



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:41 PM UTC

PDB ID : 1R7I / pdb_00001r7i
Title : HMG-CoA Reductase from *P. mevalonii*, native structure at 2.2 angstroms resolution.
Authors : Watson, J.M.; Steussy, C.N.; Burgner, J.W.; Lawrence, C.M.; Tabernero, L.; Rodwell, V.W.; Stauffacher, C.V.
Deposited on : 2003-10-21
Resolution : 2.21 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

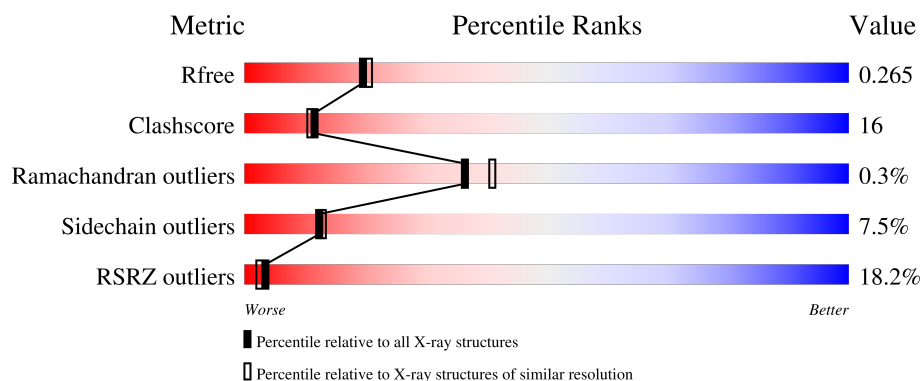
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	428	
1	B	428	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	1003	-	-	X	-

2 Entry composition [i](#)

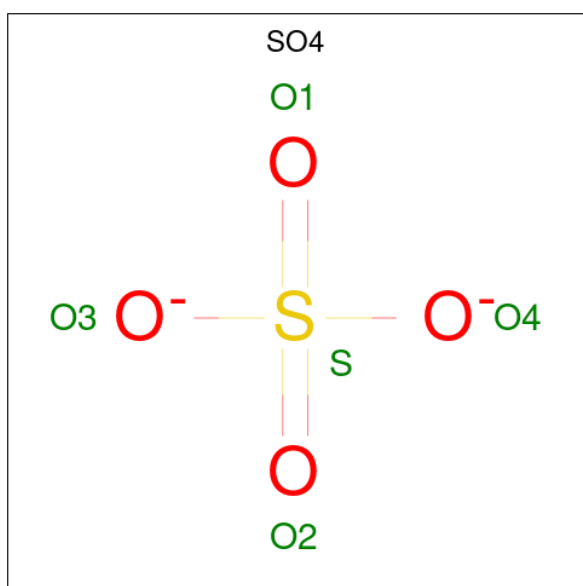
There are 4 unique types of molecules in this entry. The entry contains 5833 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-hydroxy-3-methylglutaryl-coenzyme A reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2761	1730	499	518	14			
1	B	375	Total	C	N	O	S	0	0	0
			2782	1743	502	523	14			

- 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	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

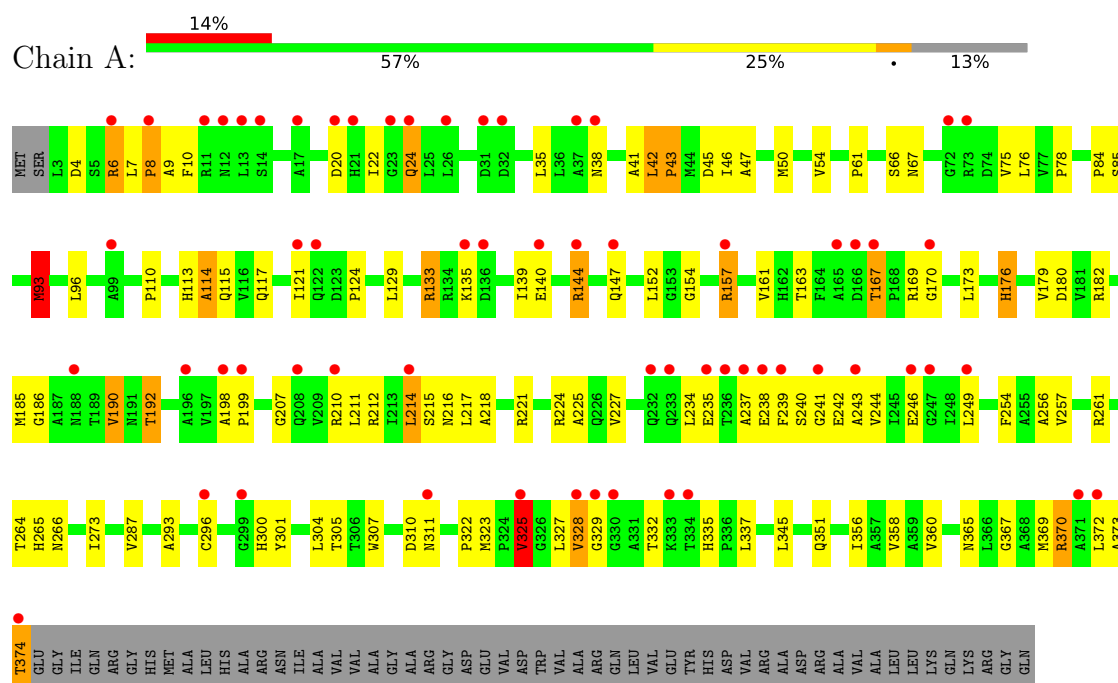
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total	O	0	0
			133	133		
4	B	130	Total	O	0	0
			130	130		

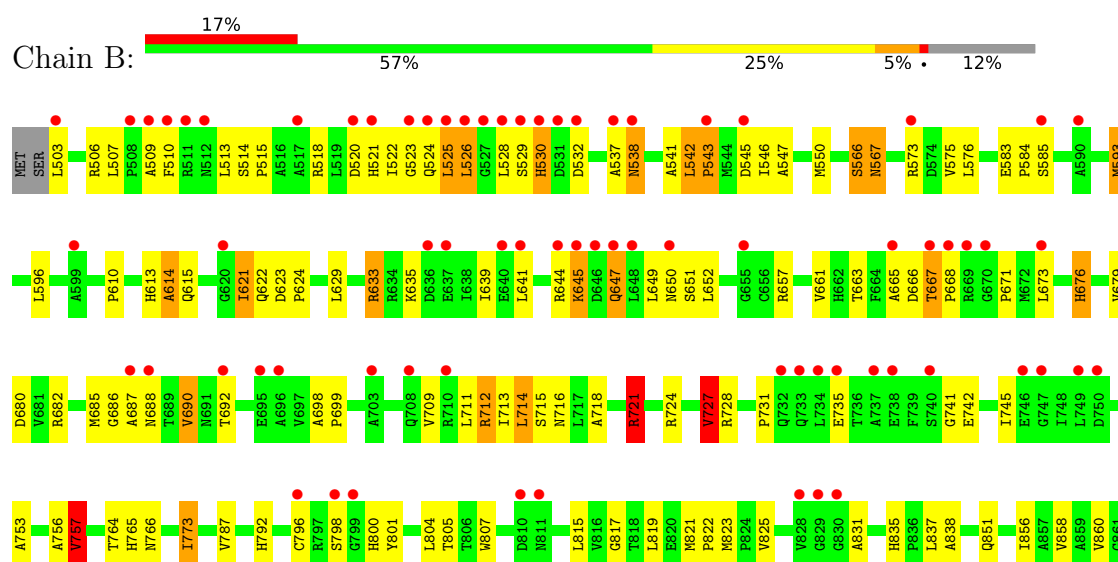
3 Residue-property plots

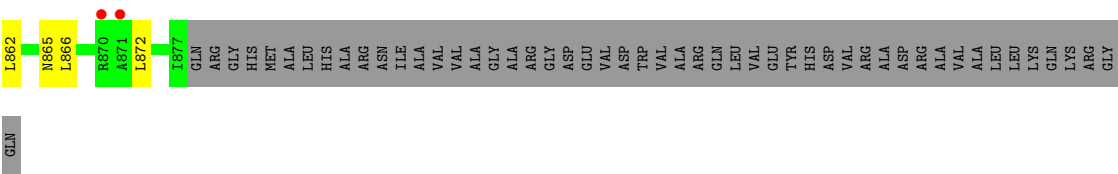
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	226.19Å 226.19Å 226.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.66 – 2.21 26.66 – 2.21	Depositor EDS
% Data completeness (in resolution range)	87.0 (26.66-2.21) 87.1 (26.66-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.256 , 0.270 0.254 , 0.265	Depositor DCC
R_{free} test set	3489 reflections (7.78%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5833	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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, GOL

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	1.03	17/2804 (0.6%)	1.22	29/3815 (0.8%)
1	B	1.04	16/2825 (0.6%)	1.22	30/3843 (0.8%)
All	All	1.03	33/5629 (0.6%)	1.22	59/7658 (0.8%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	MET	SD-CE	-17.41	1.36	1.79
1	B	685	MET	SD-CE	-16.67	1.37	1.79
1	B	550	MET	SD-CE	-16.50	1.38	1.79
1	A	185	MET	SD-CE	-15.54	1.40	1.79
1	B	593	MET	SD-CE	-11.05	1.51	1.79
1	A	93	MET	SD-CE	-10.27	1.53	1.79
1	B	727	VAL	CB-CG2	-9.06	1.22	1.52
1	B	727	VAL	CB-CG1	-8.40	1.24	1.52
1	A	227	VAL	CB-CG2	-8.28	1.25	1.52
1	A	227	VAL	CB-CG1	-7.83	1.26	1.52
1	B	724	ARG	CZ-NH1	-7.68	1.22	1.32
1	A	224	ARG	CZ-NH2	-7.53	1.23	1.33
1	A	212	ARG	CZ-NH1	-7.38	1.22	1.32
1	A	224	ARG	CZ-NH1	-7.34	1.22	1.32
1	B	692	THR	CB-CG2	-7.21	1.28	1.52
1	B	724	ARG	CZ-NH2	-7.15	1.24	1.33
1	B	825	VAL	CB-CG2	-6.96	1.29	1.52
1	B	712	ARG	CZ-NH1	-6.88	1.23	1.32
1	A	192	THR	CB-CG2	-6.88	1.29	1.52
1	A	325	VAL	CB-CG1	-6.83	1.30	1.52
1	A	38	ASN	CG-OD1	-6.79	1.10	1.23
1	A	157	ARG	CZ-NH1	-6.66	1.23	1.32
1	A	35	LEU	C-O	6.27	1.31	1.24
1	A	45	ASP	CG-OD2	-6.24	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	545	ASP	CG-OD2	-5.62	1.14	1.25
1	A	257	VAL	CB-CG1	-5.59	1.34	1.52
1	A	325	VAL	CB-CG2	-5.59	1.34	1.52
1	B	757	VAL	CB-CG2	-5.58	1.34	1.52
1	B	825	VAL	CB-CG1	-5.57	1.34	1.52
1	B	538	ASN	CG-OD1	-5.53	1.13	1.23
1	B	757	VAL	CB-CG1	-5.40	1.34	1.52
1	B	526	LEU	C-O	5.06	1.30	1.24
1	A	257	VAL	CB-CG2	-5.02	1.35	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	546	ILE	N-CA-C	-11.03	100.13	110.82
1	A	46	ILE	N-CA-C	-9.66	101.45	110.82
1	A	212	ARG	NE-CZ-NH2	9.27	127.55	119.20
1	B	712	ARG	NE-CZ-NH2	9.00	127.30	119.20
1	B	724	ARG	NE-CZ-NH2	8.76	127.08	119.20
1	B	685	MET	N-CA-C	-8.48	101.98	111.82
1	A	185	MET	N-CA-C	-8.35	102.13	111.82
1	A	224	ARG	NH1-CZ-NH2	-7.99	108.91	119.30
1	A	243	ALA	N-CA-C	-7.80	102.86	111.36
1	B	686	GLY	N-CA-C	7.66	124.03	114.37
1	A	234	LEU	N-CA-C	7.62	122.77	113.17
1	A	186	GLY	N-CA-C	7.49	123.80	114.37
1	B	667	THR	N-CA-CB	7.17	124.10	111.18
1	B	773	ILE	N-CA-C	7.17	117.77	110.82
1	B	721	ARG	NE-CZ-NH2	7.11	125.60	119.20
1	B	724	ARG	NH1-CZ-NH2	-7.02	110.17	119.30
1	B	727	VAL	CB-CA-C	-6.98	98.50	110.30
1	A	224	ARG	NE-CZ-NH2	6.94	125.44	119.20
1	B	524	GLN	N-CA-C	6.92	119.84	111.40
1	B	667	THR	CB-CA-C	-6.85	97.61	109.32
1	A	35	LEU	CA-C-O	-6.68	112.29	119.97
1	B	757	VAL	CB-CA-C	-6.46	104.13	111.55
1	A	157	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	A	227	VAL	CG1-CB-CG2	-6.24	97.07	110.80
1	B	721	ARG	NE-CZ-NH1	-6.21	115.28	121.50
1	A	273	ILE	N-CA-C	6.21	116.84	110.82
1	A	133	ARG	NE-CZ-NH1	-6.06	115.44	121.50
1	B	679	VAL	N-CA-C	6.03	116.81	108.12
1	A	133	ARG	NE-CZ-NH2	5.96	124.57	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	821	MET	N-CA-C	5.96	113.50	108.13
1	B	545	ASP	CA-C-N	-5.93	112.26	120.74
1	B	545	ASP	C-N-CA	-5.93	112.26	120.74
1	A	179	VAL	N-CA-C	5.92	116.39	108.11
1	B	831	ALA	N-CA-C	-5.80	106.17	113.18
1	A	24	GLN	CB-CA-C	-5.78	101.76	110.90
1	B	567	ASN	N-CA-C	5.68	122.91	110.80
1	A	373	ALA	N-CA-C	-5.64	106.40	113.28
1	A	311	ASN	N-CA-C	5.54	118.08	111.71
1	B	838	ALA	N-CA-C	-5.49	105.21	111.14
1	B	613	HIS	CB-CA-C	-5.48	100.24	109.50
1	B	666	ASP	N-CA-C	5.46	117.54	108.20
1	B	727	VAL	CG1-CB-CG2	-5.42	98.88	110.80
1	A	327	LEU	N-CA-C	-5.37	106.89	113.50
1	A	114	ALA	N-CA-C	-5.37	99.66	108.41
1	B	712	ARG	CG-CD-NE	5.35	123.78	112.00
1	A	144	ARG	N-CA-C	-5.34	107.31	113.88
1	B	614	ALA	N-CA-C	-5.34	99.71	108.41
1	B	757	VAL	N-CA-C	5.32	116.38	111.81
1	A	237	ALA	N-CA-C	-5.26	105.67	111.71
1	A	370	ARG	N-CA-C	-5.25	105.64	111.36
1	A	45	ASP	OD1-CG-OD2	-5.21	110.39	122.90
1	B	545	ASP	OD1-CG-OD2	-5.20	110.41	122.90
1	A	35	LEU	CA-C-N	-5.20	113.99	122.26
1	A	35	LEU	C-N-CA	-5.20	113.99	122.26
1	A	113	HIS	CB-CA-C	-5.14	100.81	109.50
1	A	6	ARG	CB-CA-C	-5.05	102.74	110.81
1	A	157	ARG	NE-CZ-NH1	-5.01	116.49	121.50
1	B	566	SER	N-CA-C	5.01	117.88	110.46
1	B	583	GLU	N-CA-C	5.00	115.97	109.72

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	2761	0	2805	92	0
1	B	2782	0	2825	88	0
2	A	10	0	0	0	1
2	B	5	0	0	1	0
3	A	12	0	12	7	0
4	A	133	0	0	2	0
4	B	130	0	0	8	0
All	All	5833	0	5642	179	1

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 16.

All (179) 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)
3:A:1003:GOL:O3	3:A:1003:GOL:C3	1.66	1.43
3:A:1004:GOL:O3	3:A:1004:GOL:C3	1.66	1.40
1:A:235:GLU:HG2	1:A:241:GLY:N	1.56	1.17
1:A:235:GLU:HG2	1:A:241:GLY:H	0.88	1.02
1:B:721:ARG:HD3	1:B:851:GLN:HE22	1.29	0.95
1:A:235:GLU:CG	1:A:241:GLY:H	1.78	0.95
1:A:6:ARG:C	1:A:8:PRO:HD3	1.99	0.87
1:A:167:THR:HG23	1:A:169:ARG:H	1.38	0.86
1:A:114:ALA:HB2	1:A:190:VAL:HG13	1.58	0.85
1:B:709:VAL:CG1	1:B:712:ARG:HD2	2.08	0.84
1:B:614:ALA:HB2	1:B:690:VAL:HG13	1.60	0.84
1:A:93:MET:CE	1:A:96:LEU:HD12	2.08	0.83
1:B:699:PRO:HG2	4:B:3423:HOH:O	1.78	0.82
1:A:238:GLU:HG3	1:A:239:PHE:CD1	2.14	0.81
1:A:4:ASP:OD1	1:A:6:ARG:HG2	1.81	0.81
1:A:7:LEU:O	1:A:10:PHE:HB2	1.81	0.79
1:A:6:ARG:CB	1:A:8:PRO:HD3	2.13	0.79
1:B:647:GLN:HA	1:B:650:ASN:HD22	1.49	0.77
1:B:796:CYS:HB2	4:B:3127:HOH:O	1.83	0.77
1:B:593:MET:HE2	1:B:866:LEU:HG	1.67	0.77
1:A:167:THR:HG22	1:A:170:GLY:O	1.85	0.76
1:B:510:PHE:HA	1:B:513:LEU:HD12	1.66	0.76
1:B:721:ARG:HD3	1:B:851:GLN:NE2	2.00	0.75
1:A:6:ARG:HB3	1:A:8:PRO:HD3	1.67	0.74
1:A:238:GLU:HG3	1:A:239:PHE:CE1	2.25	0.72
1:A:323:MET:HE2	1:A:325:VAL:CG1	2.20	0.72
1:B:688:ASN:HB3	4:B:3383:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ARG:CB	1:A:8:PRO:CD	2.70	0.70
1:B:507:LEU:HD12	1:B:566:SER:HB3	1.74	0.70
1:A:235:GLU:HG2	1:A:241:GLY:CA	2.21	0.70
1:B:709:VAL:HG11	1:B:712:ARG:HD2	1.72	0.69
1:A:370:ARG:O	1:A:374:THR:HB	1.90	0.69
3:A:1003:GOL:O3	3:A:1003:GOL:C2	2.35	0.69
1:A:221:ARG:HE	1:A:351:GLN:HE22	1.38	0.69
1:B:709:VAL:HG12	1:B:712:ARG:HD2	1.75	0.69
3:A:1004:GOL:O3	3:A:1004:GOL:C2	2.37	0.69
1:A:372:LEU:HB3	1:B:711:LEU:HD22	1.74	0.68
1:A:242:GLU:H	1:A:242:GLU:CD	2.02	0.68
1:A:93:MET:HE3	1:A:93:MET:HA	1.76	0.67
1:A:114:ALA:CB	1:A:190:VAL:HG13	2.25	0.66
1:A:211:LEU:HD22	1:B:872:LEU:HB3	1.77	0.66
1:B:735:GLU:CD	1:B:741:GLY:H	2.04	0.66
1:A:307:TRP:HE1	1:A:365:ASN:ND2	1.94	0.65
1:A:6:ARG:HB2	1:A:8:PRO:HD2	1.79	0.65
1:A:266:ASN:HD21	1:A:304:LEU:H	1.46	0.64
1:A:135:LYS:O	1:A:139:ILE:HG13	1.98	0.64
1:B:645:LYS:N	1:B:645:LYS:HD2	2.10	0.64
1:B:614:ALA:CB	1:B:690:VAL:HG13	2.28	0.64
1:B:773:ILE:HD13	4:B:3125:HOH:O	1.98	0.63
1:B:807:TRP:HE1	1:B:865:ASN:ND2	1.96	0.63
3:A:1003:GOL:C3	3:A:1003:GOL:HO3	2.09	0.63
1:B:530:HIS:CD2	1:B:530:HIS:H	2.16	0.62
1:A:216:ASN:HD22	1:B:764:THR:HA	1.64	0.62
1:A:6:ARG:HB2	1:A:8:PRO:CD	2.29	0.62
1:A:7:LEU:N	1:A:8:PRO:CD	2.63	0.62
1:B:541:ALA:O	1:B:543:PRO:HD3	1.99	0.61
1:A:221:ARG:HE	1:A:351:GLN:NE2	1.98	0.61
1:B:766:ASN:HD21	1:B:804:LEU:H	1.49	0.61
1:A:264:THR:HA	1:B:716:ASN:HD22	1.64	0.61
1:A:6:ARG:HB3	1:A:8:PRO:CD	2.29	0.60
1:A:93:MET:HE1	1:A:96:LEU:HD12	1.83	0.60
1:B:507:LEU:HB3	1:B:510:PHE:HB2	1.83	0.60
1:B:731:PRO:O	1:B:741:GLY:HA3	2.01	0.60
1:A:296:CYS:HB3	1:A:301:TYR:HA	1.83	0.60
1:A:4:ASP:CG	1:A:6:ARG:HG2	2.27	0.59
1:A:115:GLN:HE21	1:A:176:HIS:HE1	1.50	0.59
1:B:615:GLN:HE21	1:B:676:HIS:HE1	1.50	0.58
1:B:690:VAL:HG11	1:B:714:LEU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1004:GOL:C3	3:A:1004:GOL:HO3	2.09	0.57
1:B:765:HIS:HD2	4:B:3526:HOH:O	1.86	0.57
1:A:7:LEU:HD12	1:A:66:SER:HB3	1.87	0.56
1:A:240:SER:O	1:A:244:VAL:HG23	2.06	0.56
1:A:93:MET:HE3	1:A:96:LEU:HD12	1.86	0.56
1:A:110:PRO:HA	1:A:221:ARG:HG3	1.87	0.55
1:A:6:ARG:C	1:A:8:PRO:CD	2.76	0.55
1:B:621:ILE:HD12	1:B:624:PRO:HA	1.88	0.55
1:A:238:GLU:OE2	1:A:239:PHE:CE1	2.60	0.54
1:B:542:LEU:HD13	1:B:547:ALA:HB2	1.89	0.54
1:B:644:ARG:C	1:B:645:LYS:HD2	2.33	0.54
1:A:140:GLU:O	1:A:144:ARG:HG3	2.07	0.54
1:A:190:VAL:HG11	1:A:214:LEU:HB2	1.88	0.54
1:A:115:GLN:HE21	1:A:176:HIS:CE1	2.25	0.54
1:A:242:GLU:O	1:A:246:GLU:HG2	2.07	0.54
1:B:641:LEU:O	1:B:645:LYS:HD3	2.07	0.54
1:B:615:GLN:HE21	1:B:676:HIS:CE1	2.25	0.54
1:A:372:LEU:HD11	3:A:1003:GOL:O2	2.08	0.53
1:B:610:PRO:HA	1:B:721:ARG:HG3	1.90	0.53
1:B:787:VAL:CG2	1:B:823:MET:HE1	2.39	0.53
1:B:523:GLY:HA2	1:B:528:LEU:HD12	1.91	0.52
1:B:721:ARG:HH21	1:B:851:GLN:NE2	2.07	0.52
1:B:680:ASP:OD1	1:B:682:ARG:HD2	2.09	0.52
1:A:335:HIS:CE1	1:A:337:LEU:HB2	2.45	0.52
1:B:731:PRO:HG3	1:B:745:ILE:HD12	1.92	0.52
1:B:509:ALA:O	1:B:513:LEU:HG	2.10	0.52
1:B:698:ALA:N	1:B:699:PRO:HD2	2.25	0.51
1:B:663:THR:HG22	1:B:673:LEU:HD13	1.92	0.51
1:A:287:VAL:CG2	1:A:323:MET:HE1	2.41	0.51
1:A:180:ASP:OD1	1:A:182:ARG:HD2	2.11	0.50
1:A:323:MET:HE2	1:A:325:VAL:HG12	1.93	0.50
1:A:198:ALA:N	1:A:199:PRO:HD2	2.26	0.50
1:B:515:PRO:HD2	4:B:3504:HOH:O	2.12	0.50
1:A:93:MET:CE	1:A:93:MET:HA	2.42	0.50
1:A:121:ILE:HD12	1:A:124:PRO:HA	1.93	0.49
1:A:167:THR:CG2	1:A:169:ARG:H	2.18	0.48
1:B:526:LEU:HD13	1:B:528:LEU:HD21	1.94	0.48
1:B:663:THR:HG22	1:B:673:LEU:CD1	2.44	0.48
1:A:41:ALA:O	1:A:43:PRO:HD3	2.12	0.48
1:A:42:LEU:HD13	1:A:47:ALA:HB2	1.94	0.48
1:B:661:VAL:CG1	1:B:673:LEU:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HB3	1:A:10:PHE:HB2	1.96	0.48
1:B:593:MET:CE	1:B:596:LEU:HD12	2.43	0.47
1:B:529:SER:O	1:B:532:ASP:HB2	2.15	0.47
1:B:756:ALA:O	1:B:800:HIS:HE1	1.97	0.47
1:B:727:VAL:HG22	1:B:862:LEU:HD21	1.97	0.46
1:A:167:THR:HG22	1:A:170:GLY:N	2.31	0.46
1:A:78:PRO:HD2	1:A:345:LEU:HD21	1.97	0.46
1:A:215:SER:HA	1:B:764:THR:OG1	2.16	0.46
1:A:84:PRO:O	1:A:85:SER:HB2	2.16	0.46
1:B:753:ALA:O	1:B:757:VAL:HG23	2.16	0.46
1:A:307:TRP:HE1	1:A:365:ASN:HD21	1.64	0.46
1:B:635:LYS:O	1:B:639:ILE:HG13	2.15	0.46
1:B:742:GLU:OE1	1:B:742:GLU:N	2.47	0.45
1:A:22:ILE:HD12	1:A:76:LEU:HD13	1.98	0.45
1:A:242:GLU:CD	1:A:242:GLU:N	2.72	0.45
1:B:835:HIS:CE1	1:B:837:LEU:HB2	2.52	0.45
1:A:161:VAL:CG1	1:A:173:LEU:HD11	2.47	0.45
1:A:287:VAL:CG1	1:A:323:MET:HE1	2.45	0.45
1:B:584:PRO:O	1:B:585:SER:HB2	2.17	0.45
1:B:856:ILE:O	1:B:860:VAL:HG23	2.17	0.45
1:B:522:ILE:HD12	1:B:576:LEU:HD13	1.99	0.44
1:B:566:SER:O	1:B:567:ASN:HB2	2.18	0.44
1:B:819:LEU:HD23	1:B:858:VAL:O	2.17	0.44
1:A:254:PHE:CE2	1:A:261:ARG:HD3	2.53	0.44
1:A:328:VAL:O	1:A:332:THR:HB	2.18	0.44
1:B:641:LEU:O	1:B:644:ARG:HG2	2.17	0.44
1:B:798:SER:C	1:B:800:HIS:H	2.26	0.44
1:A:93:MET:SD	1:A:367:GLY:HA2	2.58	0.44
1:B:667:THR:HB	1:B:668:PRO:CD	2.49	0.43
1:A:163:THR:HG22	1:A:173:LEU:HD13	1.98	0.43
1:A:265:HIS:HD2	4:A:3343:HOH:O	2.01	0.43
1:A:217:LEU:HD13	1:A:293:ALA:HB3	2.01	0.43
1:A:356:ILE:O	1:A:360:VAL:HG23	2.19	0.43
1:B:514:SER:O	1:B:518:ARG:HG3	2.18	0.43
1:B:792:HIS:HD2	1:B:801:TYR:OH	2.02	0.43
1:A:238:GLU:OE2	1:A:239:PHE:HE1	2.02	0.43
1:B:687:ALA:HA	1:B:714:LEU:HD13	2.00	0.43
1:A:66:SER:O	1:A:67:ASN:HB2	2.19	0.42
1:A:8:PRO:O	1:A:9:ALA:HB3	2.19	0.42
1:A:218:ALA:O	1:A:322:PRO:HB3	2.18	0.42
1:A:369:MET:HE3	4:A:3343:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:VAL:CG1	1:B:823:MET:HE1	2.49	0.42
1:A:54:VAL:O	1:B:518:ARG:HD2	2.19	0.42
1:B:731:PRO:HG3	1:B:745:ILE:CD1	2.49	0.42
1:A:264:THR:OG1	1:B:715:SER:HA	2.20	0.42
1:A:310:ASP:OD1	1:A:310:ASP:C	2.62	0.42
1:B:506:ARG:O	1:B:507:LEU:C	2.62	0.42
1:A:167:THR:CG2	1:A:170:GLY:O	2.63	0.42
1:A:41:ALA:O	1:A:43:PRO:CD	2.68	0.41
1:B:623:ASP:OD1	1:B:623:ASP:N	2.52	0.41
1:A:154:GLY:HA2	1:A:157:ARG:HH21	1.85	0.41
1:A:256:ALA:O	1:A:300:HIS:HE1	2.04	0.41
1:B:807:TRP:CZ3	1:B:817:GLY:HA3	2.56	0.41
1:A:121:ILE:HG23	1:A:207:GLY:HA3	2.02	0.41
1:B:649:LEU:CD1	1:B:682:ARG:HG2	2.50	0.41
1:B:765:HIS:HE1	1:B:805:THR:OG1	2.03	0.41
1:B:525:LEU:HD21	1:B:576:LEU:HD11	2.02	0.41
1:B:665:ALA:O	1:B:671:PRO:HA	2.20	0.41
1:B:851:GLN:HG2	4:B:3538:HOH:O	2.21	0.41
1:A:117:GLN:OE1	1:A:210:ARG:HB3	2.21	0.41
1:B:688:ASN:ND2	2:B:1001:SO4:O2	2.53	0.41
1:B:713:ILE:CG1	1:B:714:LEU:N	2.84	0.41
1:A:265:HIS:HE1	1:A:305:THR:OG1	2.04	0.41
1:B:537:ALA:C	1:B:538:ASN:HD22	2.28	0.41
1:A:225:ALA:HB2	1:A:358:VAL:HG23	2.02	0.40
1:B:718:ALA:O	1:B:822:PRO:HB3	2.20	0.40
1:B:633:ARG:HD2	1:B:633:ARG:C	2.47	0.40
1:B:641:LEU:HD21	4:B:3423:HOH:O	2.20	0.40
1:B:503:LEU:O	1:B:503:LEU:HG	2.21	0.40
1:B:728:ARG:HA	1:B:815:LEU:O	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	Interatomic distance (Å)	Clash overlap (Å)
2:A:1002:SO4:O2	2:A:1002:SO4:O2[13_456]	2.02	0.18

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	370/428 (86%)	349 (94%)	19 (5%)	2 (0%)	24	26
1	B	373/428 (87%)	355 (95%)	18 (5%)	0	100	100
All	All	743/856 (87%)	704 (95%)	37 (5%)	2 (0%)	36	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	GLY
1	A	328	VAL

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	285/327 (87%)	265 (93%)	20 (7%)	14	15
1	B	287/327 (88%)	264 (92%)	23 (8%)	11	11
All	All	572/654 (88%)	529 (92%)	43 (8%)	12	13

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PRO
1	A	20	ASP
1	A	24	GLN
1	A	42	LEU

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Mol	Chain	Res	Type
1	A	43	PRO
1	A	61	PRO
1	A	75	VAL
1	A	93	MET
1	A	129	LEU
1	A	133	ARG
1	A	147	GLN
1	A	152	LEU
1	A	167	THR
1	A	176	HIS
1	A	190	VAL
1	A	192	THR
1	A	214	LEU
1	A	249	LEU
1	A	325	VAL
1	A	374	THR
1	B	520	ASP
1	B	521	HIS
1	B	525	LEU
1	B	530	HIS
1	B	542	LEU
1	B	543	PRO
1	B	573	ARG
1	B	575	VAL
1	B	621	ILE
1	B	622	GLN
1	B	629	LEU
1	B	633	ARG
1	B	645	LYS
1	B	647	GLN
1	B	651	SER
1	B	652	LEU
1	B	657	ARG
1	B	676	HIS
1	B	690	VAL
1	B	714	LEU
1	B	721	ARG
1	B	727	VAL
1	B	757	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	69	GLN
1	A	115	GLN
1	A	122	GLN
1	A	150	ASN
1	A	162	HIS
1	A	176	HIS
1	A	216	ASN
1	A	265	HIS
1	A	266	ASN
1	A	300	HIS
1	A	339	GLN
1	A	351	GLN
1	A	365	ASN
1	B	538	ASN
1	B	567	ASN
1	B	569	GLN
1	B	647	GLN
1	B	650	ASN
1	B	662	HIS
1	B	676	HIS
1	B	708	GLN
1	B	716	ASN
1	B	765	HIS
1	B	766	ASN
1	B	792	HIS
1	B	800	HIS
1	B	839	GLN
1	B	851	GLN
1	B	865	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 ⓘ

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	B	1001	-	4,4,4	0.34	0	6,6,6	0.07	0
3	GOL	A	1004	-	5,5,5	4.26	2 (40%)	5,5,5	0.29	0
2	SO4	A	1000	-	4,4,4	0.46	0	6,6,6	0.26	0
2	SO4	A	1002	-	4,4,4	0.44	0	6,6,6	0.11	0
3	GOL	A	1003	-	5,5,5	4.04	2 (40%)	5,5,5	0.48	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
3	GOL	A	1003	-	-	2/4/4/4	-
3	GOL	A	1004	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1004	GOL	C3-C2	-7.55	1.23	1.51
3	A	1003	GOL	C3-C2	-7.05	1.24	1.51
3	A	1004	GOL	O3-C3	5.70	1.66	1.42
3	A	1003	GOL	O3-C3	5.66	1.66	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1004	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	1004	GOL	O2-C2-C3-O3
3	A	1003	GOL	C1-C2-C3-O3
3	A	1003	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	SO4	1	0
3	A	1004	GOL	3	0
2	A	1002	SO4	0	1
3	A	1003	GOL	4	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 ⓘ

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	372/428 (86%)	0.98	62 (16%) 4 3	18, 30, 58, 99	0
1	B	375/428 (87%)	1.10	74 (19%) 3 2	17, 30, 59, 87	0
All	All	747/856 (87%)	1.04	136 (18%) 3 2	17, 30, 59, 99	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ARG	5.3
1	B	524	GLN	4.8
1	B	525	LEU	4.6
1	B	710	ARG	4.5
1	A	299	GLY	4.4
1	A	328	VAL	4.2
1	B	646	ASP	4.2
1	B	645	LYS	4.2
1	B	530	HIS	4.1
1	A	329	GLY	4.1
1	B	647	GLN	4.1
1	A	21	HIS	4.1
1	A	330	GLY	4.1
1	B	503	LEU	4.0
1	A	170	GLY	4.0
1	A	144	ARG	3.9
1	A	374	THR	3.9
1	A	237	ALA	3.8
1	A	166	ASP	3.8
1	A	239	PHE	3.6
1	B	667	THR	3.6
1	B	517	ALA	3.6
1	B	665	ALA	3.6
1	B	746	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	521	HIS	3.6
1	B	737	ALA	3.6
1	B	670	GLY	3.5
1	B	532	ASP	3.5
1	A	208	GLN	3.5
1	A	249	LEU	3.5
1	B	871	ALA	3.5
1	A	238	GLU	3.5
1	A	24	GLN	3.5
1	B	798	SER	3.5
1	B	531	ASP	3.4
1	A	210	ARG	3.4
1	A	136	ASP	3.4
1	A	23	GLY	3.4
1	B	527	GLY	3.3
1	B	669	ARG	3.2
1	B	641	LEU	3.2
1	B	692	THR	3.2
1	B	830	GLY	3.2
1	A	236	THR	3.2
1	A	167	THR	3.1
1	A	311	ASN	3.1
1	B	708	GLN	3.1
1	B	732	GLN	3.1
1	B	545	ASP	3.0
1	A	73	ARG	3.0
1	A	122	GLN	3.0
1	B	512	ASN	3.0
1	B	688	ASN	3.0
1	A	8	PRO	3.0
1	A	165	ALA	2.9
1	A	243	ALA	2.9
1	A	334	THR	2.9
1	A	235	GLU	2.9
1	A	296	CYS	2.9
1	A	247	GLY	2.9
1	B	528	LEU	2.9
1	A	121	ILE	2.9
1	A	246	GLU	2.9
1	B	829	GLY	2.9
1	A	37	ALA	2.9
1	B	644	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	811	ASN	2.8
1	B	695	GLU	2.8
1	A	20	ASP	2.8
1	B	650	ASN	2.8
1	A	147	GLN	2.8
1	B	734	LEU	2.8
1	B	537	ALA	2.8
1	B	523	GLY	2.8
1	A	72	GLY	2.7
1	B	508	PRO	2.7
1	B	747	GLY	2.7
1	B	538	ASN	2.7
1	B	750	ASP	2.7
1	A	14	SER	2.7
1	A	32	ASP	2.7
1	A	11	ARG	2.6
1	A	140	GLU	2.6
1	B	740	SER	2.6
1	B	673	LEU	2.6
1	A	13	LEU	2.5
1	B	738	GLU	2.5
1	B	796	CYS	2.5
1	B	599	ALA	2.5
1	B	526	LEU	2.5
1	B	749	LEU	2.5
1	A	333	LYS	2.5
1	B	620	GLY	2.5
1	A	12	ASN	2.5
1	A	188	ASN	2.5
1	B	529	SER	2.4
1	B	573	ARG	2.4
1	B	687	ALA	2.4
1	B	870	ARG	2.4
1	A	26	LEU	2.4
1	A	232	GLN	2.4
1	A	241	GLY	2.4
1	A	371	ALA	2.4
1	A	135	LYS	2.4
1	B	828	VAL	2.4
1	B	733	GLN	2.4
1	A	38	ASN	2.4
1	B	799	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	543	PRO	2.3
1	B	696	ALA	2.3
1	B	640	GLU	2.3
1	B	703	ALA	2.3
1	B	585	SER	2.3
1	A	372	LEU	2.3
1	B	648	LEU	2.3
1	B	520	ASP	2.3
1	A	99	ALA	2.3
1	A	31	ASP	2.2
1	B	810	ASP	2.2
1	B	511	ARG	2.2
1	B	637	GLU	2.2
1	A	196	ALA	2.2
1	B	655	GLY	2.2
1	A	325	VAL	2.1
1	B	735	GLU	2.1
1	A	17	ALA	2.1
1	A	198	ALA	2.1
1	B	510	PHE	2.1
1	B	636	ASP	2.1
1	A	233	GLN	2.1
1	A	199	PRO	2.1
1	A	157	ARG	2.1
1	B	509	ALA	2.0
1	A	214	LEU	2.0
1	B	590	ALA	2.0
1	B	668	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1004	6/6	0.56	0.21	62,64,64,64	0
2	SO4	A	1002	5/5	0.67	0.23	65,66,69,71	0
3	GOL	A	1003	6/6	0.75	0.17	66,67,68,70	0
2	SO4	B	1001	5/5	0.84	0.19	57,60,63,65	0
2	SO4	A	1000	5/5	0.90	0.15	34,38,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.