



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2019 – 11:59 AM EDT

PDB ID : 6AC6
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

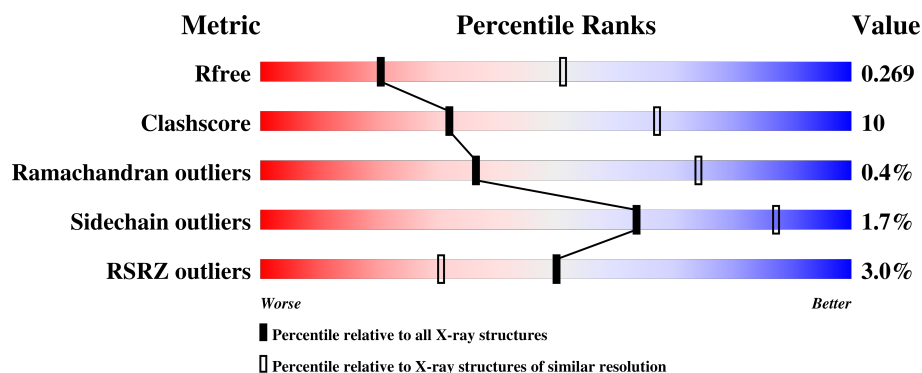
1 Overall quality at a glance

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}	111664	2374 (3.00-2.96)
Clashscore	122126	2712 (3.00-2.96)
Ramachandran outliers	120053	2626 (3.00-2.96)
Sidechain outliers	120020	2629 (3.00-2.96)
RSRZ outliers	108989	2268 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>75%</div> <div>18%</div> <div>7%</div> </div>
1	B	1235	<div> <div>3%</div> <div>71%</div> <div>21%</div> <div>7%</div> </div>

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:

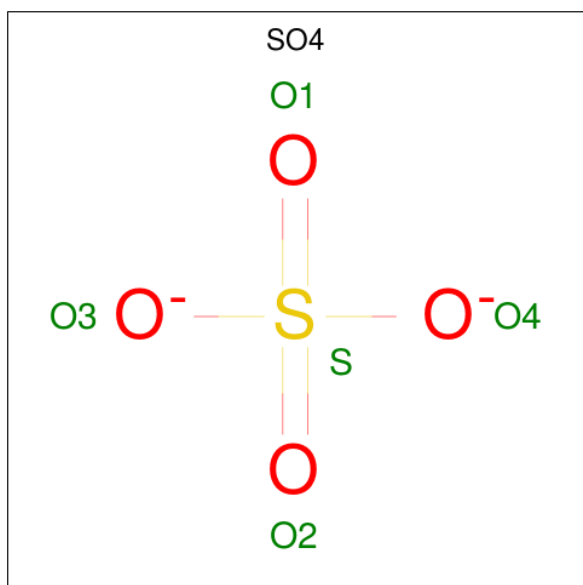
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	initiating methionine	UNP I7G7M2
A	-18	GLY	-	expression tag	UNP I7G7M2
A	-17	SER	-	expression tag	UNP I7G7M2
A	-16	SER	-	expression tag	UNP I7G7M2
A	-15	HIS	-	expression tag	UNP I7G7M2
A	-14	HIS	-	expression tag	UNP I7G7M2
A	-13	HIS	-	expression 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 (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	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		

L1193	T1036	T915	V793	G675	Q572	V474	S342	E209	L79	MSE
ASN	VAL	G916	L794	E678	L573	V475	G347	F210	R80	GLY
PRO	THR	I917	T795	I679	A581	M480	G348	W211	F83	SER
ALA	PRO	I926	S797	A680	L587	L481	D349	D212	V87	HIS
GLN	GLN	R929	V681	V681	G588	V482	A350	D213	S86	HIS
GLU	GLN	A930	R682	G589	G589	T483	P351	S216	P90	HIS
ALA	GLN	D931	S808	Q693	S590	L484	L352	F221	P91	HIS
LYS	K1044	L935	S808	Q693	S590	G491	L354	R227	S92	SER
ARG	V1052	S936	R813	T700	N594	M492	L354	S228	W93	SER
		Q937	E814	T701	T595	VAL	R369	A239	E94	GLY
		L938	L702	L702	K596	THR	W379	V240	T95	LEU
		H939	L703	L703	A599	ALA	W380	P241	L96	VAL
		Q940	H707	H707	R600	ALA	T381	E99	E99	PRO
		L941	E823	H707	R600	GLU	S386	R100	R100	GLY
		R944	V832	T710	V603	ARG	S386	T248	P103	SER
		S948	D836	R714	V611	LYS	V391	T264	T107	HIS
		R949	Q839	G717	Y614	LEU	E392	THR	R111	MSE
		R951	V840	F718	R617	ALA	A401	GLU	R120	ALA
		R958	R846	F719	Q618	LYS	ARG	THR	R120	GLY
		P959	R846	V720	Q618	ARG	GLY	VAL	R120	HIS
		L964	Q853	T721	A624	R507	SER	P270	D123	THR
		R971	K723	T722	P629	D511	GLN	V273	E124	SER
		L972	S726	K723	W631	A514	H406	V286	T125	VAL
		A973	R858	S727	Q632	L515	L415	M276	T135	T11
		T974	R860	R728	A633	D519	H418	L277	T136	L19
		R975	R862	L741	E634	V522	A425	A278	T137	P24
		M985	R872	K742	E636	V522	A425	E282	R138	
		A988	R879	D743	D637	I528	A435	V286	V154	Q27
		E993	V880	V746	A638	V532	H436	V286	D28	
		N999	V881	G751	PHE	E533	V439	T305	R32	
		H1008	V882	L755	THR	M534	E444	L308	L40	
		V1012	V887	L756	GLU	G540	A445	A312	V43	
		G1013	R888	L757	THR	L547	D446	D318	V43	
		F1014	E889	Q757	ILE	V551	T447	P319	S47	
		D1015	R894	T758	D646	A552	A448	V322	A48	
		L1016	V899	T768	V654	SER	L452	A326	R49	
		Y1017	D905	V770	M658	LYS	A460	E187	L56	
		I1018	E773	E773	P661	ARG	V463	I330	P61	
		L1019	Q774	Q774	V662	GLY	G464	K331	L62	
		L1020	R775	R775	P663	GLY	V465	R191	L63	
		V1021	F776	F776	V667	GLY	L466	I134	V64	
		G1022	H780	H780	I668	T560	P469	E338	V65	
		E1023	K781	K781	C669		L470	A339	A66	
		Y1028	R788	R788	V672	D571		S340	A67	
								W341	E78	

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) 96.5 (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 0.219 , 0.269	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)	0.29 , 51.0	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	0.26	0/8542	0.44	0/11635
1	B	0.27	0/8461	0.45	2/11529 (0.0%)
All	All	0.26	0/17003	0.45	2/23164 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	80	ARG	NE-CZ-NH2	-5.16	117.72	120.30

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	174	0
2	A	15	0	0	2	0
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	316	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 (316) 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:HD2	1:B:862:ARG:H	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1119:ILE:HA	1:A:1134:PRO:HG2	1.85	0.56
1:A:772:GLU:OE1	1:A:774:GLN:NE2	2.36	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
1:B:1101:ALA:O	1:B:1105:VAL:HG23	2.06	0.55
1:B:534:MSE:SE	1:B:547:LEU:HD13	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:ILE:HG23	1:A:1134:PRO:HD2	1.89	0.55
1:A:650:ALA:O	1:A:654:VAL:HG13	2.07	0.55
1:B:859:ASN:HA	1:B:910:THR:HG22	1.88	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:629:THR:HG22	1:B:631:TRP:H	1.73	0.54
1:B:99:GLU:OE1	1:B:846:ARG:NH1	2.40	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:178:ARG:NH2	1:B:190:VAL:HG11	2.23	0.54
1:B:164:PHE:CZ	1:B:190:VAL:HG23	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:715:MSE:CE	1:A:748:VAL:HG11	2.42	0.50
1:A:91:PRO:HD2	1:A:111:ARG:HG3	1.93	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:OG1	1:B:11:THR:O	2.24	0.50
1:A:701:THR:HG22	1:A:752:THR:HG21	1.94	0.50
1:B:124:GLU:H	1:B:124:GLU:CD	2.15	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:917:LEU:C	1:B:944:ARG:HH21	2.16	0.49
1:B:1008:HIS:O	1:B:1012:VAL:HG12	2.11	0.49
1:B:635:MSE:O	1:B:714:ARG:NH2	2.34	0.49
1:B:83:PHE:HB2	1:B:87:VAL:HG23	1.95	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:1120:THR:HG23	1:A:1134:PRO:HG3	1.95	0.48
1:A:853:GLN:OE1	1:A:921:ASN:ND2	2.47	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
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:1114:CYS:HB3	1:B:1119:ILE:HB	1.95	0.47
1:B:174:LEU:HD22	1:B:241:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1155:ARG:HB2	1:B:1158:THR:OG1	2.15	0.47
1:A:1071:TYR:HE1	1:A:1104:LEU:HD11	1.80	0.47
1:B:164:PHE:HD1	1:B:210:PHE:CE2	2.33	0.47
1:B:1129:THR:HG22	1:B:1164:PRO:HA	1.97	0.47
1:B:853:GLN:NE2	1:B:899:PHE:O	2.48	0.47
1:A:395(A):ILE:HG12	1:A:476:LEU:HD23	1.97	0.46
1:B:1133:SER:HB3	1:B:1134:PRO:HD3	1.96	0.46
1:B:43:VAL:HG13	1:B:392:GLU:HA	1.97	0.46
1:B:278:ALA:O	1:B:282:GLU:HG3	2.15	0.46
1:B:1017:TYR:O	1:B:1021:VAL:HG23	2.14	0.46
1:B:65:VAL:HG22	1:B:135:THR:HG23	1.97	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:1177:ILE:HG13	1:B:1182:LEU:HB2	1.98	0.46
1:B:183:GLY:N	1:B:187:GLU:OE2	2.36	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:1079:ASP:OD1	1:B:1079:ASP:N	2.48	0.46
1:B:369:ARG:HG3	1:B:379:TRP:CG	2.50	0.46
1:B:47:SER:OG	1:B:474:VAL:HG12	2.15	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: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:1014:PHE:O	1:B:1018:VAL:HG22	2.16	0.46
1:B:352:ILE:O	1:B:354:LEU:HD12	2.16	0.46
1:A:1120:THR:H	1:A:1134:PRO:CG	2.28	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:B:338:GLU:O	1:B:342:SER:HB3	2.16	0.46
1:B:61:PRO:HB2	1:B:312:ALA:HB2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:ALA:N	2:A:1301:SO4:O1	2.46	0.45
1:A:776:PHE:O	1:A:781:LYS:NZ	2.50	0.45
1:B:191:ARG:HD2	1:B:1094:TYR:HD1	1.82	0.45
1:A:1087:VAL:O	1:A:1091:ILE:HG13	2.16	0.45
1:A:657:ASP:N	1:A:657:ASP:OD1	2.49	0.45
1:A:1120:THR:H	1:A:1134:PRO:HG3	1.81	0.45
1:A:1148:MSE:HE2	1:A:1148:MSE:HB2	1.84	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: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:571:ASP:OD1	1:A:571:ASP:N	2.50	0.44
1:A:966:GLU:HA	1:A:969:TYR:CE2	2.51	0.44
1:B:276:MSE:HG3	1:B:286:VAL:HG11	1.98	0.44
1:B:83:PHE:HB3	1:B:86:SER:HB2	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: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:1069:GLU:OE2	1:A:1073:ARG:NH2	2.51	0.44
1:A:428:VAL:HA	1:A:466:LEU:O	2.18	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:1004:GLU:HG2	1:A:1005:GLN:N	2.33	0.44
1:A:105:VAL:HA	1:A:108:VAL:HG22	1.99	0.44
1:A:302:THR:OG1	1:A:303:THR:N	2.50	0.44
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:1059:GLU:OE1	1:A:1059:GLU:N	2.46	0.43
1:A:386:SER:HG	1:B:406:HIS:N	2.16	0.43
1:B:448:ALA:O	1:B:463:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD21	1:A:483:ILE:HD13	2.00	0.43
1:A:784:ILE:N	1:A:784:ILE:HD12	2.34	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:B:534:MSE:HB3	1:B:534:MSE:HE3	1.99	0.43
1:B:675:GLY:O	1:B:679:ILE:HD12	2.19	0.43
1:B:669:CYS:HA	1:B:797:SER:O	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:1082:ALA:O	1:A:1086:VAL:HG23	2.19	0.42
1:A:863:THR:OG1	1:A:863:THR:O	2.37	0.42
1:B:1016:LEU:O	1:B:1020:LEU:HG	2.20	0.42
1:B:721:THR:OG1	1:B:746:VAL:HA	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:571:ASP:N	1:B:571:ASP:OD1	2.53	0.42
1:B:596:LYS:O	1:B:600:ARG:HB2	2.19	0.42
1:B:894:LYS:HB2	1:B:894:LYS:HE2	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
1:B:654:VAL:O	1:B:658:MSE:HB2	2.20	0.42
1:B:123:ASP:CG	1:B:125:THR:HG22	2.40	0.42
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:B:273:VAL:O	1:B:277:LEU:HD12	2.20	0.41
1:A:676:LYS:HD3	1:A:796:MSE:HB3	2.01	0.41
1:B:1012:VAL:HG21	1:B:1016:LEU:HD23	2.02	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:A:1178:ARG:HB2	1:A:1178:ARG:HE	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:VAL:O	1:A:442:LEU:HG	2.21	0.41
1:A:428:VAL:HG11	1:A:470:LEU:HB2	2.02	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:N	1:B:814:GLU:OE2	2.53	0.41
1:A:293:LEU:HD22	1:A:293:LEU:H	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:B:879:ARG:HG2	1:B:879:ARG:H	1.69	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:A:858:HIS:NE2	1:A:863:THR:HG23	2.35	0.41
1:B:889:GLU:H	1:B:889:GLU:CD	2.23	0.41
1:B:94:GLU:HG2	1:B:951:ARG:HD2	2.03	0.41
1:A:671:ASP:N	1:A:671:ASP:OD1	2.47	0.40
1:A:138:ARG:HG3	1:A:362:PHE:CE1	2.56	0.40
1:A:434:THR:OG1	1:A:434:THR:O	2.36	0.40
1:A:912:ILE:HD12	1:A:912:ILE:H	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:808:SER:HB3	1:B:1022:GLY:HA2	2.03	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:756:LEU:HD11	1:B:780:HIS:HA	2.03	0.40
1:B:788:ARG:NH1	1:B:813:ARG:HH12	2.19	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	1140/1235 (92%)	1081 (95%)	56 (5%)	3 (0%)	43	78
1	B	1137/1235 (92%)	1070 (94%)	61 (5%)	6 (0%)	31	70
All	All	2277/2470 (92%)	2151 (94%)	117 (5%)	9 (0%)	36	74

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

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%)	809 (98%)	18 (2%)	55	83
1	B	807/961 (84%)	798 (99%)	9 (1%)	76	92
All	All	1634/1922 (85%)	1607 (98%)	27 (2%)	63	87

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	114	LEU
1	A	198	PHE
1	A	231	GLU
1	A	334	ARG
1	A	389	SER
1	A	467	LYS
1	A	537	ARG
1	A	646	ASP
1	A	676	LYS
1	A	815	MSE
1	A	879	ARG
1	A	888	ASN
1	A	1067	ARG
1	A	1144	ARG
1	A	1176	ARG
1	A	1180	LEU
1	A	1203	MSE
1	B	198	PHE
1	B	211	TRP
1	B	519	ASP
1	B	587	LEU
1	B	669	CYS
1	B	682	ARG
1	B	860	ARG
1	B	985	MSE
1	B	1064	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	594	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	1301	-	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	A	1302	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	A	1303	-	4,4,4	0.17	0	6,6,6	0.07	0
2	SO4	B	1301	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	B	1302	-	4,4,4	0.16	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.

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	1129/1235 (91%)	0.11	34 (3%)	50 30	43, 76, 115, 138	0
1	B	1128/1235 (91%)	0.10	33 (2%)	51 31	46, 82, 116, 153	0
All	All	2257/2470 (91%)	0.11	67 (2%)	50 30	43, 78, 115, 153	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	717	GLY	4.6
1	B	463	VAL	4.5
1	A	552	ALA	4.3
1	B	540	GLY	4.2
1	B	349	ASP	4.1
1	A	551	TYR	3.8
1	B	682	ARG	3.5
1	A	746	VAL	3.5
1	A	1172	VAL	3.3
1	B	213	ASP	3.2
1	B	633	ALA	3.2
1	B	491	GLY	3.2
1	B	964	LEU	3.2
1	A	762	TRP	3.1
1	B	445	ALA	3.0
1	A	550	GLU	3.0
1	A	563	LEU	2.9
1	B	581	ALA	2.9
1	A	743	ASP	2.9
1	B	444	GLU	2.9
1	B	515	LEU	2.8
1	A	1127	ALA	2.8
1	A	559	GLY	2.8
1	A	691	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	765	LEU	2.7
1	B	720	VAL	2.7
1	B	551	TYR	2.7
1	B	480	ASN	2.7
1	A	561	ASP	2.7
1	A	261	GLU	2.7
1	A	789	THR	2.7
1	B	464	GLY	2.6
1	A	791	VAL	2.6
1	B	425	ALA	2.5
1	A	582	PRO	2.5
1	A	246	LEU	2.5
1	A	286	VAL	2.4
1	A	631	TRP	2.4
1	A	663	PRO	2.4
1	B	817	THR	2.4
1	A	174	LEU	2.4
1	B	347	GLY	2.3
1	A	693	GLN	2.3
1	B	350	ALA	2.3
1	B	460	ALA	2.3
1	A	760	VAL	2.3
1	B	719	PRO	2.3
1	A	761	THR	2.3
1	A	494	VAL	2.2
1	B	277	LEU	2.2
1	A	732	ALA	2.2
1	A	675	GLY	2.2
1	A	1176	ARG	2.2
1	B	483	ILE	2.1
1	B	465	VAL	2.1
1	B	415	LEU	2.1
1	B	484	ILE	2.1
1	B	449	ALA	2.1
1	A	564	TYR	2.1
1	A	1168	ALA	2.0
1	B	448	ALA	2.0
1	A	231	GLU	2.0
1	B	470	LEU	2.0
1	A	759	GLY	2.0
1	B	741	LEU	2.0
1	B	590	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	272	THR	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 carbohydrates 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(\AA^2)	Q<0.9
2	SO4	B	1302	5/5	0.81	0.16	121,128,130,135	0
2	SO4	A	1303	5/5	0.97	0.17	78,81,90,90	0
2	SO4	A	1302	5/5	0.97	0.18	63,63,64,64	0
2	SO4	B	1301	5/5	0.98	0.15	61,66,69,76	0
2	SO4	A	1301	5/5	0.98	0.13	63,69,78,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.