASN ILE ASP LYS LEU GLY GLY S2520 L2524 V2527 A2530 I2543 L2552 A2553 K2554 L2564 I2571 M2575 S2576 P2577 A2580 W2585 H2595 L2598 Q2599 I2600 L2607 E2608 G2609 Q2610 N2619
Y2620 V2621 S2622 W2623 W2624 N2632 I2636 A2640 D2643 Q2644 P2645 D2646 L2649 R2650 A2658 HIS GLN ASN ASP THR LEU GLU HIS ASP MSE ALA SER GLU GLU ASN ASP GLY PHE GLY L2678 G2681 E2682 V2689 N2693 K2696 GLY ILE D2699 V2712 N2716 M2719
S2722 H2728 Q2731 P2732 F2733 V2734 D2735 Q2736 W2737 N2738 D2739 T2740 D2743 M2744 M2745 A2748 N2749 R2750 F2751 D2764 V2768 V2775 L2784 E2788 R2802 V2810 A2811 A2812 M2813 Q2814 W2817 D2823 P2824 D2825 A2835 T2838 V2839 A2840 K2841 A2848 H2854 T2855 W2856
R2857 P2858 V2862 W2863 E2867 L2868 L2875 E2881 ILE ALA ALA LYS LYS GLN SER HIS GLN ALA THR ASP LEU LEU ASP ALA LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	124.74Å 185.19Å 81.36Å 90.00° 95.60° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 46.30 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.70) 99.5 (46.30-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.203 , 0.244 0.207 , 0.251	Depositor DCC
R_{free} test set	2554 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.803	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8384	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: MES, CL, FMT, DIO, SO4

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	0.64	3/4161 (0.1%)	0.72	2/5619 (0.0%)
1	B	0.59	4/4205 (0.1%)	0.70	8/5689 (0.1%)
All	All	0.61	7/8366 (0.1%)	0.71	10/11308 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2856	TRP	CD2-CE2	5.97	1.48	1.41
1	B	2856	TRP	CD2-CE2	5.91	1.48	1.41
1	B	2817	TRP	CD2-CE2	5.58	1.48	1.41
1	B	2863	TRP	CD2-CE2	5.29	1.47	1.41
1	A	2863	TRP	CD2-CE2	5.28	1.47	1.41
1	B	2585	TRP	CD2-CE2	5.13	1.47	1.41
1	A	2585	TRP	CD2-CE2	5.02	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2743	ASP	N-CA-C	8.41	133.70	111.00
1	A	2834	ASN	CB-CA-C	-7.95	94.50	110.40
1	B	2744	MSE	CB-CA-C	6.32	123.04	110.40
1	A	2314	PRO	N-CA-CB	6.11	110.63	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2745	MSE	N-CA-C	6.00	127.21	111.00
1	B	2744	MSE	N-CA-CB	5.78	121.00	110.60
1	B	2736	GLN	CB-CA-C	-5.58	99.23	110.40
1	B	2645	PRO	N-CA-CB	5.38	109.75	103.30
1	B	2743	ASP	CB-CA-C	-5.08	100.25	110.40
1	B	2376	MSE	N-CA-CB	-5.01	101.59	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2588	SER	Peptide

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	4105	0	3918	80	0
1	B	4143	0	3896	81	0
2	A	12	0	16	0	0
3	A	5	0	0	0	0
4	A	12	0	13	0	0
4	B	12	0	13	0	0
5	A	3	0	1	0	0
6	A	2	0	0	2	0
6	B	1	0	0	0	0
7	A	60	0	0	1	0
7	B	29	0	0	1	0
All	All	8384	0	7857	160	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 (160) 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:B:2736:GLN:HE22	1:B:2750:ARG:HH22	0.95	0.93
1:B:2736:GLN:HE22	1:B:2750:ARG:NH2	1.70	0.89
1:A:2777:ARG:O	1:A:2781:GLU:HG3	1.85	0.75
1:A:2737:TRP:NE1	1:A:2744:MSE:HG2	2.04	0.72
1:A:2377:SER:OG	1:A:2380:GLU:HG3	1.89	0.72
1:A:2507:GLY:O	1:A:2510:ASN:HB2	1.90	0.71
1:A:2582:MSE:HE1	1:A:2872:GLY:HA3	1.74	0.70
1:B:2343:LEU:HD22	1:B:2348:VAL:HG22	1.74	0.70
1:A:2774:ASN:O	1:A:2778:LEU:HB3	1.93	0.68
1:B:2424:LEU:HG	1:B:2458:LEU:HD13	1.75	0.67
1:B:2736:GLN:NE2	1:B:2750:ARG:HH22	1.81	0.64
1:B:2716:ASN:HB3	1:B:2719:MSE:HG3	1.78	0.64
1:A:2775:VAL:HG12	1:A:2776:VAL:N	2.12	0.63
1:A:2373:VAL:O	1:A:2373:VAL:HG12	1.99	0.62
1:B:2421:VAL:HG21	1:B:2465:VAL:CG1	2.30	0.61
1:A:2489:LEU:HD22	1:A:2493:LYS:HD2	1.83	0.61
1:B:2313:ASN:HB3	1:B:2343:LEU:HB3	1.81	0.61
1:A:2375:LEU:HD23	1:A:2453:GLN:HB3	1.84	0.60
1:B:2624:TRP:CZ2	1:B:2719:MSE:HE3	2.36	0.59
1:A:2774:ASN:O	1:A:2778:LEU:CB	2.50	0.59
1:B:2731:GLN:N	1:B:2732:PRO:HD2	2.18	0.59
1:B:2636:ILE:CG2	1:B:2712:VAL:HG22	2.32	0.58
1:B:2580:ALA:HB2	1:B:2813:MSE:HE1	1.85	0.58
1:A:2626:LEU:HD21	1:A:2650:ARG:HD2	1.86	0.57
1:B:2733:PHE:CD1	1:B:2751:PHE:HB2	2.40	0.56
1:A:2506:LYS:HE2	1:A:2509:GLY:HA3	1.87	0.56
1:B:2428:ARG:NH1	1:B:2458:LEU:HD23	2.20	0.56
1:B:2624:TRP:CZ2	1:B:2719:MSE:CE	2.89	0.56
1:A:2485:ASP:O	6:A:2906:CL:CL	2.62	0.55
1:A:2426:ASN:O	1:A:2430:GLN:HG2	2.06	0.55
1:B:2734:VAL:O	1:B:2735:ASP:C	2.45	0.54
1:A:2406:TYR:CE1	1:A:2424:LEU:HB2	2.42	0.54
1:A:2777:ARG:O	1:A:2777:ARG:HG3	2.06	0.54
1:A:2588:SER:O	1:A:2589:ASP:HB3	2.08	0.54
1:B:2736:GLN:O	1:B:2738:ASN:N	2.41	0.53
1:B:2848:ALA:HB1	1:B:2875:LEU:HD21	1.90	0.52
1:A:2508:LYS:C	1:A:2510:ASN:H	2.12	0.52
1:B:2736:GLN:C	1:B:2738:ASN:N	2.63	0.52
1:B:2350:SER:HB3	1:B:2359:LEU:HD11	1.92	0.52
1:B:2428:ARG:NH1	1:B:2458:LEU:CD2	2.72	0.52
1:B:2640:ALA:O	1:B:2643:ASP:N	2.41	0.52
1:B:2722:SER:HB2	1:B:2775:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2393:GLY:O	1:A:2397:GLN:HG3	2.10	0.51
1:B:2440:ASP:O	1:B:2441:SER:HB3	2.09	0.51
1:B:2440:ASP:O	1:B:2441:SER:CB	2.59	0.51
1:B:2543:ILE:HD13	1:B:2571:ILE:HG12	1.92	0.51
1:A:2437:GLY:HA2	1:A:2489:LEU:HD21	1.93	0.51
1:B:2429:LYS:HG3	1:B:2482:ASP:HB3	1.92	0.51
1:A:2550:ASN:N	1:A:2550:ASN:OD1	2.44	0.51
1:B:2407:HIS:O	1:B:2410:THR:HB	2.11	0.51
1:B:2428:ARG:HH11	1:B:2458:LEU:HD23	1.74	0.51
1:B:2504:VAL:CG1	1:B:2505:THR:N	2.74	0.50
1:A:2732:PRO:O	1:A:2736:GLN:HG3	2.10	0.50
6:A:2906:CL:CL	7:A:3013:HOH:O	2.57	0.50
1:B:2443:ARG:O	1:B:2447:MSE:HG2	2.12	0.50
1:A:2626:LEU:CD2	1:A:2650:ARG:HD2	2.42	0.50
1:B:2858:PRO:HB3	1:B:2867:GLU:HG2	1.94	0.50
1:A:2736:GLN:HE22	1:A:2750:ARG:NH2	2.10	0.50
1:B:2838:THR:O	1:B:2841:LYS:HB3	2.12	0.49
1:A:2453:GLN:O	1:A:2457:ARG:HG2	2.11	0.49
1:B:2732:PRO:O	1:B:2736:GLN:HG3	2.13	0.49
1:A:2771:ARG:HG3	1:A:2828:TYR:CE1	2.46	0.49
1:B:2731:GLN:N	1:B:2732:PRO:CD	2.76	0.49
1:A:2434:TYR:CD1	1:A:2447:MSE:HG3	2.48	0.49
1:A:2775:VAL:O	1:A:2776:VAL:C	2.49	0.48
1:A:2657:PRO:O	1:A:2658:ALA:HB3	2.13	0.48
1:B:2835:ALA:O	1:B:2839:VAL:HG23	2.13	0.48
1:A:2462:SER:O	1:A:2465:VAL:HG12	2.13	0.48
1:B:2441:SER:O	1:B:2444:VAL:HG23	2.14	0.48
1:B:2378:VAL:HG12	1:B:2382:LEU:HD23	1.96	0.48
1:B:2632:ASN:HD21	1:B:2719:MSE:SE	2.47	0.48
1:A:2343:LEU:HD12	1:A:2348:VAL:HG22	1.96	0.48
1:A:2520:SER:HB2	1:B:2378:VAL:HG21	1.96	0.48
1:B:2527:VAL:O	1:B:2530:ALA:HB3	2.14	0.47
1:B:2620:TYR:CD2	1:B:2650:ARG:HG2	2.49	0.47
1:A:2725:ILE:HG22	1:A:2730:PHE:HD2	1.80	0.47
1:B:2736:GLN:C	1:B:2738:ASN:H	2.16	0.47
1:B:2731:GLN:HB2	1:B:2732:PRO:HD3	1.97	0.47
1:A:2571:ILE:CG2	1:A:2604:ARG:HG2	2.45	0.47
1:A:2491:GLU:HA	1:A:2561:ILE:HB	1.96	0.47
1:A:2756:GLN:O	1:A:2760:GLN:HG2	2.15	0.46
1:B:2441:SER:O	1:B:2441:SER:OG	2.30	0.46
1:A:2494:HIS:HA	1:A:2560:ASP:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2323:ILE:HD13	1:B:2343:LEU:HB2	1.97	0.46
1:B:2636:ILE:HG21	1:B:2712:VAL:HG22	1.96	0.46
1:A:2506:LYS:HE2	1:A:2509:GLY:CA	2.45	0.46
1:A:2353:ASP:HB3	1:A:2354:GLY:H	1.49	0.46
1:A:2737:TRP:CE2	1:A:2744:MSE:HG2	2.50	0.46
1:A:2737:TRP:CD1	1:A:2744:MSE:HG2	2.51	0.46
1:A:2839:VAL:HG11	1:A:2868:LEU:HD11	1.98	0.46
1:A:2734:VAL:HG12	1:A:2735:ASP:N	2.29	0.46
1:B:2449:ALA:O	1:B:2453:GLN:HG3	2.16	0.46
1:B:2495:LEU:HD11	1:B:2564:LEU:HD22	1.98	0.45
1:A:2838:THR:O	1:A:2842:VAL:HG23	2.16	0.45
1:B:2728:HIS:HA	1:B:2731:GLN:HG2	1.97	0.45
1:B:2736:GLN:NE2	1:B:2750:ARG:NH2	2.52	0.45
1:A:2378:VAL:O	1:A:2382:LEU:HG	2.16	0.45
1:A:2829:GLN:O	1:A:2833:LYS:HG2	2.17	0.45
1:B:2417:GLU:O	1:B:2421:VAL:HG23	2.16	0.45
1:B:2811:ALA:HA	1:B:2814:GLN:HG2	1.98	0.45
1:B:2571:ILE:O	1:B:2575:MSE:HG3	2.17	0.45
1:B:2598:LEU:HB3	1:B:2621:VAL:HB	1.97	0.45
1:B:2640:ALA:O	1:B:2644:GLN:N	2.47	0.45
1:A:2352:HIS:O	1:A:2353:ASP:C	2.54	0.45
1:B:2585:TRP:HB3	1:B:2595:HIS:HB2	1.99	0.45
1:B:2857:ARG:HA	1:B:2858:PRO:HD2	1.93	0.45
1:B:2287:VAL:HG22	1:B:2296:VAL:HG22	1.99	0.44
1:A:2839:VAL:CG1	1:A:2868:LEU:HD11	2.47	0.44
1:B:2682:GLU:OE1	1:B:2788:GLU:HG2	2.17	0.44
1:B:2444:VAL:O	1:B:2447:MSE:N	2.51	0.44
1:A:2484:LEU:HD11	1:A:2564:LEU:HD23	1.99	0.44
1:A:2692:LEU:HD13	1:A:2777:ARG:HB2	2.00	0.44
1:B:2421:VAL:HG21	1:B:2465:VAL:HG12	1.97	0.43
1:B:2623:TRP:HA	7:B:3008:HOH:O	2.19	0.43
1:B:2744:MSE:O	1:B:2748:ALA:CB	2.66	0.43
1:B:2810:VAL:O	1:B:2814:GLN:HG2	2.18	0.43
1:A:2384:ALA:O	1:A:2446:ALA:HB2	2.18	0.43
1:B:2524:LEU:HD11	1:B:2552:LEU:HD13	2.01	0.43
1:A:2722:SER:OG	1:A:2824:PRO:O	2.29	0.43
1:A:2809:ASP:O	1:A:2813:MSE:HG3	2.18	0.43
1:B:2636:ILE:HG22	1:B:2712:VAL:HG22	2.00	0.43
1:B:2823:ASP:OD1	1:B:2823:ASP:C	2.57	0.43
1:A:2406:TYR:HE1	1:A:2424:LEU:HB2	1.84	0.43
1:A:2401:ASP:O	1:A:2405:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2624:TRP:HZ2	1:B:2719:MSE:HE3	1.84	0.43
1:A:2395:SER:HA	1:A:2486:ASN:OD1	2.19	0.42
1:A:2450:LEU:O	1:A:2454:VAL:HG23	2.20	0.42
1:A:2782:ARG:NH2	1:A:2831:LEU:O	2.52	0.42
1:A:2346:ASN:O	1:A:2361:ARG:HA	2.19	0.42
1:B:2802:ARG:HH11	1:B:2802:ARG:HG2	1.84	0.42
1:A:2494:HIS:HE1	1:A:2557:LYS:O	2.01	0.42
1:A:2497:LEU:HG	1:A:2523:VAL:HG22	2.02	0.42
1:B:2375:LEU:HA	1:B:2453:GLN:OE1	2.19	0.42
1:A:2327:ILE:HD11	1:A:2343:LEU:HD22	2.02	0.42
1:A:2771:ARG:HG3	1:A:2828:TYR:CZ	2.55	0.42
1:A:2512:ALA:O	1:A:2516:LYS:HG2	2.19	0.42
1:B:2576:SER:HA	1:B:2577:PRO:HD2	1.93	0.42
1:A:2582:MSE:CE	1:A:2803:ILE:HD12	2.50	0.41
1:A:2784:LEU:O	1:A:2788:GLU:HG3	2.21	0.41
1:B:2620:TYR:CE2	1:B:2650:ARG:HG2	2.55	0.41
1:B:2744:MSE:O	1:B:2748:ALA:HB3	2.20	0.41
1:A:2507:GLY:C	1:A:2510:ASN:HB2	2.40	0.41
1:A:2497:LEU:HA	1:A:2502:ASP:O	2.20	0.41
1:A:2713:LEU:HB3	1:A:2720:LEU:HD13	2.01	0.41
1:B:2600:ILE:HB	1:B:2619:ASN:HB3	2.00	0.41
1:B:2296:VAL:HG23	1:B:2311:LEU:HD23	2.01	0.41
1:A:2478:SER:OG	1:A:2604:ARG:NH2	2.54	0.41
1:A:2852:ILE:HG13	1:A:2854:HIS:O	2.20	0.41
1:B:2689:VAL:HG12	1:B:2693:ASN:HD21	1.84	0.41
1:A:2349:LEU:HD11	1:A:2463:VAL:HG11	2.03	0.41
1:A:2467:SER:O	1:A:2468:GLU:HB2	2.20	0.41
1:A:2503:PHE:CZ	1:A:2526:LYS:HB3	2.56	0.41
1:A:2571:ILE:HG22	1:A:2604:ARG:HG2	2.03	0.41
1:A:2511:LEU:HB2	1:B:2825:ASP:OD1	2.20	0.41
1:B:2598:LEU:HB2	1:B:2839:VAL:HG13	2.02	0.41
1:B:2733:PHE:CE1	1:B:2751:PHE:HA	2.56	0.41
1:A:2834:ASN:ND2	1:A:2863:TRP:O	2.54	0.40
1:B:2343:LEU:CD2	1:B:2348:VAL:HG22	2.47	0.40
1:A:2287:VAL:HG12	1:A:2296:VAL:HG12	2.04	0.40
1:A:2588:SER:O	1:A:2589:ASP:CB	2.68	0.40

There are no symmetry-related clashes.

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	529/616 (86%)	486 (92%)	41 (8%)	2 (0%)	34	60
1	B	537/616 (87%)	498 (93%)	37 (7%)	2 (0%)	34	60
All	All	1066/1232 (86%)	984 (92%)	78 (7%)	4 (0%)	34	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2589	ASP
1	A	2657	PRO
1	B	2441	SER
1	B	2737	TRP

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	412/496 (83%)	381 (92%)	31 (8%)	13	31
1	B	412/496 (83%)	378 (92%)	34 (8%)	11	25
All	All	824/992 (83%)	759 (92%)	65 (8%)	12	28

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2349	LEU
1	A	2352	HIS

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Mol	Chain	Res	Type
1	A	2353	ASP
1	A	2355	ARG
1	A	2375	LEU
1	A	2388	SER
1	A	2398	GLN
1	A	2410	THR
1	A	2419	THR
1	A	2427	LEU
1	A	2457	ARG
1	A	2468	GLU
1	A	2480	LEU
1	A	2504	VAL
1	A	2526	LYS
1	A	2550	ASN
1	A	2559	ILE
1	A	2578	VAL
1	A	2647	LEU
1	A	2655	SER
1	A	2707	GLU
1	A	2722	SER
1	A	2734	VAL
1	A	2737	TRP
1	A	2755	LEU
1	A	2777	ARG
1	A	2785	GLU
1	A	2793	SER
1	A	2825	ASP
1	A	2855	THR
1	A	2866	THR
1	B	2339	ASP
1	B	2343	LEU
1	B	2353	ASP
1	B	2355	ARG
1	B	2373	VAL
1	B	2379	THR
1	B	2382	LEU
1	B	2387	VAL
1	B	2413	HIS
1	B	2418	LEU
1	B	2419	THR
1	B	2420	SER
1	B	2427	LEU

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Mol	Chain	Res	Type
1	B	2436	LEU
1	B	2441	SER
1	B	2450	LEU
1	B	2465	VAL
1	B	2469	GLN
1	B	2480	LEU
1	B	2554	LYS
1	B	2575	MSE
1	B	2649	LEU
1	B	2719	MSE
1	B	2738	ASN
1	B	2740	THR
1	B	2745	MSE
1	B	2764	ASP
1	B	2768	VAL
1	B	2784	LEU
1	B	2813	MSE
1	B	2855	THR
1	B	2857	ARG
1	B	2862	VAL
1	B	2868	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2448	ASN
1	A	2510	ASN
1	A	2716	ASN
1	B	2319	GLN
1	B	2736	GLN
1	B	2756	GLN
1	B	2760	GLN
1	B	2834	ASN

5.3.3 RNA

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 9 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
4	MES	B	2901	-	12,12,12	2.27	1 (8%)	14,16,16	2.06	5 (35%)
4	MES	A	2904	-	12,12,12	2.13	1 (8%)	14,16,16	1.54	3 (21%)
3	SO4	A	2903	-	4,4,4	0.38	0	6,6,6	0.13	0
5	FMT	A	2905	-	2,2,2	0.82	0	1,1,1	0.53	0
2	DIO	A	2902	-	6,6,6	0.56	0	6,6,6	0.74	0
2	DIO	A	2901	-	6,6,6	0.62	0	6,6,6	0.93	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
4	MES	A	2904	-	-	3/6/14/14	0/1/1/1
2	DIO	A	2902	-	-	-	0/1/1/1
4	MES	B	2901	-	-	1/6/14/14	0/1/1/1
2	DIO	A	2901	-	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2901	MES	C8-S	-7.37	1.67	1.77
4	A	2904	MES	C8-S	-6.98	1.67	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2901	MES	O3S-S-C8	4.28	112.69	105.77
4	B	2901	MES	O1S-S-C8	4.16	111.93	106.92
4	A	2904	MES	O2S-S-C8	2.79	110.28	106.92
4	A	2904	MES	O1S-S-C8	2.42	109.83	106.92
4	B	2901	MES	O3S-S-O1S	-2.39	105.43	111.27
4	A	2904	MES	O3S-S-C8	2.22	109.36	105.77
4	B	2901	MES	O1-C2-C3	-2.09	107.19	111.80
4	B	2901	MES	O2S-S-C8	-2.01	104.50	106.92

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2904	MES	C8-C7-N4-C5
4	A	2904	MES	C8-C7-N4-C3
4	A	2904	MES	N4-C7-C8-S
4	B	2901	MES	C8-C7-N4-C5

There are no ring outliers.

No monomer is involved in short contacts.

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	536/616 (87%)	0.41	45 (8%)	11	9	32, 69, 134, 188	0
1	B	542/616 (87%)	0.33	30 (5%)	25	24	38, 74, 127, 162	0
All	All	1078/1232 (87%)	0.37	75 (6%)	16	14	32, 71, 132, 188	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2687	ARG	5.4
1	B	2285	LEU	5.4
1	B	2286	LEU	5.3
1	A	2343	LEU	5.3
1	A	2678	LEU	5.2
1	A	2327	ILE	4.8
1	B	2331	PHE	4.7
1	A	2296	VAL	4.3
1	A	2333	ASN	4.2
1	A	2294	PHE	4.1
1	A	2747	VAL	4.1
1	A	2737	TRP	4.0
1	A	2287	VAL	3.8
1	A	2359	LEU	3.8
1	B	2609	GLY	3.8
1	A	2349	LEU	3.8
1	A	2311	LEU	3.6
1	A	2348	VAL	3.6
1	A	2293	GLY	3.4
1	B	2327	ILE	3.3
1	A	2341	LEU	3.2
1	B	2343	LEU	3.2
1	A	2738	ASN	3.2
1	B	2284	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	2391	VAL	3.0
1	A	2681	GLY	3.0
1	B	2495	LEU	3.0
1	A	2884	ALA	3.0
1	A	2714	LEU	2.9
1	A	2285	LEU	2.9
1	A	2657	PRO	2.9
1	B	2349	LEU	2.9
1	A	2710	ALA	2.8
1	A	2357	ARG	2.8
1	B	2309	ILE	2.7
1	B	2640	ALA	2.7
1	A	2312	ASP	2.6
1	B	2610	GLN	2.6
1	A	2885	LYS	2.6
1	B	2681	GLY	2.6
1	A	2358	ILE	2.5
1	A	2590	HIS	2.5
1	B	2335	GLU	2.5
1	A	2342	PHE	2.5
1	A	2637	PHE	2.5
1	A	2325	ARG	2.5
1	B	2311	LEU	2.5
1	B	2497	LEU	2.4
1	B	2607	LEU	2.4
1	A	2688	PHE	2.4
1	B	2510	ASN	2.4
1	A	2755	LEU	2.4
1	B	2332	ASP	2.3
1	B	2854	HIS	2.3
1	A	2347	LYS	2.3
1	A	2647	LEU	2.3
1	B	2474	HIS	2.3
1	B	2294	PHE	2.3
1	A	2638	ASN	2.3
1	A	2736	GLN	2.3
1	A	2677	GLY	2.2
1	B	2313	ASN	2.2
1	B	2507	GLY	2.2
1	B	2287	VAL	2.2
1	A	2319	GLN	2.2
1	A	2648	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2308	THR	2.2
1	B	2326	PHE	2.2
1	B	2646	ASP	2.1
1	B	2328	LEU	2.1
1	A	2746	ASP	2.1
1	A	2636	ILE	2.1
1	A	2332	ASP	2.1
1	A	2685	LEU	2.1
1	B	2298	SER	2.1

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
2	DIO	A	2901	6/6	0.85	0.19	104,108,115,117	0
4	MES	A	2904	12/12	0.91	0.27	106,126,136,138	0
3	SO4	A	2903	5/5	0.93	0.22	96,100,109,110	0
4	MES	B	2901	12/12	0.94	0.20	58,63,72,73	0
5	FMT	A	2905	3/3	0.95	0.15	54,54,60,62	0
6	CL	A	2906	1/1	0.95	0.13	92,92,92,92	0
6	CL	A	2907	1/1	0.95	0.23	63,63,63,63	0
2	DIO	A	2902	6/6	0.98	0.24	63,70,71,75	0
6	CL	B	2902	1/1	0.99	0.18	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.