



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:37 AM UTC

PDB ID : 3L0M / pdb_00003l0m
Title : Crystal structure of Rab1-activation domain and P4M domain of SidM/DrrA from legionella
Authors : Zhu, Y.; Shao, F.
Deposited on : 2009-12-10
Resolution : 3.45 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

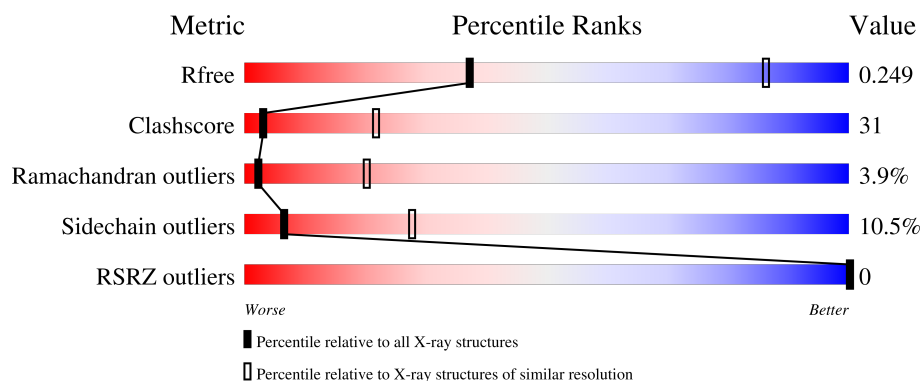
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

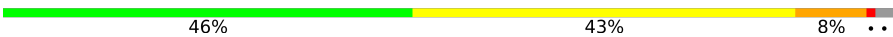
The reported resolution of this entry is 3.45 Å.

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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	336	
1	B	336	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5119 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 DrrA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	Se	0	0	0
			2578	1613	441	512	1	11			
1	B	323	Total	C	N	O	S	Se	0	0	0
			2531	1584	433	502	1	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	GLY	-	expression tag	UNP Q29ST3
A	313	PRO	-	expression tag	UNP Q29ST3
A	314	LEU	-	expression tag	UNP Q29ST3
A	315	GLY	-	expression tag	UNP Q29ST3
A	316	SER	-	expression tag	UNP Q29ST3
B	312	GLY	-	expression tag	UNP Q29ST3
B	313	PRO	-	expression tag	UNP Q29ST3
B	314	LEU	-	expression tag	UNP Q29ST3
B	315	GLY	-	expression tag	UNP Q29ST3
B	316	SER	-	expression tag	UNP Q29ST3

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	144.34Å 144.34Å 102.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.45 20.00 – 3.45	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-3.45) 98.8 (20.00-3.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 3.44Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.241 0.229 , 0.249	Depositor DCC
R_{free} test set	2728 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	127.1	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 165.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.117 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5119	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: 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	0.48	0/2603	1.04	12/3476 (0.3%)
1	B	0.45	0/2554	0.99	11/3410 (0.3%)
All	All	0.46	0/5157	1.02	23/6886 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	SER	N-CA-C	10.34	125.78	110.48
1	B	438	LYS	N-CA-C	8.79	120.63	111.14
1	A	639	GLN	N-CA-C	-8.56	102.60	112.87
1	A	314	LEU	N-CA-C	-8.47	102.96	113.38
1	A	638	SER	N-CA-C	-8.08	105.41	114.62
1	B	446	CYS	N-CA-C	-7.71	104.80	112.97
1	A	440	SER	N-CA-C	-6.91	102.97	111.40
1	A	428	VAL	N-CA-C	6.91	117.05	110.42
1	B	423	LEU	N-CA-C	-6.74	105.06	113.28
1	B	373	ASN	N-CA-C	-6.57	104.05	111.14
1	B	437	ASN	CB-CA-C	6.04	122.44	110.42
1	A	400	PRO	N-CA-C	-5.94	106.11	113.84
1	B	575	PHE	N-CA-C	-5.87	104.47	111.69
1	B	428	VAL	N-CA-C	5.57	115.81	110.74
1	A	513	GLU	N-CA-C	5.53	117.11	111.14
1	A	342	ARG	N-CA-C	-5.52	105.18	111.14
1	B	363	GLY	N-CA-C	5.46	126.13	113.18
1	A	363	GLY	N-CA-C	5.39	125.96	113.18
1	A	368	TYR	N-CA-C	-5.34	104.87	111.33
1	B	317	MSE	CA-C-N	5.32	125.31	120.21
1	B	317	MSE	C-N-CA	5.32	125.31	120.21
1	B	517	SER	N-CA-C	5.07	117.92	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	SER	N-CA-CB	-5.01	102.67	110.29

There are no chirality outliers.

There are no planarity outliers.

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	2578	0	2609	148	0
1	B	2531	0	2563	179	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
All	All	5119	0	5172	323	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 31.

All (323) 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:544:ARG:HD2	1:B:610:LEU:HG	1.31	1.10
1:A:526:LEU:HD13	1:A:530:LEU:HD11	1.49	0.93
1:A:539:GLU:HG3	1:A:540:GLY:H	1.35	0.91
1:B:468:LEU:HD13	1:B:519:LEU:HD21	1.56	0.86
1:B:604:LEU:HD22	1:B:621:SER:HB3	1.58	0.85
1:A:568:LYS:HD2	1:A:608:GLN:HE21	1.41	0.84
1:A:572:LEU:HG	1:A:628:MSE:HE1	1.60	0.84
1:A:468:LEU:HD13	1:A:519:LEU:HD21	1.60	0.83
1:B:399:SER:C	1:B:401:LYS:H	1.87	0.82
1:A:568:LYS:HD2	1:A:608:GLN:NE2	1.94	0.82
1:A:562:MSE:O	1:A:567:LEU:HD12	1.81	0.80
1:B:339:ARG:HG2	1:B:339:ARG:HH11	1.45	0.80
1:A:561:GLN:H	1:A:561:GLN:HE21	1.31	0.77
1:A:559:TYR:HA	1:A:562:MSE:HG3	1.66	0.76
1:B:339:ARG:HE	1:B:343:ILE:HD11	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ARG:HD2	1:A:610:LEU:HG	1.68	0.76
1:B:339:ARG:O	1:B:339:ARG:HD3	1.85	0.76
1:B:369:LEU:HD21	1:B:409:LEU:HD11	1.67	0.76
1:A:425:GLU:HG3	1:A:522:LYS:HZ2	1.50	0.76
1:A:587:SER:O	1:A:591:ILE:HG13	1.85	0.76
1:A:596:LYS:HD3	1:A:601:TYR:CE2	2.22	0.74
1:A:333:ARG:O	1:A:337:VAL:HG13	1.87	0.74
1:A:560:GLN:C	1:A:562:MSE:H	1.94	0.74
1:B:465:SER:O	1:B:469:VAL:HG23	1.85	0.74
1:A:526:LEU:CD1	1:A:530:LEU:HD11	2.18	0.74
1:A:429:GLU:HB2	1:A:485:ILE:HD13	1.70	0.73
1:A:604:LEU:O	1:A:619:THR:HG21	1.87	0.73
1:A:425:GLU:HG3	1:A:522:LYS:NZ	2.03	0.73
1:B:567:LEU:C	1:B:567:LEU:HD23	2.14	0.73
1:B:422:THR:HG22	1:B:423:LEU:H	1.53	0.73
1:A:539:GLU:HG3	1:A:540:GLY:N	2.03	0.72
1:B:369:LEU:HD13	1:B:439:MSE:HE3	1.71	0.72
1:A:547:ALA:HB3	1:A:564:GLY:HA2	1.72	0.72
1:B:439:MSE:HE1	1:B:474:PHE:CZ	2.25	0.70
1:B:439:MSE:HE1	1:B:474:PHE:CE2	2.27	0.69
1:B:544:ARG:HD2	1:B:610:LEU:CG	2.17	0.69
1:A:494:MSE:O	1:A:498:ILE:HG13	1.92	0.69
1:A:589:LYS:O	1:A:592:VAL:HG12	1.93	0.68
1:B:399:SER:C	1:B:401:LYS:N	2.51	0.68
1:B:409:LEU:O	1:B:409:LEU:HD23	1.94	0.68
1:B:315:GLY:O	1:B:316:SER:HB3	1.93	0.68
1:B:494:MSE:O	1:B:498:ILE:HG13	1.93	0.68
1:B:530:LEU:HD12	1:B:530:LEU:H	1.58	0.68
1:B:526:LEU:HD13	1:B:530:LEU:HD11	1.75	0.67
1:A:604:LEU:HD22	1:A:621:SER:HB3	1.78	0.66
1:A:426:SER:O	1:B:418:ARG:NH1	2.28	0.66
1:B:604:LEU:O	1:B:619:THR:HG21	1.95	0.66
1:A:416:TYR:CD1	1:A:519:LEU:HD22	2.31	0.66
1:B:544:ARG:HG2	1:B:545:TYR:CD2	2.29	0.66
1:B:557:GLU:O	1:B:560:GLN:HG2	1.97	0.65
1:B:339:ARG:NE	1:B:343:ILE:HD11	2.12	0.65
1:B:568:LYS:HD2	1:B:608:GLN:NE2	2.13	0.64
1:A:619:THR:HG23	1:A:622:VAL:H	1.61	0.64
1:B:336:GLY:O	1:B:340:VAL:HG23	1.98	0.64
1:B:325:MSE:O	1:B:329:VAL:HG23	1.97	0.64
1:B:571:ILE:HD12	1:B:603:ILE:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:GLU:CG	1:A:540:GLY:H	2.08	0.64
1:B:469:VAL:HG13	1:B:498:ILE:HG23	1.80	0.64
1:B:369:LEU:HD11	1:B:436:VAL:HG13	1.81	0.63
1:A:544:ARG:CD	1:A:610:LEU:HG	2.28	0.62
1:A:549:THR:HG21	1:A:560:GLN:HA	1.81	0.62
1:A:369:LEU:HD11	1:A:436:VAL:HG13	1.80	0.62
1:B:543:HIS:CD2	1:B:546:THR:H	2.18	0.62
1:A:560:GLN:HA	1:A:560:GLN:NE2	2.15	0.61
1:B:549:THR:HG21	1:B:560:GLN:HA	1.83	0.61
1:B:571:ILE:CD1	1:B:603:ILE:HG21	2.31	0.61
1:B:530:LEU:HD12	1:B:530:LEU:N	2.15	0.60
1:B:554:ASN:HB2	1:B:599:ASP:OD2	2.00	0.60
1:A:639:GLN:HE21	1:A:639:GLN:HA	1.66	0.60
1:B:568:LYS:HD2	1:B:608:GLN:HE21	1.67	0.60
1:B:339:ARG:HG2	1:B:339:ARG:NH1	2.10	0.60
1:B:357:ASN:OD1	1:B:398:ILE:HG23	2.02	0.59
1:A:507:SER:O	1:A:508:ASN:C	2.45	0.59
1:A:582:ALA:HB2	1:A:591:ILE:HD12	1.85	0.59
1:B:389:LEU:O	1:B:389:LEU:HG	2.03	0.58
1:A:550:GLU:C	1:A:552:PHE:H	2.11	0.58
1:B:544:ARG:HG2	1:B:545:TYR:CE2	2.39	0.58
1:B:525:ASN:OD1	1:B:528:GLU:HB3	2.03	0.58
1:B:613:GLN:C	1:B:615:LEU:H	2.10	0.58
1:B:406:LEU:HD23	1:B:444:MSE:SE	2.54	0.57
1:A:561:GLN:HE21	1:A:561:GLN:N	2.02	0.57
1:B:560:GLN:C	1:B:562:MSE:H	2.11	0.57
1:B:595:LEU:O	1:B:598:LYS:HB2	2.05	0.57
1:B:544:ARG:NH1	1:B:544:ARG:HB2	2.20	0.57
1:B:605:ALA:HA	1:B:619:THR:HG21	1.85	0.57
1:B:575:PHE:CD1	1:B:595:LEU:HD13	2.39	0.57
1:B:622:VAL:O	1:B:626:GLU:HG3	2.04	0.56
1:B:314:LEU:HD12	1:B:317:MSE:SE	2.55	0.56
1:B:349:ALA:HB3	1:B:389:LEU:HD13	1.87	0.56
1:B:543:HIS:CG	1:B:544:ARG:N	2.71	0.56
1:A:456:PRO:O	1:A:458:PRO:HD3	2.05	0.56
1:A:568:LYS:CE	1:A:604:LEU:HA	2.36	0.56
1:A:638:SER:C	1:A:640:GLU:N	2.63	0.56
1:A:560:GLN:HA	1:A:560:GLN:HE21	1.71	0.56
1:A:326:LEU:HD22	1:B:611:THR:HG23	1.89	0.55
1:A:514:THR:O	1:A:517:SER:HB3	2.07	0.55
1:A:521:SER:O	1:A:522:LYS:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ARG:HG2	1:A:545:TYR:CD2	2.42	0.55
1:A:638:SER:C	1:A:640:GLU:H	2.14	0.55
1:B:346:LEU:HD23	1:B:384:LEU:HD13	1.88	0.55
1:B:584:ASP:OD1	1:B:587:SER:HB2	2.06	0.55
1:A:561:GLN:H	1:A:561:GLN:NE2	2.02	0.55
1:B:447:LYS:HD3	1:B:447:LYS:C	2.32	0.55
1:B:489:ASN:HB2	1:B:577:ASP:OD2	2.06	0.55
1:B:562:MSE:HE2	1:B:562:MSE:HA	1.89	0.55
1:A:325:MSE:O	1:A:325:MSE:HG2	2.07	0.55
1:A:373:ASN:ND2	1:A:377:LYS:HE2	2.21	0.55
1:B:568:LYS:CE	1:B:604:LEU:HA	2.37	0.54
1:B:393:LEU:HD12	1:B:446:CYS:O	2.07	0.54
1:A:575:PHE:CE1	1:A:595:LEU:HD22	2.43	0.54
1:A:557:GLU:HG3	1:A:558:LYS:H	1.72	0.54
1:B:568:LYS:O	1:B:572:LEU:HB2	2.08	0.54
1:B:422:THR:HG22	1:B:423:LEU:N	2.23	0.54
1:A:568:LYS:O	1:A:572:LEU:HB2	2.08	0.53
1:A:600:GLU:HA	1:A:603:ILE:HD12	1.90	0.53
1:B:334:GLU:C	1:B:336:GLY:N	2.65	0.53
1:B:539:GLU:HG3	1:B:540:GLY:N	2.23	0.53
1:A:315:GLY:O	1:A:316:SER:HB3	2.08	0.53
1:B:557:GLU:HG3	1:B:558:LYS:H	1.73	0.53
1:B:334:GLU:C	1:B:336:GLY:H	2.16	0.53
1:B:454:ALA:O	1:B:456:PRO:HD3	2.09	0.53
1:B:436:VAL:O	1:B:437:ASN:C	2.50	0.53
1:B:365:ILE:HD11	1:B:405:ILE:CG2	2.39	0.53
1:B:416:TYR:CD1	1:B:416:TYR:O	2.63	0.52
1:A:322:ALA:O	1:A:326:LEU:HB2	2.09	0.52
1:A:410:TRP:HD1	1:A:437:ASN:HD21	1.58	0.51
1:B:504:LEU:CD1	1:B:514:THR:HB	2.41	0.51
1:A:429:GLU:HB3	1:A:430:PRO:HD3	1.91	0.51
1:A:571:ILE:HD13	1:A:600:GLU:HB2	1.92	0.51
1:B:410:TRP:CD1	1:B:437:ASN:OD1	2.63	0.51
1:A:515:LEU:C	1:A:517:SER:H	2.18	0.51
1:B:362:LYS:O	1:B:364:ASN:N	2.43	0.51
1:B:369:LEU:CD1	1:B:439:MSE:HE3	2.38	0.51
1:A:610:LEU:HD22	1:A:614:LEU:HD11	1.92	0.51
1:B:547:ALA:HB3	1:B:564:GLY:HA2	1.91	0.51
1:B:319:TYR:CE2	1:B:323:LYS:HD2	2.46	0.51
1:A:398:ILE:HB	1:A:403:TYR:CE2	2.45	0.51
1:A:442:PHE:CD1	1:A:442:PHE:C	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:LEU:C	1:B:567:LEU:CD2	2.83	0.51
1:B:465:SER:HB2	1:B:505:GLU:OE1	2.11	0.51
1:B:356:ALA:HB3	1:B:443:PHE:CE2	2.46	0.50
1:A:557:GLU:O	1:A:559:TYR:N	2.44	0.50
1:A:572:LEU:HG	1:A:628:MSE:CE	2.36	0.50
1:B:339:ARG:HD3	1:B:339:ARG:C	2.36	0.50
1:B:546:THR:CG2	1:B:547:ALA:N	2.74	0.50
1:A:515:LEU:C	1:A:517:SER:N	2.68	0.50
1:B:561:GLN:H	1:B:561:GLN:NE2	2.10	0.50
1:A:469:VAL:HG13	1:A:498:ILE:HG23	1.94	0.49
1:A:435:ALA:HB1	1:B:423:LEU:HG	1.93	0.49
1:B:486:TRP:CZ3	1:B:524:GLU:HA	2.46	0.49
1:B:539:GLU:HG3	1:B:540:GLY:H	1.77	0.49
1:A:613:GLN:C	1:A:615:LEU:H	2.21	0.49
1:B:314:LEU:O	1:B:315:GLY:O	2.31	0.49
1:B:429:GLU:HG3	1:B:485:ILE:HD13	1.94	0.49
1:A:434:SER:O	1:A:435:ALA:C	2.55	0.49
1:A:334:GLU:HG2	1:A:335:LEU:N	2.28	0.49
1:B:410:TRP:HD1	1:B:437:ASN:OD1	1.95	0.49
1:A:480:ASP:C	1:A:482:THR:H	2.21	0.48
1:A:601:TYR:C	1:A:601:TYR:CD1	2.90	0.48
1:A:550:GLU:OE2	1:A:551:ASN:HB2	2.13	0.48
1:A:480:ASP:OD2	1:A:481:PRO:N	2.47	0.48
1:A:521:SER:C	1:A:522:LYS:HD3	2.38	0.48
1:A:478:VAL:HG21	1:B:423:LEU:HD22	1.94	0.48
1:B:449:SER:HB2	1:B:450:PRO:HD2	1.96	0.48
1:B:605:ALA:HA	1:B:619:THR:CG2	2.43	0.48
1:B:371:ALA:O	1:B:374:GLU:HB2	2.13	0.48
1:B:480:ASP:C	1:B:482:THR:H	2.21	0.48
1:A:599:ASP:O	1:A:603:ILE:HG13	2.14	0.48
1:B:393:LEU:C	1:B:395:ASP:H	2.22	0.48
1:B:399:SER:O	1:B:401:LYS:N	2.46	0.48
1:B:596:LYS:HD3	1:B:601:TYR:CE2	2.48	0.48
1:A:600:GLU:HA	1:A:603:ILE:CD1	2.44	0.48
1:B:353:TRP:O	1:B:353:TRP:CE3	2.67	0.48
1:B:390:ARG:HB3	1:B:391:PRO:HD3	1.96	0.48
1:A:355:ASN:O	1:A:358:SER:HB3	2.13	0.48
1:A:552:PHE:CE2	1:A:602:ARG:NH1	2.82	0.47
1:A:567:LEU:O	1:A:567:LEU:HD23	2.13	0.47
1:B:561:GLN:H	1:B:561:GLN:HE21	1.61	0.47
1:B:564:GLY:O	1:B:567:LEU:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LYS:HE2	1:A:604:LEU:HA	1.96	0.47
1:B:575:PHE:O	1:B:579:LEU:HB2	2.14	0.47
1:A:526:LEU:O	1:A:527:SER:C	2.57	0.47
1:B:314:LEU:O	1:B:315:GLY:C	2.56	0.47
1:B:543:HIS:HD2	1:B:546:THR:H	1.59	0.47
1:A:489:ASN:OD1	1:A:491:LYS:HB2	2.15	0.47
1:B:515:LEU:C	1:B:517:SER:N	2.71	0.47
1:B:355:ASN:O	1:B:358:SER:HB3	2.14	0.47
1:A:349:ALA:HB2	1:A:378:PHE:HE2	1.79	0.46
1:A:575:PHE:CD1	1:A:595:LEU:HD13	2.51	0.46
1:B:567:LEU:HD21	1:B:571:ILE:CD1	2.45	0.46
1:A:416:TYR:CZ	1:A:472:MSE:HE3	2.50	0.46
1:A:326:LEU:C	1:A:329:VAL:HG12	2.40	0.46
1:B:560:GLN:HA	1:B:560:GLN:NE2	2.31	0.46
1:A:575:PHE:CZ	1:A:595:LEU:HD22	2.50	0.46
1:A:546:THR:CG2	1:A:547:ALA:N	2.79	0.46
1:A:339:ARG:O	1:A:343:ILE:HG13	2.16	0.46
1:B:507:SER:O	1:B:508:ASN:C	2.58	0.46
1:B:543:HIS:CD2	1:B:544:ARG:N	2.84	0.46
1:A:399:SER:C	1:A:401:LYS:N	2.74	0.45
1:A:413:ALA:O	1:A:417:SER:HB2	2.16	0.45
1:A:561:GLN:N	1:A:561:GLN:NE2	2.61	0.45
1:B:447:LYS:HD3	1:B:447:LYS:O	2.16	0.45
1:A:460:PHE:CE2	1:A:462:VAL:HG22	2.51	0.45
1:A:489:ASN:O	1:A:490:THR:C	2.60	0.45
1:B:350:LYS:HE2	1:B:392:GLU:O	2.17	0.45
1:A:486:TRP:CG	1:A:487:MSE:N	2.83	0.45
1:A:542:GLU:OE2	1:A:542:GLU:HA	2.16	0.45
1:B:448:LEU:HD13	1:B:449:SER:O	2.14	0.45
1:B:561:GLN:NE2	1:B:561:GLN:N	2.65	0.45
1:A:369:LEU:HD12	1:A:474:PHE:CD2	2.52	0.45
1:A:437:ASN:C	1:A:437:ASN:HD22	2.22	0.45
1:B:536:THR:O	1:B:566:ALA:HA	2.17	0.45
1:A:315:GLY:O	1:A:316:SER:CB	2.64	0.45
1:A:460:PHE:HE2	1:A:462:VAL:HG22	1.81	0.45
1:B:364:ASN:C	1:B:364:ASN:HD22	2.24	0.45
1:B:502:GLN:O	1:B:505:GLU:N	2.50	0.45
1:A:567:LEU:HD23	1:A:571:ILE:HG13	1.99	0.45
1:B:601:TYR:CD1	1:B:601:TYR:C	2.95	0.45
1:A:560:GLN:C	1:A:562:MSE:N	2.61	0.44
1:A:326:LEU:O	1:A:329:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:TRP:CG	1:A:487:MSE:H	2.35	0.44
1:A:489:ASN:OD1	1:A:489:ASN:C	2.61	0.44
1:A:594:GLU:O	1:A:598:LYS:HD2	2.17	0.44
1:A:634:GLU:C	1:A:636:ILE:H	2.25	0.44
1:B:468:LEU:CD1	1:B:519:LEU:HD21	2.37	0.44
1:B:575:PHE:HD1	1:B:625:PHE:CE1	2.36	0.44
1:B:416:TYR:CD1	1:B:519:LEU:HD22	2.52	0.44
1:B:515:LEU:O	1:B:517:SER:N	2.51	0.44
1:A:619:THR:CG2	1:A:622:VAL:HG23	2.47	0.44
1:B:362:LYS:O	1:B:362:LYS:HG3	2.17	0.44
1:B:514:THR:O	1:B:518:VAL:HG23	2.18	0.44
1:B:544:ARG:HB2	1:B:544:ARG:HH11	1.83	0.44
1:A:493:LEU:O	1:A:493:LEU:HG	2.17	0.44
1:B:498:ILE:O	1:B:499:ALA:C	2.61	0.44
1:B:393:LEU:C	1:B:395:ASP:N	2.75	0.43
1:B:360:LEU:HB2	1:B:368:TYR:CD1	2.53	0.43
1:B:364:ASN:C	1:B:364:ASN:ND2	2.74	0.43
1:B:487:MSE:C	1:B:488:HIS:CD2	2.96	0.43
1:B:550:GLU:C	1:B:550:GLU:CD	2.85	0.43
1:A:550:GLU:CD	1:A:551:ASN:N	2.76	0.43
1:B:349:ALA:CB	1:B:389:LEU:HD13	2.48	0.43
1:B:367:GLY:C	1:B:369:LEU:N	2.76	0.43
1:B:599:ASP:C	1:B:601:TYR:H	2.25	0.43
1:A:370:LYS:NZ	1:A:373:ASN:HD22	2.17	0.43
1:A:422:THR:HG22	1:A:423:LEU:N	2.33	0.43
1:B:346:LEU:CD2	1:B:384:LEU:HD13	2.48	0.43
1:B:489:ASN:OD1	1:B:491:LYS:HB2	2.17	0.43
1:A:525:ASN:O	1:A:526:LEU:C	2.62	0.43
1:A:530:LEU:N	1:A:530:LEU:HD12	2.33	0.43
1:B:416:TYR:OH	1:B:494:MSE:HE1	2.17	0.43
1:B:429:GLU:O	1:B:430:PRO:C	2.60	0.43
1:A:360:LEU:HD21	1:A:406:LEU:HD13	2.00	0.43
1:B:487:MSE:C	1:B:488:HIS:HD2	2.27	0.43
1:B:587:SER:O	1:B:591:ILE:HG13	2.18	0.43
1:B:539:GLU:CG	1:B:540:GLY:H	2.32	0.43
1:B:543:HIS:CG	1:B:546:THR:OG1	2.72	0.43
1:A:468:LEU:O	1:A:469:VAL:C	2.62	0.43
1:B:317:MSE:HE2	1:B:321:ASP:HB3	2.01	0.42
1:B:463:GLY:O	1:B:464:LYS:C	2.62	0.42
1:A:365:ILE:C	1:A:367:GLY:H	2.27	0.42
1:B:352:LEU:O	1:B:355:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:LEU:HD21	1:B:444:MSE:HB2	2.01	0.42
1:B:576:LYS:HD2	1:B:576:LYS:O	2.19	0.42
1:A:480:ASP:OD2	1:A:481:PRO:HD2	2.20	0.42
1:B:480:ASP:OD2	1:B:481:PRO:N	2.53	0.42
1:B:562:MSE:O	1:B:567:LEU:HD12	2.20	0.42
1:B:575:PHE:O	1:B:579:LEU:CB	2.68	0.42
1:A:341:THR:HA	1:A:344:GLU:HB2	2.02	0.42
1:A:349:ALA:HB2	1:A:378:PHE:CE2	2.54	0.42
1:B:539:GLU:CG	1:B:540:GLY:N	2.82	0.42
1:A:313:PRO:HB2	1:A:314:LEU:H	1.53	0.42
1:B:409:LEU:HD23	1:B:409:LEU:C	2.44	0.42
1:A:543:HIS:CG	1:A:544:ARG:N	2.86	0.42
1:B:571:ILE:HG21	1:B:600:GLU:O	2.20	0.42
1:B:386:GLU:HG3	1:B:442:PHE:CE2	2.55	0.42
1:B:436:VAL:HA	1:B:439:MSE:HE2	2.01	0.42
1:A:530:LEU:O	1:A:531:SER:HB2	2.20	0.41
1:B:355:ASN:HD22	1:B:355:ASN:HA	1.62	0.41
1:B:546:THR:HG23	1:B:564:GLY:CA	2.50	0.41
1:A:550:GLU:C	1:A:552:PHE:N	2.77	0.41
1:A:572:LEU:HD12	1:A:572:LEU:HA	1.88	0.41
1:A:338:GLN:C	1:A:340:VAL:N	2.77	0.41
1:A:436:VAL:O	1:A:437:ASN:C	2.63	0.41
1:B:326:LEU:O	1:B:329:VAL:HB	2.20	0.41
1:B:560:GLN:C	1:B:562:MSE:N	2.79	0.41
1:A:567:LEU:HD21	1:A:571:ILE:HD11	2.02	0.41
1:A:609:GLY:O	1:A:610:LEU:C	2.63	0.41
1:A:630:GLU:OE2	1:A:630:GLU:HA	2.20	0.41
1:B:484:LYS:HB3	1:B:484:LYS:HE2	1.86	0.41
1:B:557:GLU:O	1:B:559:TYR:N	2.53	0.41
1:A:389:LEU:HD23	1:A:446:CYS:HB3	2.02	0.41
1:B:445:ASP:C	1:B:447:LYS:H	2.29	0.41
1:B:370:LYS:HA	1:B:370:LYS:HD2	1.93	0.41
1:B:486:TRP:HZ3	1:B:524:GLU:HA	1.85	0.41
1:A:568:LYS:HE2	1:A:604:LEU:HD23	2.03	0.41
1:A:619:THR:OG1	2:A:1:SO4:S	2.79	0.41
1:A:620:SER:O	1:A:623:SER:HB3	2.20	0.41
1:B:544:ARG:O	1:B:544:ARG:HG3	2.21	0.41
1:B:560:GLN:HB2	1:B:561:GLN:NE2	2.36	0.41
1:B:564:GLY:O	1:B:565:ASP:C	2.64	0.41
1:A:359:MSE:HB2	1:A:368:TYR:HA	2.03	0.41
1:B:389:LEU:HD23	1:B:446:CYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:THR:HG21	1:B:560:GLN:CA	2.50	0.41
1:B:613:GLN:C	1:B:615:LEU:N	2.78	0.41
1:A:314:LEU:O	1:A:315:GLY:C	2.62	0.40
1:A:427:THR:OG1	1:A:428:VAL:N	2.54	0.40
1:B:365:ILE:C	1:B:367:GLY:H	2.27	0.40
1:B:472:MSE:O	1:B:473:GLN:C	2.64	0.40
1:B:603:ILE:HG22	1:B:604:LEU:N	2.36	0.40
1:A:468:LEU:HD23	1:A:468:LEU:HA	1.93	0.40
1:A:592:VAL:HG13	1:A:593:ALA:N	2.36	0.40
1:B:365:ILE:HD11	1:B:405:ILE:HG23	2.04	0.40
1:B:592:VAL:O	1:B:596:LYS:HG2	2.21	0.40
1:A:319:TYR:CZ	1:A:323:LYS:HE2	2.56	0.40
1:A:425:GLU:HG3	1:A:425:GLU:O	2.19	0.40
1:A:438:LYS:HE2	1:A:438:LYS:HB3	1.89	0.40
1:A:454:ALA:O	1:A:456:PRO:HD3	2.22	0.40
1:A:546:THR:HG23	1:A:564:GLY:HA3	2.02	0.40
1:A:554:ASN:HB2	1:A:599:ASP:OD2	2.21	0.40
1:B:422:THR:O	1:B:426:SER:HB3	2.21	0.40
1:A:437:ASN:C	1:A:437:ASN:ND2	2.78	0.40
1:B:365:ILE:C	1:B:367:GLY:N	2.79	0.40
1:B:369:LEU:HD11	1:B:436:VAL:CG1	2.50	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 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	326/336 (97%)	272 (83%)	42 (13%)	12 (4%)	2	21
1	B	319/336 (95%)	263 (82%)	43 (14%)	13 (4%)	2	19
All	All	645/672 (96%)	535 (83%)	85 (13%)	25 (4%)	2	20

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	GLY
1	A	544	ARG
1	A	550	GLU
1	A	557	GLU
1	A	558	LYS
1	B	363	GLY
1	B	544	ARG
1	B	557	GLU
1	B	558	LYS
1	A	315	GLY
1	A	508	ASN
1	B	315	GLY
1	B	533	LYS
1	B	565	ASP
1	B	508	ASN
1	B	543	HIS
1	A	533	LYS
1	B	542	GLU
1	A	543	HIS
1	A	610	LEU
1	B	486	TRP
1	B	516	GLU
1	A	556	LYS
1	B	607	GLY
1	A	318	PRO

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 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	284/281 (101%)	256 (90%)	28 (10%)	7	30
1	B	278/281 (99%)	247 (89%)	31 (11%)	6	26
All	All	562/562 (100%)	503 (90%)	59 (10%)	6	28

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	325	MSE
1	A	326	LEU
1	A	331	LYS
1	A	334	GLU
1	A	337	VAL
1	A	342	ARG
1	A	369	LEU
1	A	383	ASN
1	A	397	THR
1	A	406	LEU
1	A	425	GLU
1	A	462	VAL
1	A	467	ILE
1	A	482	THR
1	A	516	GLU
1	A	524	GLU
1	A	537	LYS
1	A	546	THR
1	A	550	GLU
1	A	561	GLN
1	A	563	ARG
1	A	565	ASP
1	A	576	LYS
1	A	583	THR
1	A	598	LYS
1	A	600	GLU
1	A	611	THR
1	A	639	GLN
1	B	337	VAL
1	B	339	ARG
1	B	369	LEU
1	B	398	ILE
1	B	406	LEU
1	B	422	THR
1	B	425	GLU
1	B	427	THR
1	B	447	LYS
1	B	448	LEU
1	B	462	VAL
1	B	495	ASN
1	B	501	ILE
1	B	504	LEU
1	B	514	THR

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Mol	Chain	Res	Type
1	B	516	GLU
1	B	524	GLU
1	B	526	LEU
1	B	537	LYS
1	B	546	THR
1	B	561	GLN
1	B	562	MSE
1	B	563	ARG
1	B	565	ASP
1	B	567	LEU
1	B	583	THR
1	B	600	GLU
1	B	603	ILE
1	B	608	GLN
1	B	611	THR
1	B	612	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	ASN
1	A	364	ASN
1	A	373	ASN
1	A	437	ASN
1	A	502	GLN
1	A	509	ASN
1	A	525	ASN
1	A	543	HIS
1	A	551	ASN
1	A	560	GLN
1	A	561	GLN
1	A	608	GLN
1	A	613	GLN
1	A	639	GLN
1	B	345	ASN
1	B	355	ASN
1	B	364	ASN
1	B	373	ASN
1	B	509	ASN
1	B	543	HIS
1	B	560	GLN
1	B	561	GLN

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Mol	Chain	Res	Type
1	B	608	GLN
1	B	613	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 ⓘ

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	B	2	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	A	1	-	4,4,4	0.33	0	6,6,6	0.19	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	SO4	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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($\text{\AA}^2$)	Q<0.9
1	A	317/336 (94%)	-1.02	0 100 100	69, 134, 189, 200	0
1	B	312/336 (92%)	-0.90	0 100 100	75, 151, 197, 200	0
All	All	629/672 (93%)	-0.96	0 100 100	69, 142, 193, 200	0

There are no RSRZ outliers to report.

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($\text{\AA}^2$)	Q<0.9
2	SO4	B	2	5/5	0.99	0.06	193,195,197,202	0
2	SO4	A	1	5/5	1.00	0.06	146,146,147,150	0

6.5 Other polymers [i](#)

There are no such residues in this entry.