



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2024 – 08:24 PM EST

PDB ID : 1Y1O
Title : X-ray crystal Structure of Penicillin-binding protein-related factor A from *Bacillus stearothermophilus*
Authors : Osipiuk, J.; Li, H.; Moy, S.; Collart, F.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2004-11-19
Resolution : 2.20 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

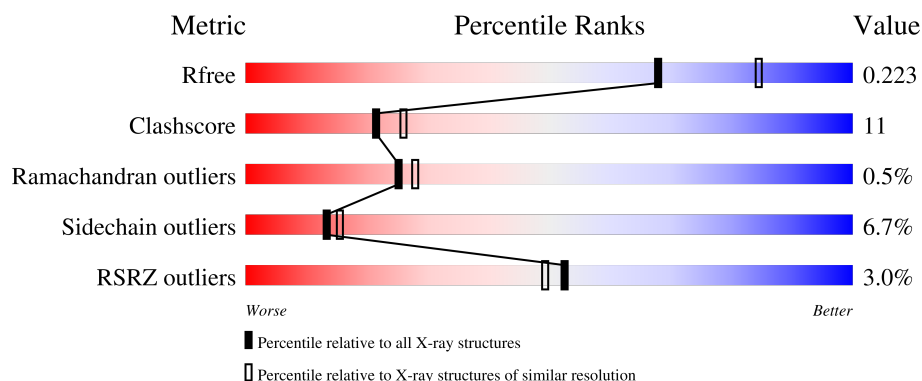
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	203	<div> <div>0%</div> <div> <div></div> <div>67%</div> <div>13%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	203	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>20%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	203	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>14%</div> <div>•</div> <div>17%</div> </div> </div>
1	D	203	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>19%</div> <div>•</div> <div>17%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5713 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 Penicillin-binding protein-related factor A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	Se	0	0	0
			1378	882	245	248	1	2			
1	B	168	Total	C	N	O	S	Se	0	0	0
			1378	882	245	248	1	2			
1	C	168	Total	C	N	O	S	Se	0	0	0
			1378	882	245	248	1	2			
1	D	168	Total	C	N	O	S	Se	0	0	0
			1378	882	245	248	1	2			

- 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		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

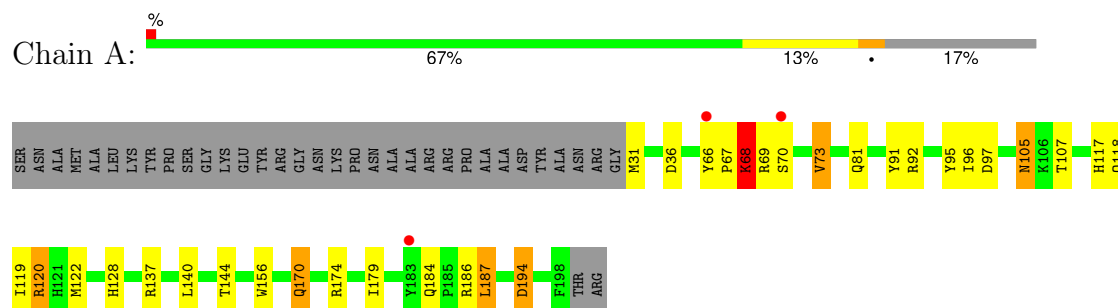
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	37	Total	O	0	0
			37	37		
4	C	45	Total	O	0	0
			45	45		
4	D	31	Total	O	0	0
			31	31		

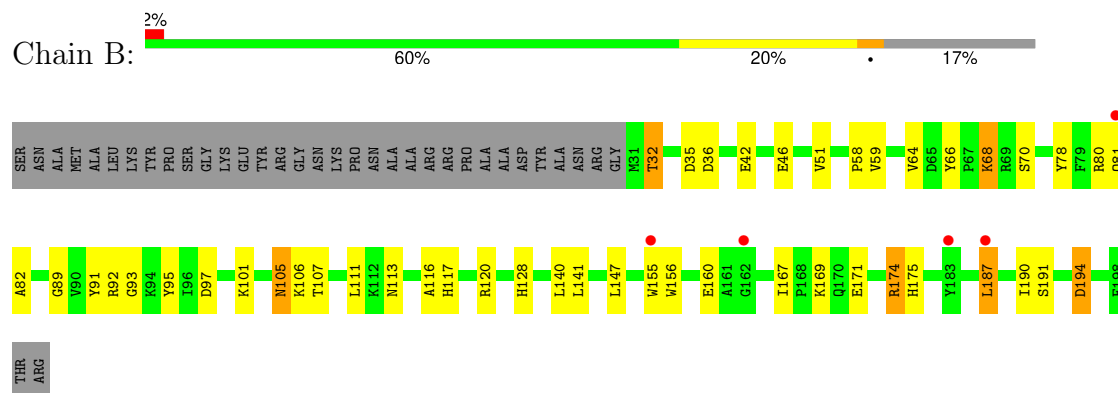
3 Residue-property plots [i](#)

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.

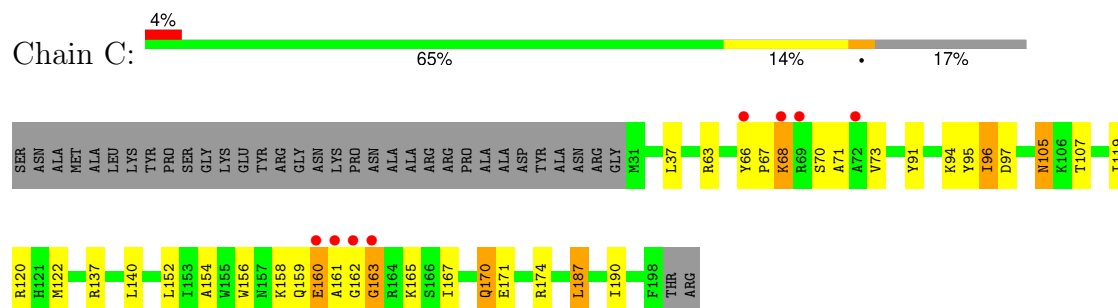
- Molecule 1: Penicillin-binding protein-related factor A



- Molecule 1: Penicillin-binding protein-related factor A

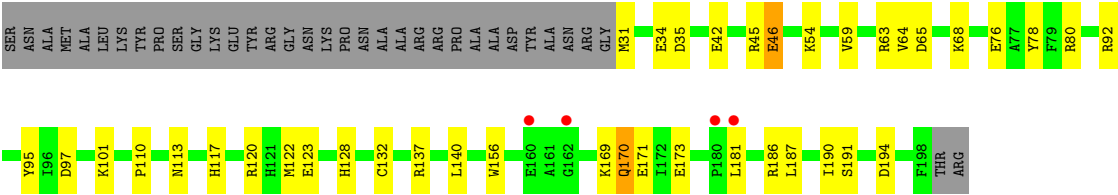


- Molecule 1: Penicillin-binding protein-related factor A



- Molecule 1: Penicillin-binding protein-related factor A





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.26Å 81.02Å 106.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.10 – 2.20 34.10 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.10-2.20) 97.6 (34.10-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.197 , 0.248 0.210 , 0.223	Depositor DCC
R_{free} test set	2039 reflections (5.82%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5713	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% 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, NI

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	0.75	0/1413	0.76	2/1912 (0.1%)
1	B	0.72	0/1413	0.72	0/1912
1	C	0.74	0/1413	0.74	1/1912 (0.1%)
1	D	0.69	0/1413	0.71	0/1912
All	All	0.73	0/5652	0.73	3/7648 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ILE	CG1-CB-CG2	-5.50	99.31	111.40
1	C	96	ILE	CG1-CB-CG2	-5.36	99.61	111.40
1	A	137	ARG	NE-CZ-NH2	-5.05	117.78	120.30

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	1378	0	1355	24	1
1	B	1378	0	1355	39	1
1	C	1378	0	1355	27	1
1	D	1378	0	1355	30	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	0	0	0
2	B	20	0	0	1	0
2	C	10	0	0	0	0
2	D	15	0	0	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	31	0	0	3	0
4	B	37	0	0	2	0
4	C	45	0	0	1	0
4	D	31	0	0	0	0
All	All	5713	0	5420	118	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 11.

All (118) 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:D:31:MSE:HE2	1:D:186:ARG:NH1	1.68	1.08
1:A:36:ASP:HB3	1:A:187:LEU:HD11	1.20	1.08
1:B:68:LYS:HD2	1:B:68:LYS:H	1.23	1.00
1:B:92:ARG:NH1	1:B:194:ASP:OD1	1.96	0.97
1:B:147:LEU:HD21	1:B:155:TRP:HZ3	1.30	0.97
1:C:160:GLU:HG3	1:C:161:ALA:H	1.30	0.94
1:D:181:LEU:HD22	1:D:187:LEU:HD22	1.50	0.91
1:B:91:TYR:OH	1:B:194:ASP:OD2	1.88	0.91
1:B:147:LEU:HD21	1:B:155:TRP:CZ3	2.08	0.88
1:D:101:LYS:HD2	1:D:113:ASN:HB3	1.56	0.87
1:B:68:LYS:H	1:B:68:LYS:CD	1.86	0.84
1:D:181:LEU:HD22	1:D:187:LEU:CD2	2.08	0.84
1:C:170:GLN:HE21	1:C:170:GLN:H	1.24	0.84
1:C:68:LYS:H	1:C:68:LYS:HD2	1.44	0.83
1:D:31:MSE:CE	1:D:186:ARG:NH1	2.44	0.81
1:A:187:LEU:HD12	1:A:187:LEU:N	1.96	0.81
1:D:31:MSE:CE	1:D:186:ARG:HH12	1.95	0.80
4:A:344:HOH:O	1:B:128:HIS:HD2	1.65	0.80
1:C:160:GLU:HG3	1:C:161:ALA:N	1.97	0.79
1:D:31:MSE:HE1	1:D:35:ASP:HB3	1.64	0.79
1:B:174:ARG:HG3	1:B:174:ARG:HH11	1.47	0.79
1:A:170:GLN:H	1:A:170:GLN:HE21	1.28	0.78
1:B:32:THR:HG22	1:B:35:ASP:H	1.49	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:360:HOH:O	1:D:128:HIS:HD2	1.68	0.76
1:D:31:MSE:HE2	1:D:186:ARG:HH12	1.49	0.76
1:D:31:MSE:HE2	1:D:186:ARG:HH11	1.52	0.74
1:A:81:GLN:NE2	1:A:117:HIS:CD2	2.58	0.72
1:A:186:ARG:HB2	1:A:187:LEU:HD12	1.71	0.72
1:B:81:GLN:HE21	1:B:117:HIS:CE1	2.08	0.71
1:B:36:ASP:HB3	1:B:187:LEU:HD21	1.74	0.69
1:B:82:ALA:O	1:B:117:HIS:CD2	2.46	0.68
1:D:31:MSE:CE	1:D:35:ASP:HB3	2.24	0.68
1:D:137:ARG:NH2	1:D:187:LEU:HD21	2.08	0.68
1:D:110:PRO:O	1:D:113:ASN:ND2	2.28	0.67
1:B:174:ARG:HG3	1:B:174:ARG:NH1	2.11	0.65
1:B:155:TRP:CE3	1:B:167:ILE:HD13	2.33	0.64
1:D:137:ARG:HH22	1:D:187:LEU:HD21	1.61	0.63
1:B:147:LEU:CD2	1:B:155:TRP:HZ3	2.10	0.63
1:B:81:GLN:NE2	1:B:117:HIS:CE1	2.66	0.63
1:C:105:ASN:HD22	1:C:107:THR:H	1.46	0.63
1:D:120:ARG:NH1	1:D:123:GLU:OE2	2.31	0.63
1:C:137:ARG:NH2	1:C:187:LEU:HD23	2.14	0.62
1:B:68:LYS:HD2	1:B:68:LYS:N	2.07	0.61
1:B:105:ASN:HD22	1:B:107:THR:H	1.48	0.61
1:A:92:ARG:NH1	1:A:194:ASP:OD1	2.36	0.58
1:D:181:LEU:CD2	1:D:187:LEU:HD22	2.29	0.58
1:A:95:TYR:CE2	1:A:97:ASP:HB2	2.39	0.56
1:A:91:TYR:OH	1:A:194:ASP:OD2	2.13	0.56
1:A:81:GLN:HE22	1:A:117:HIS:CD2	2.23	0.56
1:C:122:MSE:SE	1:C:152:LEU:HD23	2.56	0.56
1:D:95:TYR:CE2	1:D:97:ASP:HB2	2.41	0.56
1:B:81:GLN:HE21	1:B:117:HIS:HE1	1.49	0.55
1:A:31:MSE:N	4:A:350:HOH:O	2.40	0.55
1:A:174:ARG:NH2	2:D:311:SO4:O3	2.40	0.55
1:B:174:ARG:HH11	1:B:174:ARG:CG	2.19	0.55
1:A:36:ASP:CB	1:A:187:LEU:HD11	2.14	0.54
1:B:106:LYS:HE3	1:B:140:LEU:HD23	1.91	0.53
1:C:170:GLN:HE21	1:C:170:GLN:N	2.01	0.52
1:C:37:LEU:HD23	1:C:187:LEU:HD13	1.91	0.52
1:C:167:ILE:HG23	1:C:171:GLU:HG2	1.93	0.51
1:D:63:ARG:HD2	1:D:76:GLU:OE1	2.09	0.51
1:A:105:ASN:HD22	1:A:107:THR:H	1.57	0.51
1:A:186:ARG:HB2	1:A:187:LEU:CD1	2.39	0.51
1:B:36:ASP:CB	1:B:187:LEU:HD21	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ARG:NH2	1:C:187:LEU:CD2	2.73	0.51
1:D:46:GLU:OE2	1:D:46:GLU:HA	2.11	0.51
1:D:170:GLN:HG2	1:D:171:GLU:N	2.25	0.51
1:C:95:TYR:CE2	1:C:97:ASP:HB2	2.46	0.51
1:C:159:GLN:HB3	1:C:165:LYS:HZ3	1.76	0.51
1:B:42:GLU:O	1:B:46:GLU:HG3	2.11	0.50
1:B:116:ALA:O	1:B:120:ARG:HG2	2.12	0.50
1:C:91:TYR:HB3	1:C:96:ILE:CD1	2.42	0.50
1:A:73:VAL:HG13	1:B:78:TYR:CE1	2.45	0.50
1:B:93:GLY:O	4:B:310:HOH:O	2.19	0.50
1:B:95:TYR:CE2	1:B:97:ASP:HB2	2.47	0.48
1:C:70:SER:OG	1:C:71:ALA:N	2.45	0.48
1:C:162:GLY:O	1:C:163:GLY:O	2.31	0.48
1:D:31:MSE:CE	1:D:35:ASP:CB	2.92	0.48
1:D:169:LYS:HE2	1:D:173:GLU:OE2	2.14	0.47
1:A:119:ILE:HG13	1:A:156:TRP:CD2	2.49	0.47
2:B:306:SO4:O1	1:C:174:ARG:NH2	2.46	0.47
1:B:82:ALA:O	1:B:117:HIS:NE2	2.47	0.47
1:B:111:LEU:HD21	1:B:167:ILE:HD11	1.97	0.47
1:C:154:ALA:O	1:C:158:LYS:HB2	2.14	0.47
1:D:92:ARG:NH1	1:D:194:ASP:OD1	2.48	0.46
1:A:66:TYR:HA	1:A:67:PRO:HD3	1.82	0.46
1:A:81:GLN:NE2	4:A:347:HOH:O	2.43	0.46
1:D:42:GLU:HG2	1:D:45:ARG:NH2	2.31	0.46
1:B:160:GLU:OE1	1:B:160:GLU:HA	2.16	0.46
1:C:66:TYR:HA	1:C:67:PRO:HD3	1.71	0.45
1:C:94:LYS:O	1:C:96:ILE:HD12	2.16	0.45
1:D:31:MSE:HE1	1:D:186:ARG:HH12	1.77	0.45
1:B:171:GLU:HG3	1:B:175:HIS:HD2	1.80	0.45
1:B:36:ASP:HB3	1:B:187:LEU:CD2	2.43	0.45
1:D:31:MSE:HE3	1:D:35:ASP:CB	2.47	0.45
1:C:120:ARG:HH22	1:C:156:TRP:HZ3	1.65	0.45
1:D:31:MSE:HE3	1:D:35:ASP:HB2	1.99	0.45
1:A:118:GLN:O	1:A:122:MSE:HG3	2.17	0.44
1:C:73:VAL:HG22	1:D:78:TYR:HE1	1.81	0.44
1:A:144:THR:HG22	1:A:179:ILE:HD12	1.98	0.44
1:B:141:LEU:HD13	1:B:169:LYS:HE3	2.00	0.44
1:C:160:GLU:CG	1:C:161:ALA:N	2.76	0.44
1:B:51:VAL:O	1:B:89:GLY:HA3	2.17	0.44
1:B:58:PRO:HB2	1:B:80:ARG:HG2	1.99	0.43
1:C:167:ILE:CG2	1:C:171:GLU:HG2	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:GLU:OE2	1:D:54:LYS:HE3	2.17	0.43
1:C:120:ARG:NH2	1:C:156:TRP:HZ3	2.17	0.42
1:C:119:ILE:HG13	1:C:156:TRP:CD2	2.54	0.42
1:A:120:ARG:HD3	1:A:120:ARG:HA	1.70	0.42
1:B:91:TYR:CZ	1:B:194:ASP:OD2	2.70	0.42
1:A:67:PRO:HG2	1:A:70:SER:HB3	2.02	0.41
1:B:101:LYS:NZ	1:B:113:ASN:O	2.53	0.41
1:A:128:HIS:HD2	4:B:321:HOH:O	2.03	0.41
1:C:68:LYS:H	1:C:68:LYS:CD	2.20	0.41
1:B:120:ARG:HA	1:B:120:ARG:HD3	1.90	0.41
1:D:122:MSE:HG2	1:D:132:CYS:SG	2.61	0.41
1:A:68:LYS:HB2	1:A:69:ARG:H	1.71	0.40
1:B:105:ASN:ND2	1:B:107:THR:H	2.17	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:B:66:TYR:OH	1:D:68:LYS:O[3_545]	2.09	0.11
1:A:66:TYR:OH	1:C:66:TYR:OH[1_545]	2.18	0.02

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	166/203 (82%)	161 (97%)	4 (2%)	1 (1%)	22	23
1	B	166/203 (82%)	163 (98%)	3 (2%)	0	100	100
1	C	166/203 (82%)	158 (95%)	6 (4%)	2 (1%)	11	9
1	D	166/203 (82%)	163 (98%)	3 (2%)	0	100	100
All	All	664/812 (82%)	645 (97%)	16 (2%)	3 (0%)	25	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	160	GLU
1	C	163	GLY
1	A	68	LYS

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	145/168 (86%)	136 (94%)	9 (6%)	15	18
1	B	145/168 (86%)	133 (92%)	12 (8%)	9	9
1	C	145/168 (86%)	138 (95%)	7 (5%)	21	28
1	D	145/168 (86%)	134 (92%)	11 (8%)	11	12
All	All	580/672 (86%)	541 (93%)	39 (7%)	13	15

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	73	VAL
1	A	105	ASN
1	A	120	ARG
1	A	140	LEU
1	A	170	GLN
1	A	184	GLN
1	A	187	LEU
1	A	194	ASP
1	B	32	THR
1	B	59	VAL
1	B	64	VAL
1	B	68	LYS
1	B	70	SER
1	B	105	ASN
1	B	156	TRP
1	B	174	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	187	LEU
1	B	190	ILE
1	B	191	SER
1	B	194	ASP
1	C	63	ARG
1	C	68	LYS
1	C	105	ASN
1	C	140	LEU
1	C	170	GLN
1	C	187	LEU
1	C	190	ILE
1	D	46	GLU
1	D	59	VAL
1	D	64	VAL
1	D	65	ASP
1	D	80	ARG
1	D	117	HIS
1	D	140	LEU
1	D	156	TRP
1	D	170	GLN
1	D	190	ILE
1	D	191	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	105	ASN
1	A	117	HIS
1	A	170	GLN
1	A	195	ASN
1	B	81	GLN
1	B	105	ASN
1	B	117	HIS
1	B	128	HIS
1	B	175	HIS
1	C	105	ASN
1	C	159	GLN
1	C	170	GLN
1	C	195	ASN
1	D	81	GLN
1	D	124	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	128	HIS
1	D	195	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 ⓘ

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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	C	308	-	4,4,4	0.31	0	6,6,6	0.44	0
2	SO4	C	307	-	4,4,4	0.33	0	6,6,6	0.23	0
2	SO4	D	311	-	4,4,4	0.26	0	6,6,6	0.41	0
2	SO4	B	306	-	4,4,4	0.32	0	6,6,6	0.23	0
2	SO4	A	301	-	4,4,4	0.29	0	6,6,6	0.25	0
2	SO4	D	309	-	4,4,4	0.18	0	6,6,6	0.43	0
2	SO4	D	310	-	4,4,4	0.28	0	6,6,6	0.37	0
2	SO4	B	304	-	4,4,4	0.29	0	6,6,6	0.29	0
2	SO4	A	302	-	4,4,4	0.27	0	6,6,6	0.40	0
2	SO4	B	305	-	4,4,4	0.25	0	6,6,6	0.25	0
2	SO4	B	303	-	4,4,4	0.20	0	6,6,6	0.38	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	311	SO4	1	0
2	B	306	SO4	1	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	166/203 (81%)	-0.02	3 (1%) 67 64	22, 33, 53, 69	0
1	B	166/203 (81%)	0.17	5 (3%) 52 49	23, 38, 52, 57	0
1	C	166/203 (81%)	0.06	8 (4%) 36 33	22, 33, 55, 64	0
1	D	166/203 (81%)	0.16	4 (2%) 59 56	22, 37, 48, 55	0
All	All	664/812 (81%)	0.09	20 (3%) 52 49	22, 35, 52, 69	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	162	GLY	3.3
1	B	155	TRP	3.1
1	C	66	TYR	2.9
1	C	68	LYS	2.7
1	C	161	ALA	2.7
1	D	162	GLY	2.6
1	A	183	TYR	2.6
1	B	187	LEU	2.5
1	B	183	TYR	2.4
1	D	160	GLU	2.4
1	B	81	GLN	2.2
1	A	66	TYR	2.2
1	D	180	PRO	2.2
1	A	70	SER	2.1
1	D	181	LEU	2.1
1	C	72	ALA	2.1
1	C	163	GLY	2.1
1	C	160	GLU	2.0
1	C	69	ARG	2.0
1	B	162	GLY	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 monosaccharides 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	D	310	5/5	0.78	0.11	83,83,84,84	0
2	SO4	C	308	5/5	0.87	0.11	63,64,65,65	0
2	SO4	B	305	5/5	0.87	0.10	70,70,71,72	0
2	SO4	D	311	5/5	0.87	0.15	60,61,63,63	0
2	SO4	A	302	5/5	0.88	0.08	63,65,66,67	0
2	SO4	B	304	5/5	0.88	0.09	72,73,74,75	0
2	SO4	A	301	5/5	0.88	0.14	56,58,59,60	0
2	SO4	C	307	5/5	0.90	0.10	51,52,54,54	0
2	SO4	B	306	5/5	0.91	0.14	60,61,62,62	0
2	SO4	B	303	5/5	0.92	0.13	52,53,57,58	0
2	SO4	D	309	5/5	0.93	0.10	54,54,55,57	0
3	NI	C	322	1/1	0.99	0.02	29,29,29,29	0
3	NI	A	321	1/1	1.00	0.03	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.