



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:06 PM UTC

PDB ID : 6AC6 / pdb_00006ac6
Title : Ab initio crystal structure of Selenomethionine labelled Mycobacterium smegmatis Mfd
Authors : Putta, S.; Fox, G.C.; Walsh, M.A.; Rao, D.N.; Nagaraja, V.; Natesh, R.
Deposited on : 2018-07-25
Resolution : 2.99 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

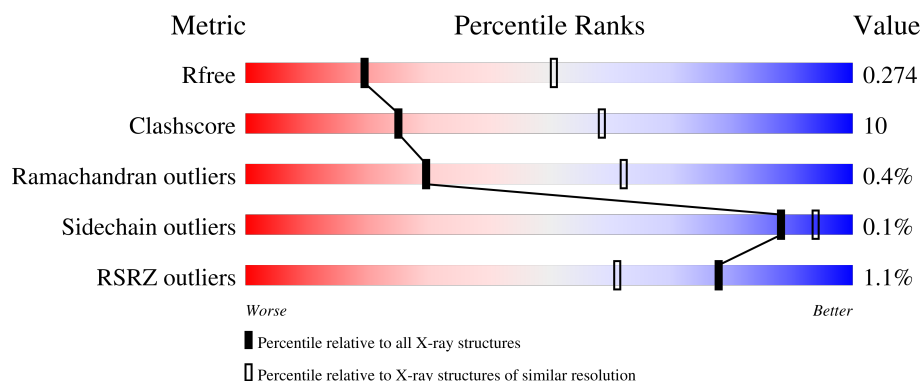
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	1235	76% 17% 7%
1	B	1235	71% 22% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16853 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 Mycobacterium smegmatis Mfd.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1154	Total	C	N	O	S	Se	0	0	0
			8417	5293	1487	1606	6	25			
1	B	1153	Total	C	N	O	S	Se	0	0	0
			8337	5253	1473	1580	6	25			

There are 40 discrepancies between the modelled and reference sequences:

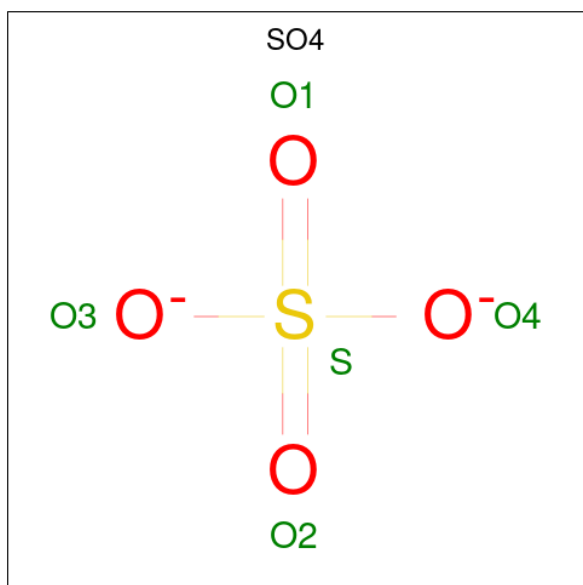
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	initiating methionine	UNP I7G7M2
A	-18	GLY	-	expression tag	UNP I7G7M2
A	-17	SER	-	expression tag	UNP I7G7M2
A	-16	SER	-	expression tag	UNP I7G7M2
A	-15	HIS	-	expression tag	UNP I7G7M2
A	-14	HIS	-	expression tag	UNP I7G7M2
A	-13	HIS	-	expression tag	UNP I7G7M2
A	-12	HIS	-	expression tag	UNP I7G7M2
A	-11	HIS	-	expression tag	UNP I7G7M2
A	-10	HIS	-	expression tag	UNP I7G7M2
A	-9	SER	-	expression tag	UNP I7G7M2
A	-8	SER	-	expression tag	UNP I7G7M2
A	-7	GLY	-	expression tag	UNP I7G7M2
A	-6	LEU	-	expression tag	UNP I7G7M2
A	-5	VAL	-	expression tag	UNP I7G7M2
A	-4	PRO	-	expression tag	UNP I7G7M2
A	-3	ARG	-	expression tag	UNP I7G7M2
A	-2	GLY	-	expression tag	UNP I7G7M2
A	-1	SER	-	expression tag	UNP I7G7M2
A	0	HIS	-	expression tag	UNP I7G7M2
B	-19	MSE	-	initiating methionine	UNP I7G7M2
B	-18	GLY	-	expression tag	UNP I7G7M2
B	-17	SER	-	expression tag	UNP I7G7M2
B	-16	SER	-	expression tag	UNP I7G7M2
B	-15	HIS	-	expression tag	UNP I7G7M2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP I7G7M2
B	-13	HIS	-	expression tag	UNP I7G7M2
B	-12	HIS	-	expression tag	UNP I7G7M2
B	-11	HIS	-	expression tag	UNP I7G7M2
B	-10	HIS	-	expression tag	UNP I7G7M2
B	-9	SER	-	expression tag	UNP I7G7M2
B	-8	SER	-	expression tag	UNP I7G7M2
B	-7	GLY	-	expression tag	UNP I7G7M2
B	-6	LEU	-	expression tag	UNP I7G7M2
B	-5	VAL	-	expression tag	UNP I7G7M2
B	-4	PRO	-	expression tag	UNP I7G7M2
B	-3	ARG	-	expression tag	UNP I7G7M2
B	-2	GLY	-	expression tag	UNP I7G7M2
B	-1	SER	-	expression tag	UNP I7G7M2
B	0	HIS	-	expression tag	UNP I7G7M2

- 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	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		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	37	Total	O	0	0
			37	37		

V1086	R951	V840	R714	V611	GLY	P353	F210	L79	MSE
E1089	Y958	R846	G717	Y614	GLY	L354	S216	R80	GLY
Y1094	P959	Q853	T721	R617	LYS	R369	F221	F83	SER
A1101	L964	I857	K723	Q618	LEU	V379	R227	S86	HIS
V1105	R971	H858	S726	A624	ALA	V380	S228	V87	HIS
C1114	L972	R860	R727	T629	LYS	T381	A239	F90	HIS
I1119	A973	V861	F728	P830	ARG	S386	V240	P91	HIS
T1129	I975	R862	D743	K631	D511	V391	P241	W93	SER
M985	R872	R879	V746	M635	A514	A401	T248	T95	GLY
S1133	R879	V880	G751	E636	L515	ARG	T264	L96	VAL
P1134	V881	V882	L755	D637	D519	GLY	THR	E99	PRO
R1144	V882	M687	L756	A638	V622	SER	GLU	R100	ARG
L1145	M887	N888	T758	PHE	L529	GLN	ASN	P103	SER
R1155	E889	E889	T769	GLY	F531	H406	THR	T107	HIS
T1158	K894	K894	I770	PHE	V532	M414	P270	R111	MSE
P1164	F899	F899	V770	THR	E533	L415	VAL	R120	THR
V1172	D905	D905	E773	ILE	H534	A435	M276	R123	ALA
A1174	I906	I906	Q774	D646	V654	H436	L277	E124	GLY
I1177	I907	I907	F776	V654	L547	V439	A278	T125	ALA
R1178	V908	V908	P661	P661	A552	A445	E282	T135	PRO
D1179	C909	C909	V662	V662	SER	D446	V286	T136	GLY
L1182	L1020	L1020	P663	P663	SER	T447	M289	T137	HIS
L1193	V1021	V1021	V667	V667	LYS	A448	T305	R138	THR
S1207	G1022	G1022	C669	C669	ARG	L452	L308	V154	GLY
T1036	E1023	E1023	V672	V672	GLY	V463	A312	F164	THR
VAL	Y1028	Y1028	G675	G675	T560	L466	D318	L174	SER
ALA	T1036	T1036	Q675	Q675	V565	P469	P319	R178	ALA
THR	VAL	VAL	E678	E678	D571	V474	V322	D180	THR
PRO	ALA	ALA	I679	I679	Q672	V475	A326	G183	VAL
GLY	THR	THR	A680	A680	S574	L476	I330	R185	GLY
GLN	PRO	PRO	V681	V681	R575	N480	K331	G186	LYS
ALA	GLU	GLU	R682	R682	L587	L481	F336	E187	ALA
LYS	GLN	GLN	E814	E814	G588	V482	E338	I194	LYS
ARG	K1044	K1044	Q693	Q693	N594	I483	A339	A202	ARG
V1082	V1082	V1082	T320	T320	K596	ARG	S340	A66	ALA
S1063	S1063	S1063	P821	P821	A599	VAL	S341	A67	THR
E1069	E1069	E1069	P822	P822	R600	THR	S342	E78	ASN
R1073	R1073	R1073	E823	E823	A599	ASN	I352		
D1079	D1079	D1079	V632	V632	R600				
			D836	D836	V603				
			Q839	Q839					

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.71Å 158.87Å 207.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 2.99 47.19 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.19-2.99) 96.2 (47.19-2.99)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.218 , 0.270 0.223 , 0.274	Depositor DCC
R_{free} test set	2788 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16853	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.15	0/8542	0.34	0/11635
1	B	0.18	1/8461 (0.0%)	0.37	2/11529 (0.0%)
All	All	0.17	1/17003 (0.0%)	0.35	2/23164 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	MSE	SE-CE	-5.33	1.79	1.95

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	531	PHE	CA-C-N	-5.76	116.72	122.77
1	B	531	PHE	C-N-CA	-5.76	116.72	122.77

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8417	0	8131	145	0
1	B	8337	0	8022	176	0
2	A	15	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	0	0
3	A	37	0	0	2	0
3	B	37	0	0	2	0
All	All	16853	0	16153	318	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 (318) 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:452:LEU:HD13	1:B:466:LEU:HG	1.43	0.95
1:B:330:ILE:HD12	1:B:331:LYS:N	1.91	0.86
1:A:674:TYR:HB3	1:A:818:ILE:HD11	1.62	0.81
1:B:636:GLU:HG2	1:B:682:ARG:HH11	1.48	0.79
1:B:532:VAL:HG23	1:B:533:GLU:HB3	1.64	0.77
1:B:1052:VAL:HG23	1:B:1179:ASP:HA	1.67	0.77
1:B:185:ARG:NH1	1:B:202:ALA:O	2.18	0.76
1:A:635:MSE:HG2	1:A:714:ARG:HH21	1.51	0.75
1:B:330:ILE:HD12	1:B:331:LYS:H	1.50	0.74
1:A:805:LEU:HD13	1:A:1018:VAL:HG23	1.71	0.73
1:A:195:LEU:HD23	1:A:208:VAL:HB	1.71	0.71
1:B:862:ARG:H	1:B:862:ARG:HD2	1.55	0.71
1:B:880:VAL:HG22	1:B:906:ILE:HB	1.71	0.71
1:B:617:ARG:NH1	1:B:663:PRO:O	2.25	0.70
1:B:185:ARG:NH2	1:B:823:GLU:O	2.25	0.70
1:B:587:LEU:H	1:B:587:LEU:HD23	1.58	0.69
1:A:92:SER:HB2	1:A:138:ARG:HD2	1.76	0.68
1:B:931:ASP:O	1:B:971:ARG:NH2	2.27	0.67
1:A:701:THR:HG21	1:A:727:ARG:HB3	1.76	0.67
1:A:52:VAL:HG21	1:A:382:LEU:HD22	1.76	0.66
1:B:92:SER:HB3	1:B:138:ARG:HD2	1.77	0.66
1:B:1145:LEU:HD13	1:B:1193:LEU:HD11	1.78	0.66
1:A:28:ASP:OD1	1:A:31:ARG:NH2	2.29	0.66
1:A:770:VAL:HB	1:A:795:THR:HG22	1.78	0.66
1:A:541:GLY:O	1:A:1178:ARG:NH1	2.28	0.66
1:A:243:ARG:HD3	1:A:289:MSE:HE1	1.76	0.66
1:B:599:ALA:O	1:B:603:VAL:HG23	1.96	0.66
1:B:209:GLU:O	1:B:216:SER:N	2.29	0.64
1:B:1144:ARG:NH2	3:B:1402:HOH:O	2.30	0.64
1:B:305:THR:HA	1:B:308:LEU:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:LEU:HB2	1:B:466:LEU:HD21	1.81	0.63
1:B:840:VAL:HG13	1:B:926:ILE:HD13	1.80	0.63
1:A:850:ARG:HH21	1:A:950:GLU:HG2	1.64	0.62
1:B:452:LEU:HB2	1:B:466:LEU:CG	2.30	0.62
1:B:860:ARG:CZ	1:B:862:ARG:HD3	2.29	0.62
1:B:154:VAL:HB	1:B:239:ALA:HB3	1.82	0.61
1:B:415:LEU:HD11	1:B:484:ILE:HG13	1.82	0.61
1:B:452:LEU:HB2	1:B:466:LEU:HG	1.82	0.61
1:B:701:THR:HG23	1:B:726:SER:HB3	1.82	0.61
1:B:452:LEU:HB2	1:B:466:LEU:CD2	2.30	0.61
1:A:138:ARG:NH2	2:A:1302:SO4:O1	2.33	0.61
1:B:164:PHE:HZ	1:B:190:VAL:HG23	1.65	0.61
1:A:117:ARG:HG2	1:A:126:LEU:HB3	1.83	0.60
1:B:452:LEU:CD1	1:B:466:LEU:HG	2.24	0.60
1:B:678:GLU:HA	1:B:681:VAL:HG22	1.83	0.60
1:A:944:ARG:NH2	3:A:1401:HOH:O	2.32	0.59
1:A:611:VAL:HG21	1:A:1028:TYR:HB3	1.83	0.59
1:B:522:VAL:HG12	1:B:528:ILE:HG13	1.85	0.59
1:A:532:VAL:HB	1:A:548:VAL:HG23	1.83	0.58
1:B:802:PRO:HD3	1:B:993:GLU:HB3	1.83	0.58
1:B:722:VAL:HG23	1:B:723:LYS:H	1.67	0.58
1:B:929:ARG:HG3	1:B:959:PRO:HD3	1.84	0.58
1:A:1091:ILE:HG22	1:A:1096:PRO:HA	1.84	0.58
1:B:90:PHE:HB3	1:B:135:THR:HB	1.84	0.58
1:B:773:GLU:OE2	1:B:788:ARG:NH2	2.36	0.58
1:A:206:VAL:HG11	1:A:237:VAL:HG11	1.85	0.58
1:A:762:TRP:HB3	1:A:765:LEU:HB2	1.86	0.58
1:A:545:GLU:OE2	1:A:1067:ARG:NH1	2.36	0.58
1:B:935:LEU:HD11	1:B:985:MSE:SE	2.53	0.57
1:A:56:LEU:HB2	1:A:62:LEU:HD22	1.85	0.57
1:B:751:GLY:HA3	1:B:755:LEU:HD11	1.87	0.57
1:A:784:ILE:H	1:A:784:ILE:HD12	1.70	0.56
1:A:772:GLU:OE1	1:A:774:GLN:NE2	2.36	0.56
1:A:1119:ILE:HA	1:A:1134:PRO:HG2	1.85	0.56
1:B:78:GLU:HA	1:B:469:PRO:HG2	1.87	0.56
1:B:774:GLN:HB3	1:B:999:ASN:HD22	1.70	0.56
1:A:847:GLU:HG3	1:A:924:THR:HB	1.87	0.56
1:B:49:ARG:NH2	1:B:318:ASP:OD2	2.37	0.56
1:A:678:GLU:O	1:A:681:VAL:HG22	2.04	0.56
1:A:475:VAL:HG22	1:A:482:VAL:HG23	1.87	0.56
1:B:614:TYR:O	1:B:618:GLN:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:MSE:SE	1:B:547:LEU:HD13	2.56	0.55
1:B:1101:ALA:O	1:B:1105:VAL:HG23	2.06	0.55
1:A:780:HIS:O	1:A:784:ILE:HD12	2.05	0.55
1:A:882:VAL:HG23	1:A:887:MSE:HE1	1.88	0.55
1:A:83:PHE:HB2	1:A:87:VAL:HG23	1.88	0.55
1:A:847:GLU:O	1:A:850:ARG:HG2	2.06	0.55
1:A:606:ILE:O	1:A:610:LEU:HG	2.06	0.55
1:A:650:ALA:O	1:A:654:VAL:HG13	2.07	0.55
1:A:1119:ILE:HG23	1:A:1134:PRO:HD2	1.89	0.55
1:B:859:ASN:HA	1:B:910:THR:HG22	1.88	0.55
1:B:124:GLU:CD	1:B:124:GLU:H	2.15	0.55
1:A:1012:VAL:HG22	1:A:1016:LEU:HD23	1.88	0.54
1:A:522:VAL:HG23	1:A:528:ILE:HD13	1.88	0.54
1:A:1109:ARG:HH21	1:A:1206:PHE:HA	1.71	0.54
1:B:414:MSE:HE1	1:B:482:VAL:HG11	1.88	0.54
1:B:917:LEU:C	1:B:944:ARG:HH21	2.16	0.54
1:B:99:GLU:OE1	1:B:846:ARG:NH1	2.40	0.54
1:B:629:THR:HG22	1:B:631:TRP:H	1.73	0.54
1:B:1073:ARG:NH2	1:B:1086:VAL:HG12	2.23	0.54
1:A:544:ARG:NH2	1:A:1049:ASP:OD1	2.41	0.54
1:B:164:PHE:CZ	1:B:190:VAL:HG23	2.43	0.54
1:B:178:ARG:NH2	1:B:190:VAL:HG11	2.23	0.54
1:B:938:LEU:HD11	1:B:975:ILE:HG21	1.88	0.54
1:B:603:VAL:HG13	1:B:1021:VAL:HG22	1.90	0.53
1:B:32:ARG:NH1	1:B:391:VAL:HG21	2.22	0.53
1:B:948:SER:OG	1:B:949:ARG:N	2.38	0.53
1:A:407:ASN:O	1:A:411:ILE:HG13	2.08	0.53
1:B:28:ASP:O	1:B:32:ARG:HG3	2.08	0.53
1:A:427:VAL:HG11	1:A:438:VAL:HG11	1.91	0.53
1:B:221:PHE:HA	1:B:228:SER:HA	1.90	0.53
1:B:19:LEU:HG	1:B:481:LEU:HD11	1.90	0.52
1:A:884:HIS:CD2	1:A:887:MSE:HE3	2.44	0.52
1:A:195:LEU:HD22	1:A:210:PHE:HE1	1.75	0.52
1:A:303:THR:OG1	1:A:304:LEU:N	2.43	0.52
1:B:700:THR:OG1	1:B:703:LEU:HD12	2.10	0.52
1:B:194:ILE:HG13	1:B:209:GLU:HG2	1.91	0.52
1:B:624:ALA:HB2	1:B:661:PRO:HB3	1.92	0.52
1:A:227:ARG:HD3	1:A:1089:GLU:HG3	1.90	0.52
1:B:100:ARG:HG3	1:B:340:SER:HB3	1.92	0.52
1:A:1109:ARG:NH2	1:A:1206:PHE:HA	2.26	0.51
1:B:565:VAL:HG11	1:B:573:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:LEU:HB3	1:B:565:VAL:HG13	1.92	0.51
1:B:533:GLU:HG3	1:B:534:MSE:N	2.25	0.51
1:A:727:ARG:NH2	1:A:893:GLU:OE2	2.43	0.51
1:B:768:ILE:HB	1:B:793:VAL:HG22	1.91	0.51
1:A:1044:LYS:O	1:A:1115:ARG:NH1	2.44	0.51
1:B:935:LEU:HD23	1:B:971:ARG:HG3	1.92	0.51
1:B:326:ALA:O	1:B:330:ILE:HG13	2.11	0.51
1:B:93:TRP:CE2	1:B:103:PRO:HG3	2.46	0.51
1:B:120:ARG:NH1	1:B:123:ASP:OD2	2.44	0.51
1:B:137:THR:HB	1:B:322:VAL:HG13	1.91	0.51
1:B:594:ASN:ND2	3:B:1403:HOH:O	2.32	0.51
1:A:624:ALA:HB2	1:A:661:PRO:HA	1.92	0.50
1:A:91:PRO:HD2	1:A:111:ARG:HG3	1.93	0.50
1:A:715:MSE:CE	1:A:748:VAL:HG11	2.42	0.50
1:A:607:ALA:O	1:A:611:VAL:HG22	2.12	0.50
1:A:693:GLN:HE22	1:A:744:GLY:HA2	1.76	0.50
1:A:847:GLU:OE2	1:A:850:ARG:NH1	2.44	0.50
1:B:11:THR:O	1:B:11:THR:OG1	2.24	0.50
1:A:701:THR:HG22	1:A:752:THR:HG21	1.94	0.50
1:A:162:MSE:HE1	1:A:215:ILE:HD11	1.94	0.50
1:B:435:ALA:O	1:B:439:VAL:HG13	2.12	0.49
1:B:1008:HIS:O	1:B:1012:VAL:HG12	2.11	0.49
1:B:83:PHE:HB2	1:B:87:VAL:HG23	1.95	0.49
1:B:635:MSE:O	1:B:714:ARG:NH2	2.34	0.49
1:B:180:ASP:HB2	1:B:1063:SER:HB2	1.95	0.49
1:B:823:GLU:OE2	1:B:823:GLU:N	2.45	0.49
1:A:366:GLU:OE1	1:A:369:ARG:NH1	2.46	0.48
1:A:829:LEU:HG	1:A:951:ARG:HD3	1.93	0.48
1:A:547:LEU:HD22	1:A:1068:LEU:HD11	1.94	0.48
1:B:43:VAL:HG21	1:B:386:SER:HA	1.94	0.48
1:B:882:VAL:HA	1:B:908:VAL:O	2.12	0.48
1:A:741:LEU:HD12	1:A:762:TRP:HA	1.96	0.48
1:A:853:GLN:OE1	1:A:921:ASN:ND2	2.47	0.48
1:A:1120:THR:HG23	1:A:1134:PRO:HG3	1.95	0.48
1:B:971:ARG:O	1:B:974:THR:OG1	2.30	0.48
1:B:635:MSE:HE1	1:B:682:ARG:HD3	1.96	0.48
1:A:780:HIS:O	1:A:784:ILE:CD1	2.61	0.48
1:A:1166:PRO:HG2	1:A:1177:ILE:HD13	1.95	0.48
1:B:937:GLN:OE1	1:B:937:GLN:N	2.47	0.48
1:A:154:VAL:HB	1:A:239:ALA:HB3	1.95	0.48
1:A:195:LEU:HD22	1:A:210:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:HD22	1:B:308:LEU:HD11	1.96	0.47
1:B:857:ILE:HD11	1:B:914:GLU:HG3	1.96	0.47
1:A:19:LEU:O	1:A:22:SER:HB3	2.14	0.47
1:A:87:VAL:HG22	1:A:132:VAL:HB	1.95	0.47
1:A:635:MSE:HE2	1:A:635:MSE:HB3	1.85	0.47
1:B:174:LEU:HD22	1:B:241:PRO:HG3	1.96	0.47
1:B:1114:CYS:HB3	1:B:1119:ILE:HB	1.95	0.47
1:A:1163:VAL:HG21	1:A:1189:LEU:HD11	1.97	0.47
1:A:11:THR:HB	1:A:14:ALA:HB2	1.96	0.47
1:A:947:ARG:HD3	3:A:1401:HOH:O	2.14	0.47
1:A:1071:TYR:HE1	1:A:1104:LEU:HD11	1.80	0.47
1:B:1155:ARG:HB2	1:B:1158:THR:OG1	2.15	0.47
1:B:164:PHE:HD1	1:B:210:PHE:CE2	2.33	0.47
1:B:853:GLN:NE2	1:B:899:PHE:O	2.48	0.47
1:B:1129:THR:HG22	1:B:1164:PRO:HA	1.97	0.47
1:A:395(A):ILE:HG12	1:A:476:LEU:HD23	1.97	0.46
1:B:43:VAL:HG13	1:B:392:GLU:HA	1.97	0.46
1:B:1133:SER:HB3	1:B:1134:PRO:HD3	1.96	0.46
1:B:123:ASP:CG	1:B:125:THR:HG22	2.40	0.46
1:B:278:ALA:O	1:B:282:GLU:HG3	2.15	0.46
1:B:65:VAL:HG22	1:B:135:THR:HG23	1.97	0.46
1:B:1017:TYR:O	1:B:1021:VAL:HG23	2.14	0.46
1:A:183:GLY:HA2	1:A:223:ILE:HD12	1.96	0.46
1:B:832:VAL:HG21	1:B:972:LEU:HB3	1.97	0.46
1:B:958:TYR:CG	1:B:964:LEU:HD11	2.50	0.46
1:B:183:GLY:N	1:B:187:GLU:OE2	2.36	0.46
1:B:1177:ILE:HG13	1:B:1182:LEU:HB2	1.98	0.46
1:B:40:LEU:HB3	1:B:380:TRP:CD1	2.51	0.46
1:B:872:ARG:NH2	1:B:880:VAL:O	2.47	0.46
1:B:47:SER:OG	1:B:474:VAL:HG12	2.15	0.46
1:B:369:ARG:HG3	1:B:379:TRP:CG	2.50	0.46
1:B:693:GLN:NE2	1:B:743:ASP:O	2.47	0.46
1:B:728:PHE:HE1	1:B:894:LYS:HD3	1.81	0.46
1:B:1079:ASP:OD1	1:B:1079:ASP:N	2.48	0.46
1:A:487:THR:HG22	1:A:492:ASN:O	2.15	0.46
1:A:567:MSE:SE	1:A:570:LEU:HD11	2.65	0.46
1:B:352:ILE:O	1:B:354:LEU:HD12	2.16	0.46
1:B:1014:PHE:O	1:B:1018:VAL:HG22	2.16	0.46
1:A:23:ASP:OD2	1:A:25:SER:HB3	2.16	0.46
1:A:753:HIS:HB2	1:A:780:HIS:CE1	2.51	0.46
1:A:1120:THR:H	1:A:1134:PRO:CG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:PRO:HB2	1:B:312:ALA:HB2	1.98	0.46
1:B:338:GLU:O	1:B:342:SER:HB3	2.16	0.46
1:A:676:LYS:HD2	1:A:796:MSE:HE3	1.98	0.45
1:B:475:VAL:HG13	1:B:482:VAL:HG22	1.97	0.45
1:B:667:VAL:HG12	1:B:795:THR:HB	1.98	0.45
1:A:49:ARG:HA	1:A:52:VAL:HG22	1.98	0.45
1:B:1012:VAL:CG2	1:B:1016:LEU:HD23	2.47	0.45
1:A:1071:TYR:CE1	1:A:1104:LEU:HD11	2.52	0.45
1:B:889:GLU:CD	1:B:889:GLU:H	2.23	0.45
1:A:776:PHE:O	1:A:781:LYS:NZ	2.50	0.45
1:A:1156:ALA:N	2:A:1301:SO4:O1	2.46	0.45
1:B:191:ARG:HD2	1:B:1094:TYR:HD1	1.82	0.45
1:A:657:ASP:OD1	1:A:657:ASP:N	2.49	0.45
1:A:1087:VAL:O	1:A:1091:ILE:HG13	2.16	0.45
1:A:1120:THR:H	1:A:1134:PRO:HG3	1.81	0.45
1:A:712:THR:HG22	1:A:722:VAL:HG13	1.99	0.45
1:A:851:ASP:O	1:A:902:ARG:NH2	2.49	0.45
1:A:1148:MSE:HE2	1:A:1148:MSE:HB2	1.84	0.45
1:B:770:VAL:HG22	1:B:795:THR:HA	1.98	0.45
1:B:882:VAL:O	1:B:887:MSE:HE1	2.16	0.45
1:A:320:GLU:O	1:A:324:THR:HG23	2.17	0.44
1:A:966:GLU:HA	1:A:969:TYR:CE2	2.51	0.44
1:B:83:PHE:HB3	1:B:86:SER:HB2	1.98	0.44
1:B:276:MSE:HG3	1:B:286:VAL:HG11	1.98	0.44
1:A:418:HIS:O	1:A:421:THR:HB	2.17	0.44
1:A:832:VAL:HG21	1:A:972:LEU:HB3	2.00	0.44
1:B:938:LEU:HA	1:B:941:LEU:HD12	1.99	0.44
1:A:629:THR:HG22	1:A:631:TRP:H	1.83	0.44
1:A:681:VAL:HG12	1:A:711:PHE:CE1	2.52	0.44
1:A:162:MSE:HE3	1:A:162:MSE:HB2	1.63	0.44
1:B:707:HIS:HA	1:B:710:THR:HG22	1.99	0.44
1:A:292:LEU:O	1:A:296:LEU:N	2.44	0.44
1:B:93:TRP:NE1	1:B:111:ARG:HH11	2.16	0.44
1:A:195:LEU:CD2	1:A:208:VAL:HB	2.44	0.44
1:B:452:LEU:O	1:B:466:LEU:HD21	2.18	0.44
1:A:428:VAL:HA	1:A:466:LEU:O	2.18	0.44
1:A:1069:GLU:OE2	1:A:1073:ARG:NH2	2.51	0.44
1:B:56:LEU:HB2	1:B:62:LEU:HD22	2.00	0.44
1:B:80:ARG:HG3	1:B:80:ARG:HH11	1.83	0.44
1:A:105:VAL:HA	1:A:108:VAL:HG22	1.99	0.44
1:A:1004:GLU:HG2	1:A:1005:GLN:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:LYS:HG2	1:A:796:MSE:SE	2.68	0.43
1:B:96:LEU:HD12	1:B:336:PHE:CG	2.53	0.43
1:B:935:LEU:HD12	1:B:988:ALA:HB2	1.99	0.43
1:A:428:VAL:HG21	1:A:470:LEU:HD12	1.99	0.43
1:A:633:ALA:HA	1:A:636:GLU:HG3	2.00	0.43
1:A:571:ASP:OD1	1:A:571:ASP:N	2.50	0.43
1:A:1059:GLU:OE1	1:A:1059:GLU:N	2.46	0.43
1:B:448:ALA:O	1:B:463:VAL:HG22	2.18	0.43
1:A:16:LEU:HD21	1:A:483:ILE:HD13	2.00	0.43
1:A:302:THR:OG1	1:A:303:THR:N	2.50	0.43
1:A:784:ILE:HD12	1:A:784:ILE:N	2.34	0.43
1:A:386:SER:HG	1:B:406:HIS:N	2.16	0.43
1:A:664:MSE:N	1:A:792:ASP:OD1	2.45	0.43
1:B:319:PRO:HG3	1:B:381:THR:HG23	2.01	0.43
1:A:534:MSE:HE2	1:A:1064:ASP:HB3	2.00	0.43
1:A:1191:LEU:HD23	1:A:1191:LEU:HA	1.87	0.43
1:B:24:PRO:HA	1:B:27:GLN:HB2	2.00	0.43
1:A:427:VAL:HA	1:A:484:ILE:O	2.19	0.43
1:A:731:PRO:O	1:A:735:ARG:HB3	2.19	0.43
1:A:954:ALA:C	1:A:955:TYR:HD1	2.26	0.43
1:B:534:MSE:HE3	1:B:534:MSE:HB3	1.99	0.43
1:B:669:CYS:HA	1:B:797:SER:O	2.19	0.43
1:B:675:GLY:O	1:B:679:ILE:HD12	2.19	0.43
1:B:776:PHE:HB2	1:B:781:LYS:HG3	2.00	0.42
1:B:436:HIS:O	1:B:439:VAL:HG22	2.19	0.42
1:B:445:ALA:O	1:B:447:THR:N	2.52	0.42
1:B:511:ASP:O	1:B:1069:GLU:HG3	2.20	0.42
1:A:863:THR:O	1:A:863:THR:OG1	2.37	0.42
1:A:1082:ALA:O	1:A:1086:VAL:HG23	2.19	0.42
1:B:721:THR:OG1	1:B:746:VAL:HA	2.20	0.42
1:B:1016:LEU:O	1:B:1020:LEU:HG	2.20	0.42
1:A:603:VAL:CG1	1:A:1021:VAL:HA	2.50	0.42
1:A:827:PRO:O	1:A:951:ARG:NH1	2.52	0.42
1:B:83:PHE:HB2	1:B:87:VAL:CG2	2.49	0.42
1:B:596:LYS:O	1:B:600:ARG:HB2	2.19	0.42
1:B:894:LYS:HE2	1:B:894:LYS:HB2	1.82	0.42
1:A:51:LEU:HD11	1:A:474:VAL:HG11	2.01	0.42
1:B:958:TYR:HB2	1:B:959:PRO:HD2	2.02	0.42
1:A:24:PRO:HA	1:A:27:GLN:HB2	2.02	0.42
1:A:603:VAL:HG11	1:A:1021:VAL:HA	2.01	0.42
1:B:514:ALA:O	1:B:515:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:VAL:O	1:B:658:MSE:HB2	2.20	0.42
1:B:273:VAL:O	1:B:277:LEU:HD12	2.20	0.41
1:B:600:ARG:NH2	1:B:1023:GLU:OE1	2.52	0.41
1:B:611:VAL:HG21	1:B:1028:TYR:HB3	2.02	0.41
1:A:676:LYS:HD3	1:A:796:MSE:HB3	2.01	0.41
1:B:879:ARG:HG2	1:B:905:ASP:OD2	2.20	0.41
1:B:939:HIS:HB2	1:B:975:ILE:HD11	2.02	0.41
1:B:1012:VAL:HG21	1:B:1016:LEU:HD23	2.02	0.41
1:A:428:VAL:HG11	1:A:470:LEU:HB2	2.02	0.41
1:A:438:VAL:O	1:A:442:LEU:HG	2.21	0.41
1:A:1178:ARG:HE	1:A:1178:ARG:HB2	1.57	0.41
1:B:67:ALA:O	1:B:137:THR:HG22	2.19	0.41
1:B:227:ARG:HD3	1:B:1089:GLU:HG3	2.00	0.41
1:B:418:HIS:NE2	1:B:480:ASN:OD1	2.38	0.41
1:A:222:ALA:HB2	1:A:229:ILE:HD11	2.01	0.41
1:A:879:ARG:HD3	1:B:879:ARG:HD3	2.02	0.41
1:B:814:GLU:OE2	1:B:814:GLU:N	2.53	0.41
1:A:293:LEU:H	1:A:293:LEU:HD22	1.84	0.41
1:B:107:THR:O	1:B:111:ARG:HG3	2.21	0.41
1:B:836:ASP:HB3	1:B:839:GLN:HB2	2.03	0.41
1:A:677:THR:O	1:A:681:VAL:HG13	2.20	0.41
1:A:725:LEU:HD21	1:A:754:ARG:HE	1.85	0.41
1:A:876:PRO:HB2	1:B:881:VAL:HG12	2.02	0.41
1:B:911:THR:O	1:B:915:THR:HG23	2.21	0.41
1:A:858:HIS:NE2	1:A:863:THR:HG23	2.35	0.41
1:A:1054:ALA:HB1	1:A:1104:LEU:HA	2.03	0.41
1:A:1064:ASP:OD1	1:A:1067:ARG:NH2	2.54	0.41
1:A:1091:ILE:HA	1:A:1095:GLY:O	2.21	0.41
1:B:94:GLU:HG2	1:B:951:ARG:HD2	2.03	0.41
1:B:571:ASP:OD1	1:B:571:ASP:N	2.53	0.41
1:B:879:ARG:HG2	1:B:879:ARG:H	1.69	0.41
1:A:671:ASP:OD1	1:A:671:ASP:N	2.47	0.40
1:B:519:ASP:CG	1:B:575:ARG:HH12	2.29	0.40
1:A:138:ARG:HG3	1:A:362:PHE:CE1	2.56	0.40
1:A:912:ILE:H	1:A:912:ILE:HD12	1.86	0.40
1:A:1174:ALA:HB3	1:A:1175:PRO:HD3	2.02	0.40
1:A:544:ARG:HH22	1:A:1049:ASP:HA	1.87	0.40
1:B:191:ARG:HD2	1:B:1094:TYR:CD1	2.56	0.40
1:B:594:ASN:OD1	1:B:595:THR:N	2.54	0.40
1:B:808:SER:HB3	1:B:1022:GLY:HA2	2.03	0.40
1:B:756:LEU:HD11	1:B:780:HIS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:ARG:NH1	1:B:813:ARG:HH12	2.19	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	1140/1235 (92%)	1081 (95%)	56 (5%)	3 (0%)	36	67
1	B	1137/1235 (92%)	1070 (94%)	61 (5%)	6 (0%)	24	58
All	All	2277/2470 (92%)	2151 (94%)	117 (5%)	9 (0%)	30	62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1134	PRO
1	B	588	GLY
1	A	560	THR
1	A	1134	PRO
1	B	248	THR
1	B	758	THR
1	B	463	VAL
1	B	672	VAL
1	A	183	GLY

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	827/961 (86%)	826 (100%)	1 (0%)	88	94
1	B	807/961 (84%)	806 (100%)	1 (0%)	88	94
All	All	1634/1922 (85%)	1632 (100%)	2 (0%)	88	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1203	MSE
1	B	240	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	594	ASN
1	A	618	GLN
1	A	689	GLN
1	A	780	HIS
1	A	783	HIS
1	A	901	ASN
1	A	1194	ASN
1	B	226	GLN
1	B	839	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

5 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	1302	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	B	1301	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	A	1303	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	B	1302	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	1301	-	4,4,4	0.24	0	6,6,6	0.06	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1302	SO4	1	0
2	A	1301	SO4	1	0

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	1129/1235 (91%)	-0.02	12 (1%) 78 61	43, 76, 115, 138	0
1	B	1128/1235 (91%)	0.07	12 (1%) 78 61	46, 82, 116, 153	0
All	All	2257/2470 (91%)	0.02	24 (1%) 78 61	43, 78, 115, 153	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	822	PRO	3.5
1	B	682	ARG	3.1
1	A	347	GLY	2.8
1	B	401	ALA	2.7
1	A	552	ALA	2.6
1	B	492	ASN	2.6
1	B	821	PRO	2.6
1	A	789	THR	2.5
1	A	583	SER	2.5
1	A	743	ASP	2.4
1	A	978	ASN	2.3
1	B	476	LEU	2.3
1	A	352	ILE	2.3
1	B	540	GLY	2.3
1	A	644	THR	2.3
1	B	820	THR	2.2
1	B	979	ASN	2.1
1	B	755	LEU	2.1
1	B	717	GLY	2.1
1	B	448	ALA	2.1
1	A	271	GLY	2.1
1	A	261	GLU	2.1
1	A	262	HIS	2.0
1	A	494	VAL	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($\text{\AA}^2$)	Q<0.9
2	SO4	B	1302	5/5	0.81	0.12	121,128,130,135	0
2	SO4	B	1301	5/5	0.95	0.07	61,66,69,76	0
2	SO4	A	1303	5/5	0.96	0.06	78,81,90,90	0
2	SO4	A	1301	5/5	0.96	0.05	63,69,78,79	0
2	SO4	A	1302	5/5	0.96	0.06	63,63,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.