



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1P9N / pdb_00001p9n
Title : Crystal structure of Escherichia coli MobB.
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Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2003-05-12
Resolution : 2.80 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

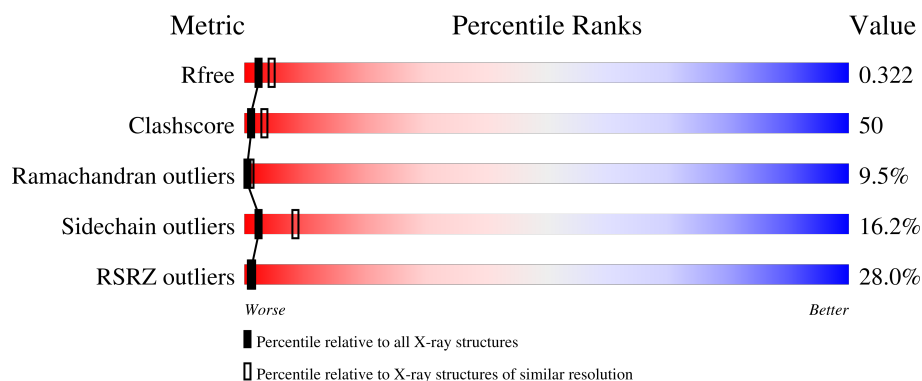
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	170	
1	B	170	

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
2	SO4	B	171	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2605 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.

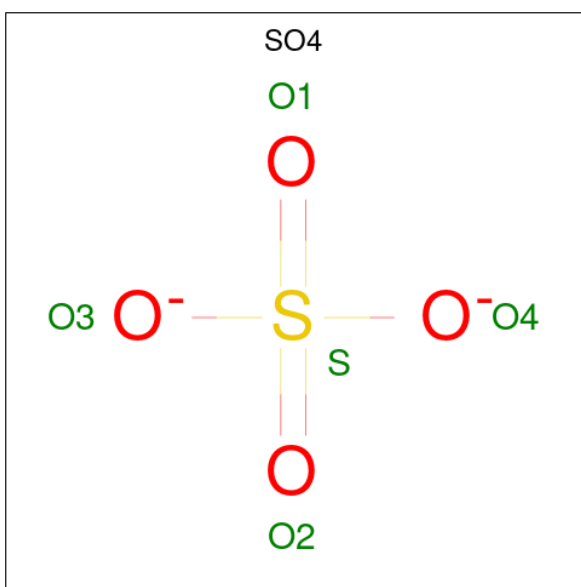
- Molecule 1 is a protein called Molybdopterin-guanine dinucleotide biosynthesis protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	Se	0	0	0
			1270	809	219	236	1	5			
1	B	162	Total	C	N	O	S	Se	0	0	0
			1270	809	219	236	1	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P32125
A	43	MSE	MET	modified residue	UNP P32125
A	74	MSE	MET	modified residue	UNP P32125
A	92	MSE	MET	modified residue	UNP P32125
A	165	MSE	MET	modified residue	UNP P32125
B	1	MSE	MET	modified residue	UNP P32125
B	43	MSE	MET	modified residue	UNP P32125
B	74	MSE	MET	modified residue	UNP P32125
B	92	MSE	MET	modified residue	UNP P32125
B	165	MSE	MET	modified residue	UNP P32125

- 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	B	1	Total	O	S	0	0
			5	4	1		

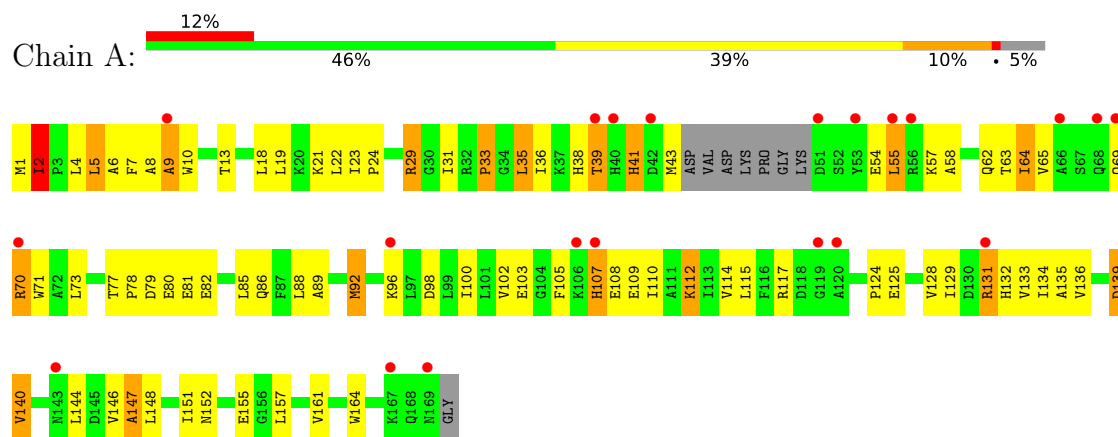
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	21	Total	O	0	0
			21	21		

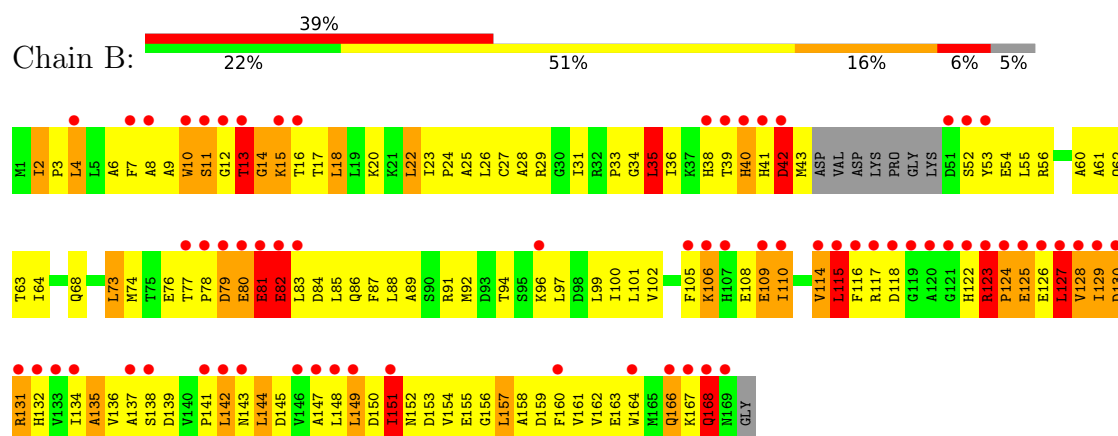
3 Residue-property plots [i](#)

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: Molybdopterin-guanine dinucleotide biosynthesis protein B



• Molecule 1: Molybdopterin-guanine dinucleotide biosynthesis protein B



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	239.00Å 239.00Å 49.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.92 – 2.80 30.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	74.8 (30.92-2.80) 91.4 (30.92-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.275 , 0.308 0.297 , 0.322	Depositor DCC
R_{free} test set	2032 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.3	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	0.85	EDS
Total number of atoms	2605	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/1288	1.08	7/1737 (0.4%)
1	B	0.54	0/1288	1.06	9/1737 (0.5%)
All	All	0.56	0/2576	1.07	16/3474 (0.5%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	LEU	N-CA-C	-7.16	106.46	114.62
1	B	27	CYS	N-CA-C	-6.93	103.80	111.36
1	B	145	ASP	N-CA-C	-6.66	102.51	113.50
1	A	2	ILE	CA-C-N	6.62	128.11	119.84
1	A	2	ILE	C-N-CA	6.62	128.11	119.84
1	B	81	GLU	N-CA-C	6.52	124.69	110.80
1	B	168	GLN	N-CA-C	-6.35	97.28	110.80
1	A	10	TRP	N-CA-C	-6.24	98.81	108.42
1	A	139	ASP	N-CA-C	-6.15	104.95	112.88
1	B	123	ARG	CA-C-N	5.87	127.17	119.84
1	B	123	ARG	C-N-CA	5.87	127.17	119.84
1	A	112	LYS	N-CA-C	5.61	118.34	108.75
1	B	40	HIS	N-CA-C	-5.56	108.28	114.62
1	B	35	LEU	N-CA-C	5.37	117.58	108.02
1	A	65	VAL	N-CA-C	5.20	114.76	107.37
1	A	136	VAL	N-CA-C	-5.03	101.24	108.53

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	1270	0	1290	100	1
1	B	1270	0	1290	176	0
2	A	5	0	0	0	0
2	B	5	0	0	2	0
3	A	34	0	0	7	1
3	B	21	0	0	5	0
All	All	2605	0	2580	254	2

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 50.

All (254) 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:114:VAL:HG12	1:B:115:LEU:H	1.22	0.98
1:A:29:ARG:HG2	1:A:29:ARG:HH11	1.31	0.94
1:A:70:ARG:HB3	1:B:76:GLU:HA	1.51	0.92
1:A:64:ILE:HD11	1:B:88:LEU:HB3	1.51	0.91
1:B:143:ASN:O	1:B:144:LEU:HG	1.71	0.89
1:B:79:ASP:HB3	3:B:179:HOH:O	1.74	0.88
1:B:131:ARG:HH11	1:B:131:ARG:HB2	1.40	0.85
1:B:106:LYS:H	1:B:106:LYS:HD2	1.43	0.84
1:A:81:GLU:OE2	1:B:68:GLN:HA	1.78	0.83
1:A:155:GLU:HG2	3:A:195:HOH:O	1.80	0.82
1:B:109:GLU:HG3	1:B:132:HIS:NE2	1.95	0.82
1:B:29:ARG:HH12	1:B:159:ASP:CG	1.88	0.81
1:A:70:ARG:HG3	1:A:70:ARG:HH11	1.45	0.81
1:B:127:LEU:HD22	1:B:129:ILE:HD11	1.62	0.80
1:A:36:ILE:HA	1:B:64:ILE:HG23	1.64	0.80
1:A:55:LEU:HD12	1:A:55:LEU:H	1.48	0.79
1:A:92:MSE:HE1	1:A:100:ILE:HD13	1.62	0.78
1:B:74:MSE:HB2	3:B:178:HOH:O	1.83	0.77
1:B:131:ARG:HB2	1:B:131:ARG:NH1	1.99	0.76
1:B:167:LYS:O	1:B:168:GLN:HG3	1.86	0.76
1:A:18:LEU:O	1:A:18:LEU:HD23	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASP:C	1:B:132:HIS:H	1.95	0.74
1:B:114:VAL:HG12	1:B:115:LEU:N	2.01	0.74
1:B:63:THR:HG22	1:B:74:MSE:HB3	1.69	0.74
1:A:38:HIS:HB2	1:A:105:PHE:CE1	2.23	0.74
1:B:134:ILE:O	1:B:135:ALA:HB2	1.89	0.73
1:B:82:GLU:OE1	1:B:82:GLU:HA	1.88	0.73
1:B:31:ILE:O	1:B:33:PRO:HD3	1.89	0.72
1:B:158:ALA:O	1:B:162:VAL:HG23	1.89	0.72
1:A:89:ALA:HA	1:A:92:MSE:HE2	1.73	0.71
1:B:23:ILE:HB	1:B:24:PRO:HD3	1.73	0.71
1:B:9:ALA:HB3	1:B:15:LYS:HD3	1.72	0.70
1:B:77:THR:C	1:B:79:ASP:H	1.98	0.70
1:B:96:LYS:HD2	1:B:96:LYS:O	1.91	0.70
1:B:2:ILE:HD11	1:B:100:ILE:HG13	1.72	0.70
1:B:56:ARG:HH11	1:B:63:THR:HG21	1.57	0.70
1:A:55:LEU:HD12	1:A:55:LEU:N	2.08	0.68
1:B:56:ARG:HD3	1:B:63:THR:CG2	2.23	0.68
1:B:94:THR:HA	1:B:97:LEU:HD12	1.76	0.68
1:B:124:PRO:C	1:B:126:GLU:H	2.02	0.68
1:A:96:LYS:HZ2	1:B:62:GLN:HG3	1.59	0.68
1:A:71:TRP:CD1	1:B:82:GLU:HG3	2.29	0.67
1:A:29:ARG:HG2	1:A:29:ARG:NH1	2.04	0.67
1:A:4:LEU:HD23	1:A:100:ILE:HB	1.77	0.67
1:B:122:HIS:NE2	1:B:126:GLU:HG3	2.10	0.67
1:A:96:LYS:NZ	1:B:62:GLN:HG3	2.10	0.66
1:B:152:ASN:HB3	3:B:176:HOH:O	1.95	0.66
1:B:38:HIS:HB2	1:B:105:PHE:CE1	2.32	0.65
1:B:26:LEU:O	1:B:31:ILE:HB	1.97	0.65
1:B:143:ASN:O	1:B:144:LEU:CG	2.44	0.65
1:B:127:LEU:O	1:B:127:LEU:HD13	1.97	0.64
1:A:23:ILE:HB	1:A:24:PRO:HD3	1.79	0.64
1:A:21:LYS:O	1:A:24:PRO:HD2	1.97	0.64
1:A:71:TRP:HD1	1:B:82:GLU:HG3	1.61	0.64
1:A:19:LEU:O	1:A:23:ILE:HG12	1.98	0.64
1:B:150:ASP:C	1:B:152:ASN:H	2.06	0.63
1:B:25:ALA:O	1:B:29:ARG:HD2	1.98	0.63
1:A:2:ILE:O	1:A:2:ILE:HG23	1.98	0.62
1:B:9:ALA:C	1:B:10:TRP:HE3	2.08	0.62
1:B:160:PHE:O	1:B:163:GLU:HB2	2.00	0.62
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.63	0.62
1:A:85:LEU:HD13	1:A:102:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:CD1	1:A:146:VAL:HG12	2.30	0.61
1:B:56:ARG:HD3	1:B:63:THR:HG21	1.82	0.61
1:B:128:VAL:HG13	1:B:128:VAL:O	2.00	0.61
1:A:31:ILE:O	1:A:33:PRO:HD3	2.00	0.60
1:B:92:MSE:HE1	1:B:100:ILE:HD13	1.83	0.60
1:B:122:HIS:NE2	1:B:126:GLU:OE1	2.34	0.60
1:B:127:LEU:O	1:B:129:ILE:N	2.35	0.60
1:B:110:ILE:HD13	1:B:110:ILE:H	1.66	0.60
1:A:110:ILE:O	1:A:132:HIS:HB3	2.00	0.60
1:A:144:LEU:HD13	1:A:146:VAL:HG12	1.84	0.60
1:A:18:LEU:HD23	1:A:18:LEU:C	2.27	0.60
1:A:29:ARG:HH11	1:A:29:ARG:CG	2.09	0.60
1:B:10:TRP:O	1:B:11:SER:O	2.20	0.60
1:A:36:ILE:HG12	1:B:64:ILE:HG21	1.84	0.59
1:A:146:VAL:O	1:A:147:ALA:C	2.45	0.59
1:B:122:HIS:HD1	1:B:122:HIS:H	1.48	0.59
1:A:55:LEU:H	1:A:55:LEU:CD1	2.15	0.59
1:A:39:THR:C	1:A:41:HIS:H	2.11	0.59
1:A:92:MSE:CE	1:A:100:ILE:HD13	2.33	0.59
1:B:134:ILE:O	1:B:135:ALA:CB	2.51	0.59
1:A:64:ILE:HG12	1:A:64:ILE:O	2.03	0.58
1:B:13:THR:HA	2:B:171:SO4:S	2.43	0.58
1:B:22:LEU:HD22	1:B:26:LEU:CD1	2.34	0.58
1:B:12:GLY:O	1:B:14:GLY:N	2.37	0.58
1:B:35:LEU:C	1:B:35:LEU:HD22	2.29	0.57
1:B:85:LEU:HD11	1:B:102:VAL:HG11	1.86	0.57
1:B:123:ARG:HG3	1:B:124:PRO:HD2	1.84	0.57
1:B:163:GLU:O	1:B:166:GLN:HG2	2.05	0.57
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.20	0.57
1:A:131:ARG:NE	3:A:172:HOH:O	2.32	0.56
1:B:125:GLU:O	1:B:127:LEU:HD12	2.05	0.56
1:A:6:ALA:HB2	1:A:110:ILE:HD11	1.87	0.56
1:A:21:LYS:C	1:A:24:PRO:HD2	2.30	0.56
1:B:42:ASP:O	1:B:43:MSE:C	2.49	0.56
1:B:123:ARG:HG2	1:B:123:ARG:HH11	1.71	0.56
1:B:25:ALA:O	1:B:28:ALA:HB3	2.06	0.56
1:B:29:ARG:NH1	1:B:159:ASP:OD1	2.39	0.55
1:A:62:GLN:HE21	1:B:96:LYS:HE2	1.72	0.55
1:B:77:THR:C	1:B:79:ASP:N	2.61	0.55
1:B:148:LEU:C	1:B:149:LEU:HD23	2.31	0.55
1:A:70:ARG:HH11	1:A:70:ARG:CG	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HD22	1:B:26:LEU:HD11	1.89	0.55
1:B:22:LEU:HD22	1:B:26:LEU:HG	1.87	0.55
1:B:10:TRP:O	1:B:11:SER:C	2.50	0.54
1:B:114:VAL:CG1	1:B:115:LEU:H	2.07	0.54
1:B:56:ARG:HD3	1:B:63:THR:HG22	1.89	0.54
1:B:29:ARG:HD2	1:B:29:ARG:H	1.71	0.54
1:B:134:ILE:HD12	1:B:164:TRP:CD1	2.43	0.54
1:A:110:ILE:HA	3:A:192:HOH:O	2.07	0.54
1:B:149:LEU:HD11	1:B:160:PHE:HD2	1.72	0.54
1:A:128:VAL:C	1:A:129:ILE:HD12	2.34	0.53
1:B:163:GLU:O	1:B:164:TRP:C	2.50	0.53
1:A:131:ARG:HD3	3:A:172:HOH:O	2.08	0.53
1:B:130:ASP:C	1:B:132:HIS:N	2.64	0.53
1:B:29:ARG:HD2	1:B:29:ARG:N	2.23	0.53
1:A:39:THR:C	1:A:41:HIS:N	2.65	0.53
1:B:80:GLU:OE2	1:B:81:GLU:HG2	2.09	0.52
1:B:117:ARG:HD2	1:B:139:ASP:OD1	2.09	0.52
1:B:136:VAL:HG12	1:B:137:ALA:N	2.25	0.52
1:B:14:GLY:O	1:B:17:THR:N	2.42	0.52
1:A:1:MSE:O	1:A:2:ILE:HG22	2.10	0.52
1:A:85:LEU:CD1	1:A:102:VAL:HG11	2.40	0.52
1:B:53:TYR:O	1:B:56:ARG:HB2	2.10	0.52
1:B:84:ASP:HB3	3:B:182:HOH:O	2.10	0.52
1:A:64:ILE:CD1	1:B:88:LEU:HB3	2.34	0.52
1:B:116:PHE:HE1	1:B:118:ASP:HB2	1.74	0.52
1:B:150:ASP:O	1:B:152:ASN:N	2.40	0.52
1:B:4:LEU:N	1:B:4:LEU:HD23	2.25	0.51
1:A:139:ASP:O	1:A:140:VAL:HG23	2.10	0.51
1:B:123:ARG:CG	1:B:124:PRO:HD2	2.41	0.51
1:B:124:PRO:O	1:B:126:GLU:N	2.43	0.51
1:B:22:LEU:O	1:B:26:LEU:HG	2.11	0.51
1:B:10:TRP:HE3	1:B:10:TRP:N	2.08	0.50
1:A:64:ILE:O	1:A:64:ILE:CG1	2.59	0.50
1:B:151:ILE:HG12	1:B:151:ILE:O	2.11	0.50
1:B:29:ARG:NH1	1:B:159:ASP:CG	2.65	0.50
1:B:39:THR:OG1	1:B:40:HIS:N	2.45	0.50
1:A:63:THR:HG23	1:B:35:LEU:HD12	1.94	0.50
1:B:123:ARG:HB2	3:B:186:HOH:O	2.10	0.50
1:B:123:ARG:HG2	1:B:123:ARG:NH1	2.26	0.49
1:A:152:ASN:HB2	3:A:173:HOH:O	2.13	0.49
1:A:70:ARG:HG3	1:A:70:ARG:NH1	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HD22	1:B:26:LEU:CG	2.42	0.49
1:B:84:ASP:C	1:B:84:ASP:OD2	2.55	0.49
1:A:69:GLN:O	1:B:77:THR:N	2.37	0.49
1:B:116:PHE:CD1	1:B:117:ARG:N	2.80	0.49
1:B:10:TRP:N	1:B:10:TRP:CE3	2.81	0.49
1:A:129:ILE:HD12	1:A:129:ILE:N	2.28	0.49
1:B:41:HIS:O	1:B:42:ASP:O	2.31	0.48
1:B:22:LEU:O	1:B:22:LEU:CD2	2.61	0.48
1:B:122:HIS:NE2	1:B:126:GLU:CG	2.75	0.48
1:A:62:GLN:HE21	1:B:96:LYS:CE	2.27	0.48
1:B:154:VAL:HG23	1:B:155:GLU:N	2.29	0.48
1:A:131:ARG:CD	3:A:172:HOH:O	2.60	0.48
1:B:12:GLY:O	1:B:13:THR:C	2.57	0.48
1:A:70:ARG:N	1:A:70:ARG:HD2	2.29	0.48
1:A:33:PRO:O	1:B:60:ALA:HA	2.14	0.47
1:B:106:LYS:H	1:B:106:LYS:CD	2.19	0.47
1:A:55:LEU:HD11	1:B:16:THR:HG23	1.95	0.47
1:A:96:LYS:HZ3	1:B:61:ALA:HB1	1.79	0.47
1:B:25:ALA:O	1:B:29:ARG:CD	2.61	0.47
1:B:81:GLU:HB2	1:B:82:GLU:H	1.31	0.47
1:A:63:THR:HG23	1:B:35:LEU:CD1	2.44	0.47
1:B:3:PRO:HG2	1:B:99:LEU:HD23	1.95	0.47
1:B:22:LEU:CD2	1:B:26:LEU:HG	2.44	0.47
1:A:29:ARG:NH1	1:A:29:ARG:CG	2.70	0.47
1:B:34:GLY:O	1:B:101:LEU:N	2.39	0.47
1:B:116:PHE:CD1	1:B:116:PHE:C	2.93	0.47
1:A:70:ARG:CG	1:A:70:ARG:NH1	2.76	0.46
1:B:22:LEU:HD22	1:B:22:LEU:O	2.16	0.46
1:B:4:LEU:HD23	1:B:4:LEU:H	1.80	0.46
1:B:54:GLU:O	1:B:56:ARG:N	2.48	0.46
1:B:18:LEU:C	1:B:18:LEU:HD22	2.41	0.46
1:B:161:VAL:O	1:B:162:VAL:C	2.58	0.46
1:A:73:LEU:C	1:A:73:LEU:HD23	2.40	0.46
1:A:1:MSE:O	1:A:2:ILE:CB	2.63	0.45
1:A:38:HIS:ND1	1:A:39:THR:N	2.64	0.45
1:A:55:LEU:N	1:A:55:LEU:CD1	2.78	0.45
1:B:127:LEU:O	1:B:127:LEU:CD1	2.62	0.45
1:B:157:LEU:O	1:B:161:VAL:HG23	2.16	0.45
1:B:79:ASP:N	1:B:79:ASP:OD1	2.45	0.45
1:B:141:PRO:O	1:B:142:LEU:HB3	2.17	0.45
1:A:108:GLU:C	1:A:109:GLU:HG3	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ALA:HA	1:B:102:VAL:O	2.17	0.45
1:A:129:ILE:HA	1:A:133:VAL:HG21	1.99	0.44
1:B:54:GLU:C	1:B:56:ARG:N	2.73	0.44
1:B:149:LEU:HD11	1:B:160:PHE:CD2	2.50	0.44
1:A:1:MSE:O	1:A:2:ILE:HB	2.17	0.44
1:A:85:LEU:HD11	1:A:108:GLU:HG2	2.00	0.44
1:A:18:LEU:C	1:A:18:LEU:CD2	2.91	0.44
1:B:7:PHE:HE2	1:B:18:LEU:HD11	1.82	0.44
1:B:35:LEU:HD22	1:B:36:ILE:N	2.32	0.44
1:B:153:ASP:CG	1:B:156:GLY:H	2.26	0.44
1:B:79:ASP:O	1:B:80:GLU:HB3	2.17	0.44
1:B:85:LEU:O	1:B:87:PHE:N	2.51	0.44
1:A:54:GLU:O	1:A:58:ALA:HB2	2.17	0.43
1:B:20:LYS:O	1:B:20:LYS:HG2	2.18	0.43
1:B:77:THR:N	1:B:78:PRO:HD3	2.32	0.43
1:B:108:GLU:HB3	1:B:110:ILE:HD12	2.00	0.43
1:A:129:ILE:HG22	1:A:129:ILE:O	2.17	0.43
1:B:85:LEU:HD21	1:B:105:PHE:CD1	2.54	0.43
1:B:138:SER:O	1:B:151:ILE:HG22	2.18	0.43
1:A:36:ILE:HG12	1:B:64:ILE:CG2	2.47	0.43
1:B:141:PRO:O	1:B:142:LEU:CB	2.66	0.43
1:A:85:LEU:CD1	1:A:108:GLU:HG2	2.48	0.43
1:B:150:ASP:C	1:B:152:ASN:N	2.71	0.43
1:A:8:ALA:HB2	1:A:112:LYS:HD3	2.01	0.43
1:A:13:THR:HG22	1:A:13:THR:O	2.17	0.43
1:A:71:TRP:CH2	1:B:91:ARG:HG3	2.54	0.43
1:A:35:LEU:C	1:A:35:LEU:HD22	2.44	0.43
1:A:38:HIS:HB2	1:A:105:PHE:CZ	2.54	0.43
1:A:5:LEU:HD22	1:A:7:PHE:CE1	2.54	0.43
1:A:35:LEU:HD22	1:A:36:ILE:N	2.34	0.43
1:A:73:LEU:HD11	1:B:92:MSE:HA	2.01	0.43
1:A:88:LEU:HD22	1:B:64:ILE:HD11	2.01	0.42
1:B:10:TRP:NE1	1:B:126:GLU:OE2	2.51	0.42
1:B:114:VAL:CG1	1:B:115:LEU:N	2.73	0.42
1:B:8:ALA:HB1	1:B:10:TRP:HZ3	1.84	0.42
1:B:105:PHE:C	1:B:108:GLU:OE1	2.62	0.42
1:B:116:PHE:HD1	1:B:117:ARG:N	2.17	0.42
1:B:154:VAL:HG23	1:B:155:GLU:H	1.83	0.42
1:A:73:LEU:C	1:A:73:LEU:CD2	2.93	0.42
1:A:124:PRO:HG2	1:A:125:GLU:OE2	2.18	0.42
1:B:15:LYS:HA	1:B:18:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:HIS:NE2	1:B:126:GLU:CD	2.78	0.42
1:B:73:LEU:HD13	1:B:73:LEU:O	2.20	0.42
1:B:13:THR:HA	2:B:171:SO4:O2	2.20	0.42
1:B:80:GLU:CD	1:B:80:GLU:C	2.87	0.42
1:B:117:ARG:HA	1:B:139:ASP:OD2	2.20	0.42
1:A:1:MSE:C	1:A:2:ILE:HG22	2.44	0.42
1:B:159:ASP:O	1:B:163:GLU:HG3	2.20	0.42
1:B:81:GLU:H	1:B:81:GLU:HG3	1.70	0.41
1:A:8:ALA:O	1:A:9:ALA:HB2	2.18	0.41
1:A:23:ILE:N	1:A:24:PRO:CD	2.83	0.41
1:B:116:PHE:HE1	1:B:118:ASP:CB	2.34	0.41
1:A:82:GLU:OE1	1:A:82:GLU:CA	2.68	0.41
1:B:13:THR:O	1:B:14:GLY:C	2.63	0.41
1:A:117:ARG:NH1	1:A:151:ILE:HD13	2.36	0.41
1:B:8:ALA:HB1	1:B:10:TRP:CZ3	2.55	0.41
1:A:77:THR:N	1:A:78:PRO:HD3	2.36	0.41
1:A:134:ILE:O	1:A:135:ALA:HB2	2.21	0.41
1:B:123:ARG:HG2	1:B:124:PRO:N	2.34	0.41
1:B:53:TYR:HA	1:B:56:ARG:CZ	2.51	0.41
1:A:29:ARG:HB3	3:A:176:HOH:O	2.21	0.41
1:A:114:VAL:O	1:A:115:LEU:HD23	2.21	0.41
1:B:38:HIS:C	1:B:38:HIS:HD1	2.29	0.41
1:B:89:ALA:C	1:B:91:ARG:N	2.79	0.41
1:B:148:LEU:C	1:B:148:LEU:HD13	2.46	0.41
1:B:132:HIS:O	1:B:134:ILE:HG23	2.21	0.40
1:B:131:ARG:HH11	1:B:131:ARG:CB	2.23	0.40
1:A:161:VAL:O	1:A:164:TRP:HB3	2.21	0.40
1:B:122:HIS:CD2	1:B:126:GLU:HG3	2.56	0.40

All (2) 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)
1:A:131:ARG:NH1	1:A:131:ARG:NH1[4_665]	1.18	1.02
3:A:183:HOH:O	3:A:183:HOH:O[7_555]	1.97	0.23

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	158/170 (93%)	132 (84%)	21 (13%)	5 (3%)	3	11
1	B	158/170 (93%)	96 (61%)	37 (23%)	25 (16%)	0	0
All	All	316/340 (93%)	228 (72%)	58 (18%)	30 (10%)	0	1

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	9	ALA
1	B	11	SER
1	B	13	THR
1	B	14	GLY
1	B	42	ASP
1	B	52	SER
1	B	80	GLU
1	B	124	PRO
1	B	127	LEU
1	B	135	ALA
1	B	151	ILE
1	A	131	ARG
1	B	15	LYS
1	B	86	GLN
1	B	114	VAL
1	B	125	GLU
1	B	128	VAL
1	B	168	GLN
1	A	147	ALA
1	B	55	LEU
1	B	142	LEU
1	B	144	LEU
1	B	147	ALA
1	A	107	HIS

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Mol	Chain	Res	Type
1	B	115	LEU
1	B	82	GLU
1	B	131	ARG
1	B	166	GLN
1	B	129	ILE

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	136/137 (99%)	114 (84%)	22 (16%)	2	8
1	B	136/137 (99%)	114 (84%)	22 (16%)	2	8
All	All	272/274 (99%)	228 (84%)	44 (16%)	2	8

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	22	LEU
1	A	29	ARG
1	A	33	PRO
1	A	35	LEU
1	A	39	THR
1	A	41	HIS
1	A	43	MSE
1	A	55	LEU
1	A	57	LYS
1	A	64	ILE
1	A	70	ARG
1	A	79	ASP
1	A	80	GLU
1	A	86	GLN
1	A	92	MSE
1	A	98	ASP
1	A	103	GLU

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Mol	Chain	Res	Type
1	A	107	HIS
1	A	140	VAL
1	A	148	LEU
1	A	157	LEU
1	B	2	ILE
1	B	4	LEU
1	B	10	TRP
1	B	13	THR
1	B	18	LEU
1	B	22	LEU
1	B	35	LEU
1	B	42	ASP
1	B	73	LEU
1	B	79	ASP
1	B	81	GLU
1	B	82	GLU
1	B	106	LYS
1	B	109	GLU
1	B	110	ILE
1	B	115	LEU
1	B	123	ARG
1	B	127	LEU
1	B	130	ASP
1	B	149	LEU
1	B	151	ILE
1	B	157	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	122	HIS
1	B	68	GLN
1	B	86	GLN
1	B	166	GLN
1	B	168	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	171	-	4,4,4	0.35	0	6,6,6	0.13	0
2	SO4	B	171	-	4,4,4	0.51	0	6,6,6	0.09	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	171	SO4	2	0

5.7 Other polymers [i](#)

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	157/170 (92%)	0.64	21 (13%) 7 5	8, 23, 64, 89	0
1	B	157/170 (92%)	1.96	67 (42%) 0 0	8, 45, 84, 92	0
All	All	314/340 (92%)	1.30	88 (28%) 1 1	8, 33, 80, 92	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	GLY	7.6
1	B	120	ALA	7.0
1	B	125	GLU	5.6
1	B	83	LEU	5.5
1	B	51	ASP	5.4
1	B	82	GLU	5.3
1	B	10	TRP	5.2
1	B	42	ASP	5.0
1	B	41	HIS	4.7
1	B	169	ASN	4.6
1	B	107	HIS	4.5
1	A	169	ASN	4.4
1	A	51	ASP	4.4
1	B	121	GLY	4.3
1	B	117	ARG	4.3
1	B	106	LYS	4.2
1	B	40	HIS	4.1
1	B	115	LEU	4.1
1	B	128	VAL	4.1
1	B	126	GLU	4.1
1	A	68	GLN	3.9
1	B	81	GLU	3.9
1	B	116	PHE	3.9
1	B	132	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	118	ASP	3.6
1	B	122	HIS	3.6
1	B	105	PHE	3.6
1	B	127	LEU	3.5
1	B	110	ILE	3.4
1	A	96	LYS	3.4
1	B	138	SER	3.4
1	A	66	ALA	3.3
1	B	7	PHE	3.3
1	B	8	ALA	3.3
1	B	4	LEU	3.3
1	B	123	ARG	3.3
1	A	167	LYS	3.3
1	B	130	ASP	3.2
1	B	167	LYS	3.2
1	B	164	TRP	3.2
1	B	11	SER	3.1
1	A	106	LYS	3.1
1	B	133	VAL	3.1
1	A	107	HIS	3.0
1	A	69	GLN	2.9
1	B	78	PRO	2.9
1	B	124	PRO	2.9
1	B	38	HIS	2.9
1	A	131	ARG	2.9
1	B	80	GLU	2.8
1	A	9	ALA	2.7
1	B	141	PRO	2.7
1	B	168	GLN	2.7
1	B	52	SER	2.7
1	B	146	VAL	2.7
1	B	137	ALA	2.7
1	B	131	ARG	2.7
1	B	142	LEU	2.6
1	B	151	ILE	2.6
1	B	143	ASN	2.6
1	A	119	GLY	2.6
1	B	134	ILE	2.6
1	B	149	LEU	2.5
1	A	120	ALA	2.5
1	A	42	ASP	2.5
1	B	114	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	147	ALA	2.3
1	A	39	THR	2.3
1	A	53	TYR	2.3
1	B	160	PHE	2.3
1	B	96	LYS	2.3
1	A	56	ARG	2.3
1	B	148	LEU	2.2
1	B	79	ASP	2.2
1	B	12	GLY	2.2
1	A	55	LEU	2.2
1	B	16	THR	2.2
1	B	109	GLU	2.2
1	B	129	ILE	2.1
1	B	166	GLN	2.1
1	B	13	THR	2.1
1	A	70	ARG	2.1
1	B	77	THR	2.1
1	A	40	HIS	2.1
1	A	143	ASN	2.1
1	B	15	LYS	2.0
1	B	39	THR	2.0
1	B	53	TYR	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	171	5/5	0.66	0.33	51,57,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	171	5/5	0.88	0.10	54,59,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.