



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 05:50 am BST

PDB ID : 1R7I  
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.; Taberner, 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

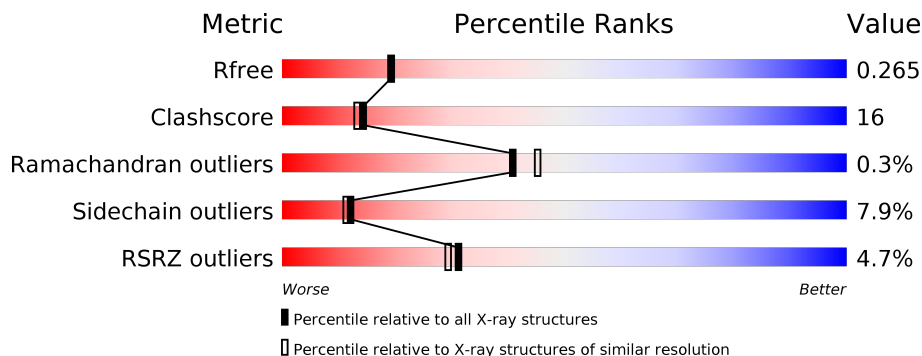
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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](#)

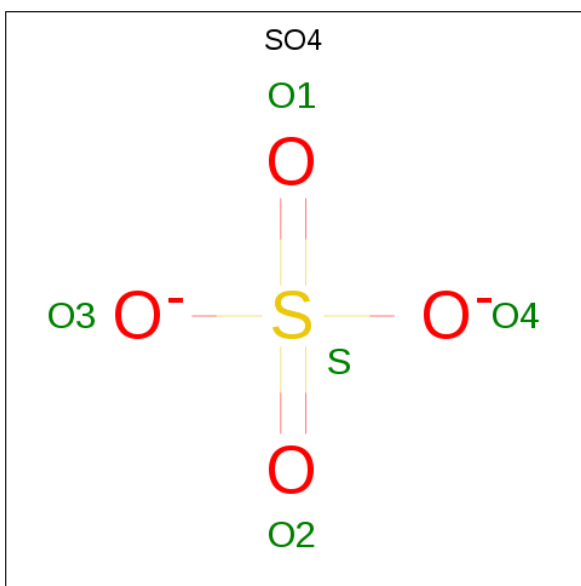
There are 4 unique types of molecules in this entry. The entry contains 5833 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	372	Total 2761	C 1730	N 499	O 518	S 14	0	0	0
1	B	375	Total 2782	C 1743	N 502	O 523	S 14	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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		



VAL  
ARG  
ALA  
ASP  
ARG  
ALA  
VAL  
ALA  
LEU  
LEU  
LYS  
GLN  
LYS  
ARG  
GLY  
GLN

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	226.19Å 226.19Å 226.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.66 – 2.21 38.79 – 2.21	Depositor EDS
% Data completeness (in resolution range)	87.0 (26.66-2.21) 87.1 (38.79-2.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 2.20Å)	Xtrriage
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 <sup>2</sup> )	28.2	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	5833	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, 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	0.87	17/2804 (0.6%)	0.97	18/3815 (0.5%)
1	B	0.88	15/2825 (0.5%)	0.99	20/3843 (0.5%)
All	All	0.88	32/5629 (0.6%)	0.98	38/7658 (0.5%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	727	VAL	CB-CG2	-14.38	1.22	1.52
1	B	727	VAL	CB-CG1	-13.34	1.24	1.52
1	A	227	VAL	CB-CG2	-13.15	1.25	1.52
1	A	227	VAL	CB-CG1	-12.45	1.26	1.52
1	B	825	VAL	CB-CG2	-11.08	1.29	1.52
1	A	325	VAL	CB-CG1	-10.88	1.30	1.52
1	A	257	VAL	CB-CG1	-8.93	1.34	1.52
1	A	325	VAL	CB-CG2	-8.93	1.34	1.52
1	B	757	VAL	CB-CG2	-8.91	1.34	1.52
1	B	825	VAL	CB-CG1	-8.90	1.34	1.52
1	B	757	VAL	CB-CG1	-8.63	1.34	1.52
1	B	724	ARG	CZ-NH1	-8.50	1.22	1.33
1	A	212	ARG	CZ-NH1	-8.18	1.22	1.33
1	A	224	ARG	CZ-NH1	-8.13	1.22	1.33
1	A	257	VAL	CB-CG2	-8.04	1.35	1.52
1	B	712	ARG	CZ-NH1	-7.64	1.23	1.33
1	A	50	MET	SD-CE	-7.47	1.36	1.77
1	A	157	ARG	CZ-NH1	-7.41	1.23	1.33
1	A	224	ARG	CZ-NH2	-7.23	1.23	1.33
1	B	692	THR	CB-CG2	-7.15	1.28	1.52
1	B	685	MET	SD-CE	-7.14	1.37	1.77
1	B	550	MET	SD-CE	-7.06	1.38	1.77
1	B	724	ARG	CZ-NH2	-6.84	1.24	1.33
1	A	192	THR	CB-CG2	-6.81	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	575	VAL	CB-CG1	-6.80	1.38	1.52
1	A	185	MET	SD-CE	-6.63	1.40	1.77
1	A	38	ASN	CG-OD1	-6.05	1.10	1.24
1	B	575	VAL	CB-CG2	-5.94	1.40	1.52
1	A	75	VAL	CB-CG2	-5.90	1.40	1.52
1	A	75	VAL	CB-CG1	-5.88	1.40	1.52
1	B	657	ARG	CZ-NH1	-5.46	1.25	1.33
1	A	45	ASP	CG-OD2	-5.15	1.13	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	ARG	NE-CZ-NH2	14.49	127.55	120.30
1	B	712	ARG	NE-CZ-NH2	14.00	127.30	120.30
1	B	724	ARG	NE-CZ-NH2	13.56	127.08	120.30
1	B	721	ARG	NE-CZ-NH2	10.59	125.60	120.30
1	B	545	ASP	CB-CG-OD1	10.36	127.63	118.30
1	B	633	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	A	224	ARG	NE-CZ-NH2	10.29	125.44	120.30
1	B	721	ARG	NE-CZ-NH1	-10.03	115.28	120.30
1	B	633	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	133	ARG	NE-CZ-NH1	-9.72	115.44	120.30
1	A	45	ASP	CB-CG-OD1	9.67	127.01	118.30
1	A	224	ARG	NH1-CZ-NH2	-9.54	108.91	119.40
1	A	157	ARG	NE-CZ-NH2	9.29	124.94	120.30
1	A	224	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	A	227	VAL	CG1-CB-CG2	-8.64	97.07	110.90
1	A	133	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	A	221	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	B	724	ARG	NH1-CZ-NH2	-8.39	110.17	119.40
1	A	157	ARG	NE-CZ-NH1	-7.63	116.49	120.30
1	B	727	VAL	CG1-CB-CG2	-7.51	98.88	110.90
1	B	667	THR	N-CA-CB	7.26	124.10	110.30
1	A	221	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	A	45	ASP	OD1-CG-OD2	-6.79	110.39	123.30
1	B	727	VAL	CB-CA-C	-6.79	98.50	111.40
1	B	545	ASP	OD1-CG-OD2	-6.78	110.41	123.30
1	B	657	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	B	825	VAL	CG1-CB-CG2	-6.29	100.84	110.90
1	A	325	VAL	CG1-CB-CG2	-6.15	101.06	110.90
1	B	712	ARG	CG-CD-NE	5.70	123.78	111.80
1	B	685	MET	CG-SD-CE	5.59	109.14	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	657	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	212	ARG	NH1-CZ-NH2	-5.37	113.50	119.40
1	B	757	VAL	CG1-CB-CG2	-5.31	102.41	110.90
1	A	133	ARG	CD-NE-CZ	5.26	130.96	123.60
1	B	667	THR	CB-CA-C	-5.18	97.61	111.60
1	A	257	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	B	613	HIS	CB-CA-C	-5.08	100.24	110.40
1	A	185	MET	CG-SD-CE	5.01	108.21	100.20

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	2761	0	2805	90	0
1	B	2782	0	2825	86	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	1	0
4	B	130	0	0	9	0
All	All	5833	0	5642	174	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 (174) 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:C3	3:A:1003:GOL:O3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLU:CG	1:A:241:GLY:H	1.78	0.95
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:A:6:ARG:C	1:A:8:PRO:HD3	1.99	0.82
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: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:B:688:ASN:HB3	4:B:3383:HOH:O	1.89	0.71
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
3:A:1003:GOL:C2	3:A:1003:GOL:O3	2.35	0.69
1:A:370:ARG:O	1:A:374:THR:HB	1.90	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: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: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:593:MET:HE2	1:B:866:LEU:HG	1.78	0.63
1:B:807:TRP:HE1	1:B:865:ASN:ND2	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1003:GOL:C3	3:A:1003:GOL:HO3	2.09	0.63
1:A:93:MET:HE3	1:A:96:LEU:HD12	1.79	0.63
1:A:242:GLU:H	1:A:242:GLU:CD	2.02	0.63
1:B:593:MET:HE1	1:B:596:LEU:HD12	1.80	0.62
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:B:735:GLU:CD	1:B:741:GLY:H	2.04	0.61
1:A:6:ARG:HB3	1:A:8:PRO:CD	2.29	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: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
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:110:PRO:HA	1:A:221:ARG:HG3	1.87	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: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:4:ASP:CG	1:A:6:ARG:HG2	2.27	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: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:A:93:MET:HE1	1:A:96:LEU:HD12	1.90	0.52
1:B:680:ASP:OD1	1:B:682:ARG:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:180:ASP:OD1	1:A:182:ARG:HD2	2.11	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:B:644:ARG:C	1:B:645:LYS:HD2	2.33	0.49
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
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:A:7:LEU:N	1:A:8:PRO:HD3	2.29	0.47
1:A:93:MET:HA	1:A:93:MET:HE3	1.97	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:215:SER:HA	1:B:764:THR:OG1	2.16	0.46
1:A:78:PRO:HD2	1:A:345:LEU:HD21	1.97	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:A:287:VAL:HG13	1:A:323:MET:HE3	1.97	0.46
1:B:635:LYS:O	1:B:639:ILE:HG13	2.15	0.46
1:A:323:MET:HE2	1:A:325:VAL:CG1	2.45	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: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:6:ARG:C	1:A:8:PRO:CD	2.76	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:566:SER:O	1:B:567:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:ILE:HD12	1:B:576:LEU:HD13	1.99	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: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:218:ALA:O	1:A:322:PRO:HB3	2.18	0.42
1:A:8:PRO:O	1:A:9:ALA:HB3	2.19	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:B:821:MET:HE2	4:B:3125:HOH:O	2.20	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:N	1:B:623:ASP:OD1	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:A:242:GLU:N	1:A:242:GLU:CD	2.72	0.41
1:A:296:CYS:HG	1:B:796:CYS:HG	1.69	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:A:225:ALA:HB2	1:A:358:VAL:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:ARG:O	1:B:658:ASP:HB2	2.21	0.40
1:B:718:ALA:O	1:B:822:PRO:HB3	2.20	0.40
1:B:641:LEU:HD21	4:B:3423:HOH:O	2.20	0.40
1:B:503:LEU:HG	1:B:503:LEU:O	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 [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	370/428 (86%)	349 (94%)	19 (5%)	2 (0%)	29	30
1	B	373/428 (87%)	355 (95%)	18 (5%)	0	100	100
All	All	743/856 (87%)	704 (95%)	37 (5%)	2 (0%)	41	45

All (2) Ramachandran outliers are listed below:

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

### 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	285/327 (87%)	264 (93%)	21 (7%)	13	13
1	B	287/327 (88%)	263 (92%)	24 (8%)	11	10
All	All	572/654 (88%)	527 (92%)	45 (8%)	12	11

All (45) 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
1	A	43	PRO
1	A	74	ASP
1	A	75	VAL
1	A	93	MET
1	A	129	LEU
1	A	133	ARG
1	A	152	LEU
1	A	167	THR
1	A	169	ARG
1	A	176	HIS
1	A	190	VAL
1	A	192	THR
1	A	210	ARG
1	A	214	LEU
1	A	249	LEU
1	A	285	ARG
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	545	ASP
1	B	573	ARG
1	B	574	ASP
1	B	575	VAL
1	B	622	GLN
1	B	629	LEU
1	B	633	ARG

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Mol	Chain	Res	Type
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	785	ARG
1	B	870	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	176	HIS
1	A	216	ASN
1	A	265	HIS
1	A	266	ASN
1	A	300	HIS
1	A	351	GLN
1	A	365	ASN
1	B	538	ASN
1	B	647	GLN
1	B	650	ASN
1	B	676	HIS
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 [i](#)

There are no RNA molecules in this entry.

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

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	1002	-	4,4,4	0.34	0	6,6,6	0.08	0
3	GOL	A	1004	-	5,5,5	4.05	2 (40%)	5,5,5	0.28	0
2	SO4	B	1001	-	4,4,4	0.23	0	6,6,6	0.09	0
3	GOL	A	1003	-	5,5,5	3.85	2 (40%)	5,5,5	0.46	0
2	SO4	A	1000	-	4,4,4	0.36	0	6,6,6	0.23	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	-6.98	1.23	1.51
3	A	1003	GOL	C3-C2	-6.51	1.24	1.51
3	A	1004	GOL	O3-C3	5.67	1.66	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	GOL	O3-C3	5.63	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
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	A	1002	SO4	0	1
3	A	1004	GOL	3	0
2	B	1001	SO4	1	0
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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	372/428 (86%)	0.15	14 (3%) 40 38	18, 30, 58, 99	0
1	B	375/428 (87%)	0.23	21 (5%) 24 23	17, 30, 59, 87	0
All	All	747/856 (87%)	0.19	35 (4%) 31 29	17, 30, 59, 99	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	647	GLN	5.0
1	B	645	LYS	4.2
1	B	530	HIS	3.9
1	B	525	LEU	3.8
1	A	238	GLU	3.5
1	A	236	THR	3.5
1	B	648	LEU	3.2
1	B	665	ALA	3.2
1	B	646	ASP	3.0
1	B	692	THR	2.9
1	A	299	GLY	2.9
1	A	237	ALA	2.9
1	A	6	ARG	2.8
1	A	235	GLU	2.8
1	B	503	LEU	2.8
1	B	732	GLN	2.8
1	A	232	GLN	2.7
1	B	640	GLU	2.7
1	B	644	ARG	2.6
1	A	239	PHE	2.5
1	B	652	LEU	2.5
1	A	73	ARG	2.3
1	B	523	GLY	2.3
1	A	24	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	573	ARG	2.3
1	B	524	GLN	2.2
1	A	144	ARG	2.2
1	B	545	ASP	2.2
1	B	531	ASP	2.2
1	A	165	ALA	2.1
1	B	532	ASP	2.1
1	A	287	VAL	2.1
1	B	651	SER	2.1
1	A	243	ALA	2.0
1	B	528	LEU	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, 95<sup>th</sup> 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	0.15	0.28	62,64,64,64	0
3	GOL	A	1003	6/6	0.73	0.30	66,67,68,70	0
2	SO4	A	1002	5/5	0.75	0.27	65,66,69,71	0
2	SO4	B	1001	5/5	0.92	0.15	57,60,63,65	0
2	SO4	A	1000	5/5	0.94	0.13	34,38,41,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.