



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:36 PM UTC

PDB ID : 5XN7 / pdb_00005xn7
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

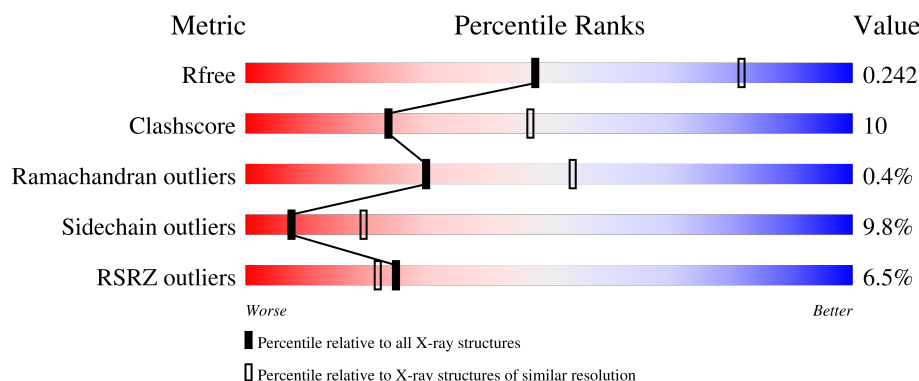
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	5% 65% 19% • • 12%
1	B	616	6% 69% 18% • 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.

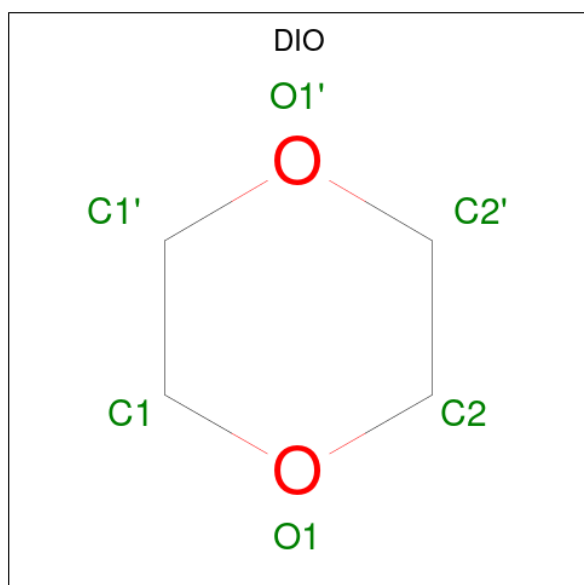
- Molecule 1 is a protein called Putative RTX-toxin.

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 (CCD ID: DIO) (formula: C₄H₈O₂).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



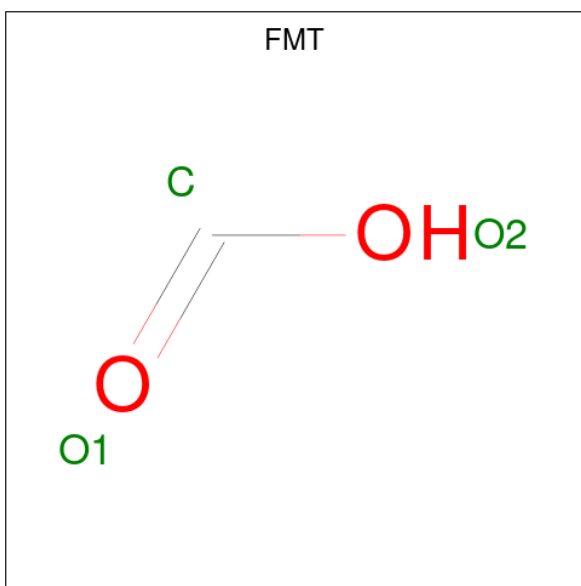
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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 (CCD ID: FMT) (formula: CH_2O_2).



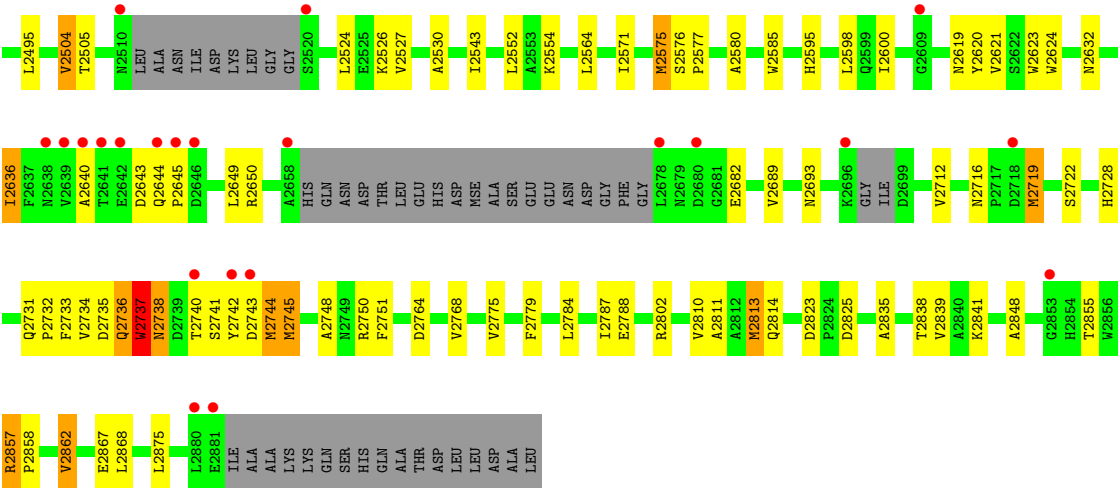
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is water.

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



4 Data and refinement statistics

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 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.70) 99.5 (50.00-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.203 , 0.244 (Not available) , 0.242	Depositor DCC
R_{free} test set	2554 reflections (5.07%)	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)	0.35 , 75.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: DIO, SO4, FMT, CL, MES

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	0.87	1/4161 (0.0%)	1.06	11/5619 (0.2%)
1	B	0.80	0/4205	1.03	14/5689 (0.2%)
All	All	0.84	1/8366 (0.0%)	1.04	25/11308 (0.2%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2442	GLY	C-O	-5.51	1.17	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2743	ASP	N-CA-C	15.42	133.70	111.96
1	A	2834	ASN	CB-CA-C	-10.94	94.50	109.71
1	B	2745	MSE	N-CA-C	10.54	127.21	112.04
1	A	2738	ASN	N-CA-C	10.34	122.63	111.36
1	B	2736	GLN	N-CA-C	9.27	122.55	111.33
1	B	2744	MSE	N-CA-C	-7.40	102.91	112.23
1	B	2744	MSE	N-CA-CB	6.95	121.00	110.30
1	A	2314	PRO	N-CA-CB	6.93	110.63	103.00
1	B	2645	PRO	N-CA-CB	6.91	109.75	103.33
1	B	2736	GLN	CB-CA-C	-6.73	99.23	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2734	VAL	N-CA-C	-6.45	104.04	110.62
1	A	2353	ASP	CB-CA-C	-6.27	109.33	116.54
1	B	2413	HIS	N-CA-C	6.26	117.69	108.86
1	B	2744	MSE	CB-CA-C	6.21	123.04	110.38
1	A	2834	ASN	N-CA-C	6.15	119.41	110.42
1	B	2743	ASP	CB-CA-C	-6.01	100.25	110.88
1	A	2657	PRO	N-CA-CB	5.65	109.19	103.25
1	A	2561	ILE	N-CA-C	5.47	116.25	110.72
1	B	2466	VAL	N-CA-C	5.47	115.67	110.53
1	A	2864	THR	N-CA-C	-5.37	102.02	108.25
1	A	2559	ILE	CB-CA-C	-5.35	102.51	111.29
1	B	2737	TRP	N-CA-CB	-5.23	101.65	110.49
1	B	2862	VAL	N-CA-C	5.10	115.25	108.11
1	A	2551	ASP	N-CA-C	-5.09	105.81	111.36
1	B	2465	VAL	CB-CA-C	-5.02	103.13	111.32

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 ⓘ

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	81	0
1	B	4143	0	3896	84	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8384	0	7857	164	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 (164) 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:2734:VAL:O	1:B:2735:ASP:C	2.45	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:2508:LYS:C	1:A:2510:ASN:H	2.12	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:2736:GLN:C	1:B:2738:ASN:N	2.63	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2736:GLN:C	1:B:2738:ASN:H	2.16	0.53
1:A:2775:VAL:O	1:A:2776:VAL:C	2.49	0.52
1:B:2848:ALA:HB1	1:B:2875:LEU:HD21	1.90	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
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:2352:HIS:O	1:A:2353:ASP:C	2.54	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:B:2835:ALA:O	1:B:2839:VAL:HG23	2.13	0.48
1:A:2657:PRO:O	1:A:2658:ALA:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2520:SER:HB2	1:B:2378:VAL:HG21	1.96	0.48
1:B:2823:ASP:OD1	1:B:2823:ASP:C	2.57	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: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
1:A:2507:GLY:C	1:A:2510:ASN:HB2	2.40	0.46
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2779:PHE:C	1:B:2779:PHE:CD2	2.96	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: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: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
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:B:2741:SER:O	1:B:2742:TYR:C	2.61	0.41
1:A:2722:SER:OG	1:A:2824:PRO:O	2.29	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: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:B:2736:GLN:O	1:B:2737:TRP:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2880:LEU:C	1:A:2882:ILE:H	2.29	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%)	30	54
1	B	537/616 (87%)	498 (93%)	37 (7%)	2 (0%)	30	54
All	All	1066/1232 (86%)	984 (92%)	78 (7%)	4 (0%)	30	54

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%)	371 (90%)	41 (10%)	7	19
1	B	412/496 (83%)	372 (90%)	40 (10%)	8	20
All	All	824/992 (83%)	743 (90%)	81 (10%)	7	19

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2287	VAL
1	A	2296	VAL
1	A	2311	LEU
1	A	2349	LEU
1	A	2352	HIS
1	A	2353	ASP
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	2543	ILE
1	A	2550	ASN
1	A	2559	ILE
1	A	2578	VAL
1	A	2588	SER
1	A	2631	SER
1	A	2647	LEU
1	A	2655	SER
1	A	2707	GLU
1	A	2722	SER
1	A	2725	ILE
1	A	2734	VAL
1	A	2737	TRP
1	A	2744	MSE
1	A	2755	LEU
1	A	2775	VAL

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Mol	Chain	Res	Type
1	A	2777	ARG
1	A	2785	GLU
1	A	2803	ILE
1	A	2825	ASP
1	A	2855	THR
1	A	2866	THR
1	A	2868	LEU
1	A	2882	ILE
1	B	2337	MSE
1	B	2339	ASP
1	B	2343	LEU
1	B	2353	ASP
1	B	2373	VAL
1	B	2379	THR
1	B	2382	LEU
1	B	2387	VAL
1	B	2410	THR
1	B	2413	HIS
1	B	2418	LEU
1	B	2419	THR
1	B	2420	SER
1	B	2427	LEU
1	B	2436	LEU
1	B	2441	SER
1	B	2450	LEU
1	B	2465	VAL
1	B	2466	VAL
1	B	2469	GLN
1	B	2480	LEU
1	B	2504	VAL
1	B	2526	LYS
1	B	2554	LYS
1	B	2575	MSE
1	B	2636	ILE
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

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Mol	Chain	Res	Type
1	B	2787	ILE
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2346	ASN
1	A	2510	ASN
1	A	2574	HIS
1	A	2606	GLN
1	A	2635	ASN
1	A	2716	ASN
1	A	2870	ASN
1	B	2319	GLN
1	B	2397	GLN
1	B	2426	ASN
1	B	2565	ASN
1	B	2569	GLN
1	B	2736	GLN
1	B	2873	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	2.33	1 (8%)	15,16,16	1.76	4 (26%)
5	FMT	A	2905	-	2,2,2	0.80	0	1,1,1	0.53	0
2	DIO	A	2902	-	6,6,6	0.56	0	6,6,6	0.76	0
4	MES	A	2904	-	12,12,12	2.18	1 (8%)	15,16,16	1.37	2 (13%)
2	DIO	A	2901	-	6,6,6	0.62	0	6,6,6	0.96	0
3	SO4	A	2903	-	4,4,4	0.47	0	6,6,6	0.13	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
2	DIO	A	2901	-	-	-	0/1/1/1
4	MES	A	2904	-	-	2/6/14/14	0/1/1/1
4	MES	B	2901	-	-	1/6/14/14	0/1/1/1
2	DIO	A	2902	-	-	-	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	-7.53	1.67	1.77
4	A	2904	MES	C8-S	-7.14	1.67	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2901	MES	O1S-S-C8	3.44	111.93	106.73
4	B	2901	MES	O3S-S-C8	3.42	112.69	106.00
4	B	2901	MES	O3S-S-O1S	-2.39	105.43	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2904	MES	O2S-S-C8	2.35	110.28	106.73
4	B	2901	MES	O1-C2-C3	-2.13	107.19	111.77
4	A	2904	MES	O1S-S-C8	2.05	109.83	106.73

There are no chirality outliers.

All (3) 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	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, 95th 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%)	0.22	30 (5%)	30 26	32, 69, 134, 188	0
1	B	542/616 (87%)	0.28	40 (7%)	20 18	38, 74, 127, 162	0
All	All	1078/1232 (87%)	0.25	70 (6%)	25 22	32, 71, 132, 188	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2299	TRP	5.6
1	A	2657	PRO	5.0
1	A	2298	SER	5.0
1	B	2331	PHE	4.7
1	A	2740	THR	4.7
1	B	2284	ASN	4.2
1	A	2660	GLN	4.2
1	B	2510	ASN	4.1
1	B	2318	ALA	3.9
1	B	2743	ASP	3.9
1	A	2328	LEU	3.9
1	A	2658	ALA	3.8
1	A	2677	GLY	3.8
1	B	2742	TYR	3.7
1	A	2333	ASN	3.7
1	A	2743	ASP	3.6
1	B	2317	ALA	3.6
1	B	2367	TRP	3.6
1	B	2678	LEU	3.4
1	A	2314	PRO	3.3
1	B	2520	SER	3.1
1	A	2739	ASP	3.1
1	A	2656	GLN	3.1
1	B	2474	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	2658	ALA	3.0
1	A	2310	LEU	3.0
1	A	2332	ASP	3.0
1	B	2646	ASP	3.0
1	A	2741	SER	3.0
1	B	2881	GLU	2.9
1	B	2638	ASN	2.9
1	A	2718	ASP	2.9
1	A	2590	HIS	2.9
1	A	2330	ASN	2.9
1	B	2316	ASP	2.8
1	B	2639	VAL	2.8
1	B	2644	GLN	2.8
1	A	2371	ALA	2.8
1	B	2285	LEU	2.7
1	B	2315	GLU	2.7
1	A	2659	HIS	2.7
1	A	2334	PHE	2.7
1	B	2853	GLY	2.6
1	B	2740	THR	2.6
1	A	2323	ILE	2.5
1	B	2309	ILE	2.5
1	B	2718	ASP	2.5
1	B	2295	GLU	2.5
1	A	2319	GLN	2.4
1	B	2609	GLY	2.4
1	B	2369	TYR	2.3
1	A	2362	LYS	2.3
1	A	2886	LYS	2.3
1	B	2289	GLU	2.3
1	B	2470	SER	2.3
1	B	2880	LEU	2.3
1	B	2641	THR	2.2
1	B	2645	PRO	2.2
1	A	2706	SER	2.2
1	B	2310	LEU	2.2
1	A	2309	ILE	2.2
1	A	2285	LEU	2.1
1	A	2776	VAL	2.1
1	B	2696	LYS	2.1
1	B	2680	ASP	2.1
1	B	2642	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2362	LYS	2.1
1	B	2640	ALA	2.1
1	A	2373	VAL	2.1
1	B	2314	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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
4	MES	A	2904	12/12	0.76	0.21	106,126,136,138	0
2	DIO	A	2901	6/6	0.77	0.24	104,108,115,117	0
3	SO4	A	2903	5/5	0.88	0.15	96,100,109,110	0
6	CL	A	2906	1/1	0.88	0.09	92,92,92,92	0
4	MES	B	2901	12/12	0.91	0.12	58,63,72,73	0
2	DIO	A	2902	6/6	0.94	0.12	63,70,71,75	0
5	FMT	A	2905	3/3	0.95	0.09	54,54,60,62	0
6	CL	A	2907	1/1	0.98	0.12	63,63,63,63	0
6	CL	B	2902	1/1	0.99	0.04	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.