



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:16 PM GMT

PDB ID : 1S3R
Title : Crystal structure of the human-specific toxin intermedilysin
Authors : Polekhina, G.; Giddings, K.S.; Tweten, R.K.; Parker, M.W.
Deposited on : 2004-01-14
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

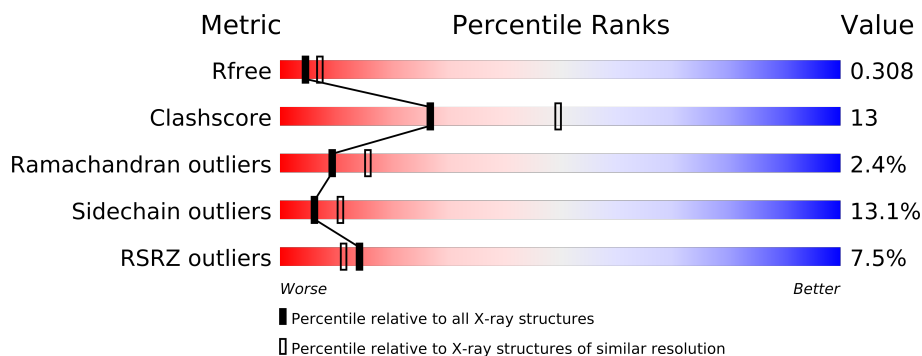
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	535	
1	B	535	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7827 atoms, of which 0 are hydrogen and 0 are deuterium.

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 intermedilysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3678	2321	644	710	3			
1	B	473	Total	C	N	O	S	0	0	0
			3678	2321	644	710	3			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP Q9LCB8
A	-1	GLY	-	EXPRESSION TAG	UNP Q9LCB8
A	0	GLY	-	EXPRESSION TAG	UNP Q9LCB8
A	1	SER	-	EXPRESSION TAG	UNP Q9LCB8
A	2	HIS	-	EXPRESSION TAG	UNP Q9LCB8
A	3	HIS	-	EXPRESSION TAG	UNP Q9LCB8
A	4	HIS	-	EXPRESSION TAG	UNP Q9LCB8
A	5	HIS	-	EXPRESSION TAG	UNP Q9LCB8
A	6	HIS	-	EXPRESSION TAG	UNP Q9LCB8
A	7	HIS	-	EXPRESSION TAG	UNP Q9LCB8
A	8	GLY	-	EXPRESSION TAG	UNP Q9LCB8
A	9	MET	-	EXPRESSION TAG	UNP Q9LCB8
A	10	ALA	-	EXPRESSION TAG	UNP Q9LCB8
A	11	SER	-	EXPRESSION TAG	UNP Q9LCB8
A	12	MET	-	EXPRESSION TAG	UNP Q9LCB8
A	13	THR	-	EXPRESSION TAG	UNP Q9LCB8
A	14	GLY	-	EXPRESSION TAG	UNP Q9LCB8
A	15	GLY	-	EXPRESSION TAG	UNP Q9LCB8
A	16	GLN	-	EXPRESSION TAG	UNP Q9LCB8
A	17	GLN	-	EXPRESSION TAG	UNP Q9LCB8
A	18	MET	-	EXPRESSION TAG	UNP Q9LCB8
A	19	GLY	-	EXPRESSION TAG	UNP Q9LCB8
A	20	ARG	-	EXPRESSION TAG	UNP Q9LCB8
A	21	ASP	-	EXPRESSION TAG	UNP Q9LCB8
A	22	LEU	-	EXPRESSION TAG	UNP Q9LCB8

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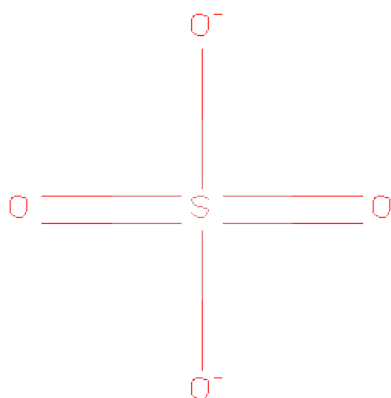
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	TYR	-	EXPRESSION TAG	UNP Q9LCB8
A	24	ASP	-	EXPRESSION TAG	UNP Q9LCB8
A	25	ASP	-	EXPRESSION TAG	UNP Q9LCB8
A	26	ASP	-	EXPRESSION TAG	UNP Q9LCB8
A	27	ASP	-	EXPRESSION TAG	UNP Q9LCB8
A	28	LYS	-	EXPRESSION TAG	UNP Q9LCB8
A	29	ASP	-	EXPRESSION TAG	UNP Q9LCB8
A	30	ARG	-	EXPRESSION TAG	UNP Q9LCB8
A	31	TRP	-	EXPRESSION TAG	UNP Q9LCB8
A	32	GLY	-	EXPRESSION TAG	UNP Q9LCB8
A	33	SER	-	EXPRESSION TAG	UNP Q9LCB8
B	-2	MET	-	EXPRESSION TAG	UNP Q9LCB8
B	-1	GLY	-	EXPRESSION TAG	UNP Q9LCB8
B	0	GLY	-	EXPRESSION TAG	UNP Q9LCB8
B	1	SER	-	EXPRESSION TAG	UNP Q9LCB8
B	2	HIS	-	EXPRESSION TAG	UNP Q9LCB8
B	3	HIS	-	EXPRESSION TAG	UNP Q9LCB8
B	4	HIS	-	EXPRESSION TAG	UNP Q9LCB8
B	5	HIS	-	EXPRESSION TAG	UNP Q9LCB8
B	6	HIS	-	EXPRESSION TAG	UNP Q9LCB8
B	7	HIS	-	EXPRESSION TAG	UNP Q9LCB8
B	8	GLY	-	EXPRESSION TAG	UNP Q9LCB8
B	9	MET	-	EXPRESSION TAG	UNP Q9LCB8
B	10	ALA	-	EXPRESSION TAG	UNP Q9LCB8
B	11	SER	-	EXPRESSION TAG	UNP Q9LCB8
B	12	MET	-	EXPRESSION TAG	UNP Q9LCB8
B	13	THR	-	EXPRESSION TAG	UNP Q9LCB8
B	14	GLY	-	EXPRESSION TAG	UNP Q9LCB8
B	15	GLY	-	EXPRESSION TAG	UNP Q9LCB8
B	16	GLN	-	EXPRESSION TAG	UNP Q9LCB8
B	17	GLN	-	EXPRESSION TAG	UNP Q9LCB8
B	18	MET	-	EXPRESSION TAG	UNP Q9LCB8
B	19	GLY	-	EXPRESSION TAG	UNP Q9LCB8
B	20	ARG	-	EXPRESSION TAG	UNP Q9LCB8
B	21	ASP	-	EXPRESSION TAG	UNP Q9LCB8
B	22	LEU	-	EXPRESSION TAG	UNP Q9LCB8
B	23	TYR	-	EXPRESSION TAG	UNP Q9LCB8
B	24	ASP	-	EXPRESSION TAG	UNP Q9LCB8
B	25	ASP	-	EXPRESSION TAG	UNP Q9LCB8
B	26	ASP	-	EXPRESSION TAG	UNP Q9LCB8
B	27	ASP	-	EXPRESSION TAG	UNP Q9LCB8
B	28	LYS	-	EXPRESSION TAG	UNP Q9LCB8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	ASP	-	EXPRESSION TAG	UNP Q9LCB8
B	30	ARG	-	EXPRESSION TAG	UNP Q9LCB8
B	31	TRP	-	EXPRESSION TAG	UNP Q9LCB8
B	32	GLY	-	EXPRESSION TAG	UNP Q9LCB8
B	33	SER	-	EXPRESSION TAG	UNP Q9LCB8

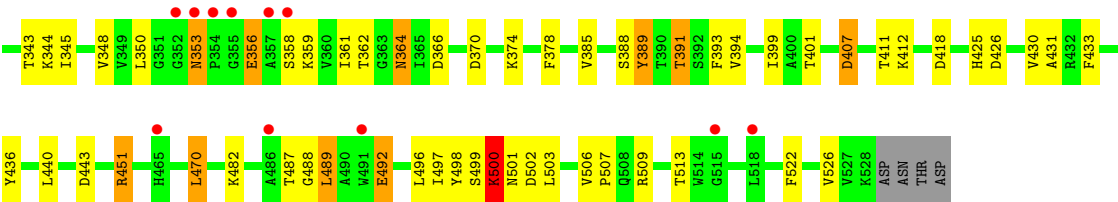
- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	205	Total	O	0	0
			205	205		
3	B	246	Total	O	0	0
			246	246		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.45Å 173.64Å 105.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.97 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.60) 99.8 (29.97-2.59)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.229 , 0.295 0.242 , 0.308	Depositor DCC
R_{free} test set	2598 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.837	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 18.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 50996 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7827	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.71	0/3755	0.83	10/5097 (0.2%)
1	B	0.93	6/3755 (0.2%)	0.92	11/5097 (0.2%)
All	All	0.83	6/7510 (0.1%)	0.88	21/10194 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	PRO	CG-CD	8.21	1.77	1.50
1	B	391	THR	CB-CG2	7.71	1.77	1.52
1	B	178	ASN	CG-ND2	7.02	1.50	1.32
1	B	389	TYR	CE1-CZ	-6.95	1.29	1.38
1	B	298	VAL	CB-CG1	5.93	1.65	1.52
1	B	127	ARG	CB-CG	5.18	1.66	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	226	ASP	CB-CG-OD2	7.17	124.76	118.30
1	A	502	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	418	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	370	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	418	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	445	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	280	ASP	CB-CG-OD2	5.76	123.49	118.30
1	B	443	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	370	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	254	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	A	263	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	524	ASP	CB-CG-OD2	5.47	123.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	130	PRO	N-CD-CG	-5.40	95.10	103.20
1	B	407	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	152	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	426	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	366	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	237	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	280	ASP	CB-CG-OD2	5.08	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3678	0	3670	94	0
1	B	3678	0	3670	100	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	205	0	0	24	1
3	B	246	0	0	31	0
All	All	7827	0	7340	193	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (193) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:391:THR:CG2	1:B:391:THR:CB	1.77	1.55
1:B:130:PRO:CG	1:B:130:PRO:CD	1.77	1.42
1:B:152:ARG:HD3	3:B:1168:HOH:O	1.51	1.09
1:B:82:GLN:HG2	3:B:1221:HOH:O	1.61	0.97
1:B:138:GLN:HG2	3:B:1250:HOH:O	1.70	0.92
1:A:214:GLN:H	1:A:218:GLN:HE21	1.23	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:322:ASP:O	1:A:326:LYS:HG2	1.77	0.84
1:B:178:ASN:O	1:B:182:ARG:HG3	1.78	0.83
1:A:119:SER:HB3	1:A:254:ARG:HH21	1.44	0.83
1:A:170:ASN:HB3	3:A:1140:HOH:O	1.81	0.81
1:B:487:THR:O	1:B:489:LEU:N	2.15	0.78
1:B:78:ILE:HA	3:B:1055:HOH:O	1.83	0.77
3:A:1166:HOH:O	1:B:451:ARG:HD3	1.85	0.76
1:B:391:THR:CA	1:B:391:THR:CG2	2.66	0.73
1:A:252:ASN:ND2	1:A:305:TYR:CE2	2.55	0.73
1:A:146:THR:HB	3:A:1186:HOH:O	1.88	0.72
1:B:277:THR:HG22	1:B:279:THR:H	1.57	0.70
1:B:506:VAL:HG11	1:B:526:VAL:HG13	1.75	0.68
1:A:252:ASN:ND2	1:A:305:TYR:CZ	2.62	0.68
1:A:214:GLN:N	1:A:218:GLN:HE21	1.91	0.67
1:A:65:ASN:OD1	1:A:267:SER:HB2	1.95	0.67
1:A:404:ASN:HB3	3:A:1061:HOH:O	1.94	0.66
1:B:65:ASN:OD1	1:B:267:SER:HB2	1.95	0.66
1:A:280:ASP:O	1:A:284:ARG:HD3	1.95	0.65
1:B:232:ALA:HB3	1:B:233:PRO:HD3	1.79	0.65
1:B:482:LYS:HE2	3:B:1192:HOH:O	1.97	0.65
1:A:119:SER:HB3	1:A:254:ARG:NH2	2.11	0.64
1:B:263:ASP:HA	3:B:1125:HOH:O	1.97	0.64
1:A:277:THR:HG22	1:A:279:THR:H	1.61	0.64
1:B:129:PHE:CD1	1:B:178:ASN:HA	2.33	0.63
1:A:506:VAL:HG11	1:A:526:VAL:HG13	1.80	0.62
1:A:342:ASN:C	1:A:342:ASN:HD22	2.03	0.62
1:A:302:ARG:NH1	3:A:1037:HOH:O	2.30	0.61
1:A:264:SER:HB3	3:A:1090:HOH:O	2.00	0.61
1:B:364:ASN:HD22	1:B:364:ASN:H	1.48	0.61
1:A:216:MET:O	1:A:220:GLN:HG3	2.01	0.59
1:A:278:PRO:O	1:A:282:ILE:HG12	2.03	0.58
1:B:84:GLU:HG3	3:B:1124:HOH:O	2.03	0.58
1:A:308:PHE:CD2	1:A:345:ILE:HD11	2.38	0.58
1:A:193:ILE:HA	1:A:197:SER:HB3	1.86	0.58
1:B:278:PRO:O	1:B:282:ILE:HG12	2.04	0.57
1:B:129:PHE:CD1	3:B:1074:HOH:O	2.58	0.57
1:B:280:ASP:O	1:B:284:ARG:HD3	2.06	0.56
1:A:181:VAL:O	1:A:185:VAL:HG23	2.06	0.56
1:B:124:ASN:O	1:B:125:ASP:C	2.42	0.56
1:B:122:SER:N	3:B:1153:HOH:O	2.39	0.56
1:B:193:ILE:HA	1:B:197:SER:HB3	1.88	0.56
1:B:271:LEU:HD12	1:B:394:VAL:HG13	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:125:ASP:O	1:B:182:ARG:NH2	2.39	0.55
1:B:358:SER:HB3	3:B:1161:HOH:O	2.07	0.55
1:B:77:ASN:HB3	3:B:1011:HOH:O	2.05	0.55
1:A:361:ILE:HG21	1:A:371:LEU:HD11	1.89	0.54
1:A:82:GLN:HB2	3:A:1059:HOH:O	2.08	0.53
1:B:96:HIS:HD1	1:B:101:TYR:HD1	1.57	0.53
1:A:331:LYS:HD2	1:A:335:GLU:OE2	2.07	0.53
1:B:178:ASN:O	1:B:182:ARG:CG	2.51	0.53
1:A:56:ASN:N	3:A:1033:HOH:O	2.41	0.52
1:B:74:ASP:O	1:B:78:ILE:HG22	2.10	0.52
1:B:329:LYS:HB2	3:B:1173:HOH:O	2.09	0.52
1:B:501:ASN:N	1:B:501:ASN:HD22	2.07	0.52
1:B:207:GLN:HE22	1:B:254:ARG:HH11	1.57	0.52
1:B:316:LYS:HD2	1:B:335:GLU:OE2	2.10	0.52
1:B:119:SER:HB3	1:B:254:ARG:HH21	1.74	0.51
1:B:195:ASN:ND2	3:B:1156:HOH:O	2.29	0.51
1:B:496:LEU:HD23	1:B:497:ILE:N	2.25	0.51
1:B:124:ASN:O	1:B:126:ASP:N	2.44	0.51
1:A:304:MET:HE2	1:A:349:VAL:HG12	1.92	0.51
1:A:57:SER:HA	3:A:1138:HOH:O	2.10	0.50
1:B:425:HIS:CD2	1:B:431:ALA:HB3	2.46	0.50
1:B:110:SER:HB3	1:B:407:ASP:OD1	2.11	0.50
1:B:97:ARG:O	1:B:98:PRO:C	2.50	0.50
1:A:207:GLN:HB3	1:A:254:ARG:HB2	1.92	0.50
1:A:329:LYS:HG3	1:A:330:LEU:H	1.76	0.50
1:B:498:TYR:CD1	1:B:522:PHE:CE1	3.00	0.50
1:B:293:VAL:HG12	1:B:393:PHE:HA	1.94	0.49
1:B:129:PHE:CE1	3:B:1074:HOH:O	2.55	0.49
1:B:470:LEU:N	1:B:470:LEU:HD23	2.28	0.49
1:A:334:THR:HG22	1:A:334:THR:O	2.13	0.49
1:A:253:PHE:HB2	1:A:304:MET:HG2	1.94	0.49
1:B:262:VAL:HG13	1:B:296:SER:HA	1.95	0.48
1:B:273:GLY:O	1:B:276:ILE:HG12	2.13	0.48
1:B:330:LEU:HD23	3:B:1202:HOH:O	2.14	0.48
1:A:74:ASP:CG	1:A:77:ASN:HB2	2.34	0.48
1:B:302:ARG:HD3	3:B:1017:HOH:O	2.14	0.48
1:B:129:PHE:CD2	1:B:178:ASN:HB2	2.49	0.48
1:B:451:ARG:HG2	3:B:1031:HOH:O	2.12	0.48
1:A:262:VAL:HG13	1:A:296:SER:HA	1.96	0.48
1:A:359:LYS:HA	3:A:1089:HOH:O	2.13	0.48
1:B:79:LEU:C	1:B:141:LEU:HD21	2.35	0.47
1:A:364:ASN:HB2	3:A:1121:HOH:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:LYS:HE2	3:B:1247:HOH:O	2.13	0.47
1:A:324:VAL:HG21	1:A:365:ILE:HD11	1.97	0.47
1:A:349:VAL:O	1:A:356:GLU:HG2	2.15	0.47
1:A:334:THR:C	1:A:335:GLU:HG3	2.33	0.47
1:B:175:ASN:O	1:B:176:PRO:C	2.52	0.47
1:B:499:SER:O	1:B:500:LYS:HB2	2.15	0.47
1:A:503:LEU:HD22	1:A:509:ARG:CZ	2.45	0.47
1:A:249:PHE:HB2	1:A:308:PHE:HB2	1.96	0.47
1:A:87:LYS:HE3	1:B:92:ARG:NH1	2.30	0.46
1:A:507:PRO:HG2	1:A:528:LYS:HG2	1.95	0.46
1:B:297:ASN:HB3	3:B:1218:HOH:O	2.14	0.46
1:A:451:ARG:HD3	3:B:1124:HOH:O	2.15	0.46
1:B:175:ASN:HB3	3:B:1205:HOH:O	2.15	0.46
1:A:353:ASN:O	1:A:356:GLU:OE1	2.34	0.46
1:B:482:LYS:HE3	3:B:1056:HOH:O	2.16	0.45
1:A:359:LYS:HB3	3:A:1074:HOH:O	2.16	0.45
1:B:116:SER:O	1:B:118:LEU:HG	2.16	0.45
1:A:478:ASN:HA	3:A:1054:HOH:O	2.16	0.45
1:B:356:GLU:O	1:B:359:LYS:O	2.34	0.45
1:A:281:LEU:HB3	1:A:286:VAL:HB	1.98	0.45
1:B:129:PHE:CG	1:B:178:ASN:HA	2.52	0.45
1:B:364:ASN:N	1:B:364:ASN:HD22	2.12	0.45
1:A:206:MET:HE1	1:A:255:GLN:HG3	1.98	0.45
1:A:425:HIS:HB3	1:A:466:TYR:HB3	1.99	0.45
1:A:342:ASN:O	1:A:342:ASN:ND2	2.49	0.45
1:A:79:LEU:C	1:A:141:LEU:HD21	2.37	0.45
1:B:216:MET:O	1:B:220:GLN:HG3	2.17	0.45
1:A:310:THR:HG22	1:A:342:ASN:HD21	1.82	0.45
1:A:139:SER:HB3	1:A:144:LEU:O	2.17	0.45
1:B:165:LYS:O	1:B:166:ASN:HB2	2.17	0.45
1:A:326:LYS:O	1:A:326:LYS:HG3	2.16	0.44
1:A:156:THR:HG23	3:A:1140:HOH:O	2.16	0.44
1:A:331:LYS:HA	3:A:1157:HOH:O	2.18	0.44
1:A:491:TRP:O	1:A:492:GLU:CB	2.66	0.44
1:A:240:SER:HA	3:A:1144:HOH:O	2.18	0.44
1:B:185:VAL:O	1:B:189:VAL:HG23	2.18	0.44
1:A:451:ARG:HG2	3:A:1118:HOH:O	2.17	0.44
1:A:58:GLU:HG3	3:A:1194:HOH:O	2.17	0.44
1:B:120:VAL:HG23	1:B:388:SER:N	2.33	0.44
1:B:489:LEU:HD12	1:B:492:GLU:O	2.17	0.44
1:A:175:ASN:O	1:A:176:PRO:C	2.56	0.44
1:B:128:ILE:HD12	1:B:389:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:326:LYS:O	1:B:326:LYS:HG2	2.18	0.44
1:A:421:LEU:HD11	1:A:511:ILE:HD12	1.99	0.44
1:B:389:TYR:CD2	1:B:389:TYR:N	2.84	0.43
1:A:94:ALA:HA	1:A:102:VAL:O	2.17	0.43
1:B:336:TYR:O	1:B:337:GLU:C	2.57	0.43
1:A:166:ASN:N	1:A:166:ASN:HD22	2.14	0.43
1:A:155:THR:HG22	1:A:157:ILE:HG13	2.00	0.43
1:A:84:GLU:HG3	3:A:1170:HOH:O	2.17	0.43
1:A:124:ASN:OD1	1:A:124:ASN:C	2.57	0.43
1:B:128:ILE:HD12	1:B:389:TYR:CE1	2.54	0.43
1:B:353:ASN:ND2	1:B:356:GLU:OE1	2.50	0.43
1:B:65:ASN:OD1	1:B:268:PRO:HD2	2.17	0.43
1:A:304:MET:HB3	1:A:349:VAL:HG12	2.01	0.43
1:B:97:ARG:O	1:B:98:PRO:O	2.37	0.43
1:B:78:ILE:CA	3:B:1055:HOH:O	2.55	0.43
1:B:122:SER:HB3	3:B:1180:HOH:O	2.18	0.43
1:B:120:VAL:HG23	1:B:388:SER:CA	2.49	0.42
1:B:318:GLN:HB3	3:B:1181:HOH:O	2.20	0.42
1:B:229:LYS:HG3	3:B:1089:HOH:O	2.18	0.42
1:A:179:SER:HB2	3:A:1005:HOH:O	2.17	0.42
1:A:410:GLU:HG2	3:A:1205:HOH:O	2.19	0.42
1:B:209:GLU:O	1:B:251:ALA:HA	2.18	0.42
1:A:119:SER:CB	1:A:254:ARG:HH21	2.25	0.42
1:A:302:ARG:NH2	1:A:304:MET:HE1	2.34	0.42
1:A:84:GLU:HA	3:A:1065:HOH:O	2.18	0.42
1:A:426:ASP:HA	1:A:464:ALA:O	2.18	0.42
1:A:342:ASN:C	1:A:342:ASN:ND2	2.72	0.42
1:A:132:ALA:HB1	1:A:147:LEU:HD21	2.01	0.42
1:B:214:GLN:HA	3:B:1019:HOH:O	2.19	0.42
1:B:503:LEU:HD22	1:B:509:ARG:CZ	2.50	0.42
1:A:164:LEU:HD13	1:A:169:SER:HA	2.01	0.42
1:A:491:TRP:O	1:A:492:GLU:HB3	2.18	0.42
1:B:253:PHE:HB2	1:B:304:MET:HG2	2.00	0.42
1:A:361:ILE:HD12	3:A:1204:HOH:O	2.19	0.42
1:B:506:VAL:HG13	1:B:507:PRO:HD2	2.02	0.42
1:A:368:LEU:O	1:A:371:LEU:N	2.53	0.42
1:B:202:VAL:HB	1:B:378:PHE:HB3	2.01	0.42
1:B:120:VAL:HG23	1:B:388:SER:HA	2.01	0.42
1:B:118:LEU:HB2	1:B:389:TYR:CE2	2.55	0.41
1:B:78:ILE:O	1:B:78:ILE:HG12	2.20	0.41
1:B:77:ASN:CB	3:B:1011:HOH:O	2.67	0.41
1:B:115:THR:HG21	3:B:1085:HOH:O	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:75:LYS:O	1:B:77:ASN:N	2.54	0.41
1:B:507:PRO:HD3	3:B:1012:HOH:O	2.20	0.41
1:A:310:THR:HG22	1:A:342:ASN:ND2	2.35	0.41
1:A:337:GLU:O	1:A:341:LYS:HG3	2.21	0.41
1:A:206:MET:CE	1:A:255:GLN:HG3	2.51	0.41
1:B:74:ASP:O	1:B:75:LYS:C	2.59	0.41
1:A:311:THR:HG22	3:A:1120:HOH:O	2.20	0.41
1:A:232:ALA:HB3	1:A:233:PRO:HD3	2.02	0.41
1:B:326:LYS:O	1:B:326:LYS:CG	2.68	0.41
1:A:118:LEU:HD12	1:A:389:TYR:CE1	2.55	0.41
1:A:202:VAL:HB	1:A:378:PHE:HB3	2.03	0.41
1:B:430:VAL:HG23	3:B:1122:HOH:O	2.20	0.41
1:A:440:LEU:O	1:A:475:ASN:ND2	2.45	0.40
1:A:470:LEU:HD23	1:A:470:LEU:N	2.37	0.40
1:A:299:SER:HB2	1:A:388:SER:OG	2.21	0.40
1:A:300:TYR:CE2	1:A:386:PRO:HG3	2.56	0.40
1:A:214:GLN:HB2	1:A:218:GLN:NE2	2.37	0.40
1:B:433:PHE:CD1	1:B:433:PHE:N	2.87	0.40
1:B:241:VAL:O	1:B:411:THR:HG21	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:1016:HOH:O	3:A:1136:HOH:O[3_546]	2.19	0.01

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	471/535 (88%)	421 (89%)	41 (9%)	9 (2%)	12	23
1	B	471/535 (88%)	414 (88%)	43 (9%)	14 (3%)	7	10
All	All	942/1070 (88%)	835 (89%)	84 (9%)	23 (2%)	9	16

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	98	PRO
1	B	125	ASP
1	B	329	LYS
1	B	333	GLY
1	B	488	GLY
1	A	235	ASN
1	A	329	LYS
1	A	334	THR
1	B	76	LEU
1	B	78	ILE
1	B	235	ASN
1	B	500	LYS
1	A	75	LYS
1	A	335	GLU
1	A	359	LYS
1	B	130	PRO
1	B	166	ASN
1	B	226	ASP
1	B	332	ALA
1	A	492	GLU
1	A	496	LEU
1	B	336	TYR
1	A	493	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	405/457 (89%)	358 (88%)	47 (12%)	8	14
1	B	405/457 (89%)	346 (85%)	59 (15%)	5	8
All	All	810/914 (89%)	704 (87%)	106 (13%)	6	11

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LEU
1	A	76	LEU
1	A	87	LYS

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Mol	Chain	Res	Type
1	A	93	GLU
1	A	97	ARG
1	A	98	PRO
1	A	108	LYS
1	A	110	SER
1	A	112	SER
1	A	115	THR
1	A	122	SER
1	A	144	LEU
1	A	152	ARG
1	A	166	ASN
1	A	174	GLU
1	A	179	SER
1	A	199	THR
1	A	206	MET
1	A	218	GLN
1	A	239	SER
1	A	240	SER
1	A	262	VAL
1	A	302	ARG
1	A	310	THR
1	A	311	THR
1	A	312	SER
1	A	326	LYS
1	A	330	LEU
1	A	331	LYS
1	A	334	THR
1	A	335	GLU
1	A	342	ASN
1	A	356	GLU
1	A	359	LYS
1	A	374	LYS
1	A	385	VAL
1	A	412	LYS
1	A	415	SER
1	A	440	LEU
1	A	451	ARG
1	A	454	SER
1	A	470	LEU
1	A	477	ARG
1	A	491	TRP
1	A	492	GLU

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Mol	Chain	Res	Type
1	A	512	SER
1	A	528	LYS
1	B	64	LEU
1	B	76	LEU
1	B	84	GLU
1	B	90	SER
1	B	92	ARG
1	B	93	GLU
1	B	100	GLU
1	B	102	VAL
1	B	108	LYS
1	B	112	SER
1	B	115	THR
1	B	122	SER
1	B	130	PRO
1	B	144	LEU
1	B	147	LEU
1	B	152	ARG
1	B	154	LYS
1	B	158	SER
1	B	174	GLU
1	B	179	SER
1	B	199	THR
1	B	217	SER
1	B	226	ASP
1	B	239	SER
1	B	240	SER
1	B	262	VAL
1	B	264	SER
1	B	302	ARG
1	B	310	THR
1	B	311	THR
1	B	312	SER
1	B	314	SER
1	B	334	THR
1	B	335	GLU
1	B	339	ILE
1	B	343	THR
1	B	344	LYS
1	B	345	ILE
1	B	348	VAL
1	B	350	LEU

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Mol	Chain	Res	Type
1	B	353	ASN
1	B	356	GLU
1	B	361	ILE
1	B	362	THR
1	B	364	ASN
1	B	374	LYS
1	B	385	VAL
1	B	399	ILE
1	B	401	THR
1	B	412	LYS
1	B	436	TYR
1	B	440	LEU
1	B	451	ARG
1	B	470	LEU
1	B	489	LEU
1	B	492	GLU
1	B	500	LYS
1	B	502	ASP
1	B	513	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	207	GLN
1	A	218	GLN
1	A	220	GLN
1	A	318	GLN
1	A	342	ASN
1	A	501	ASN
1	B	82	GLN
1	B	89	HIS
1	B	166	ASN
1	B	170	ASN
1	B	200	HIS
1	B	207	GLN
1	B	220	GLN
1	B	318	GLN
1	B	364	ASN
1	B	501	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	A	1001	-	4,4,4	0.18	0	6,6,6	0.33	0
2	SO4	A	1002	-	4,4,4	0.23	0	6,6,6	0.67	0
2	SO4	B	1003	-	4,4,4	0.34	0	6,6,6	0.57	0
2	SO4	B	1004	-	4,4,4	0.40	0	6,6,6	0.47	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	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1004	-	-	0/0/0/0	0/0/0/0

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	473/535 (88%)	0.51	49 (10%) 7 5	25, 39, 49, 61	0
1	B	473/535 (88%)	0.29	22 (4%) 30 27	15, 37, 48, 58	0
All	All	946/1070 (88%)	0.40	71 (7%) 14 11	15, 38, 48, 61	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	ALA	5.6
1	A	332	ALA	5.5
1	B	330	LEU	5.1
1	A	358	SER	4.8
1	A	355	GLY	4.7
1	A	490	ALA	4.7
1	B	333	GLY	4.6
1	A	484	LEU	4.4
1	A	488	GLY	4.4
1	A	491	TRP	4.4
1	A	354	PRO	4.2
1	A	201	ALA	4.2
1	B	329	LYS	4.2
1	A	334	THR	4.0
1	B	355	GLY	3.7
1	A	331	LYS	3.7
1	A	516	THR	3.6
1	A	519	HIS	3.6
1	B	331	LYS	3.5
1	A	330	LEU	3.4
1	B	491	TRP	3.4
1	B	353	ASN	3.3
1	A	333	GLY	3.3
1	A	356	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	332	ALA	3.3
1	B	354	PRO	3.3
1	B	358	SER	3.2
1	A	250	ILE	3.2
1	A	496	LEU	3.0
1	B	357	ALA	3.0
1	A	327	GLY	2.9
1	A	520	PRO	2.9
1	A	336	TYR	2.9
1	A	487	THR	2.9
1	B	518	LEU	2.9
1	A	328	ALA	2.9
1	A	340	LEU	2.8
1	A	514	TRP	2.7
1	A	56	ASN	2.6
1	A	120	VAL	2.6
1	B	293	VAL	2.6
1	A	492	GLU	2.6
1	A	251	ALA	2.6
1	A	485	GLY	2.5
1	B	328	ALA	2.5
1	A	528	LYS	2.5
1	A	515	GLY	2.5
1	A	119	SER	2.5
1	B	352	GLY	2.5
1	A	392	SER	2.4
1	A	489	LEU	2.3
1	A	518	LEU	2.3
1	A	483	VAL	2.3
1	B	486	ALA	2.3
1	A	495	ARG	2.3
1	A	323	ALA	2.3
1	A	493	PRO	2.3
1	B	56	ASN	2.2
1	A	166	ASN	2.2
1	A	353	ASN	2.2
1	A	474	GLY	2.2
1	B	515	GLY	2.2
1	A	388	SER	2.2
1	A	494	TRP	2.1
1	B	242	HIS	2.1
1	A	295	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	295	VAL	2.1
1	B	465	HIS	2.1
1	B	300	TYR	2.0
1	A	304	MET	2.0
1	A	252	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	1001	5/5	0.16	-0.56	45,46,47,48	0
2	SO4	A	1002	5/5	0.14	-0.85	47,50,51,52	0
2	SO4	B	1004	5/5	0.13	-1.10	42,43,46,46	0
2	SO4	B	1003	5/5	0.08	-1.61	44,44,46,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.