



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:08 PM UTC

PDB ID : 2OUK / pdb_00002ouk
Title : ABC Protein ArtP in complex with Sulphate
Authors : Thaben, P.F.; Eckey, V.; Scheffel, F.; Saenger, W.; Schneider, E.; Vahedi-Faridi, A.
Deposited on : 2007-02-11
Resolution : 2.15 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

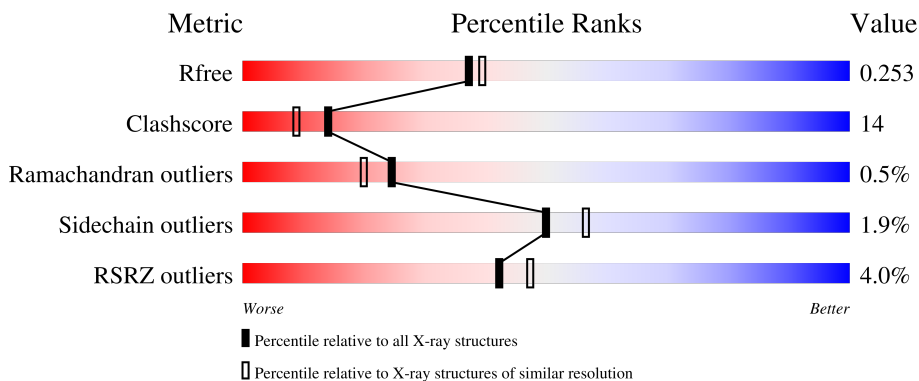
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	263	 5% 65% 24% 8%
1	B	263	 2% 68% 22% 8%
1	C	263	 6% 62% 28% 8%
1	D	263	 2% 68% 21% 8%

2 Entry composition [i](#)

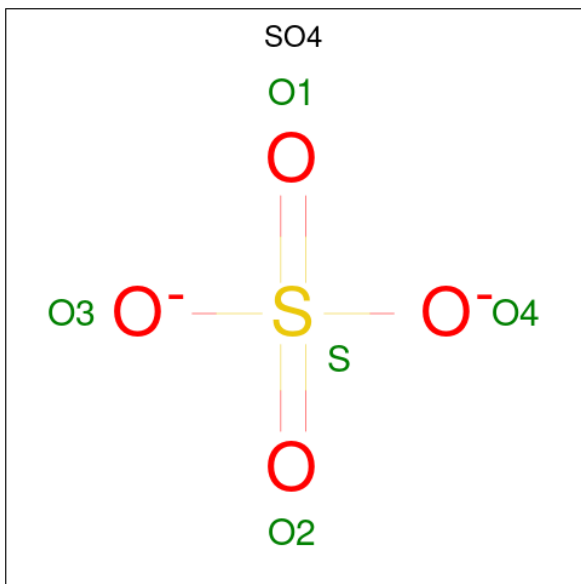
There are 3 unique types of molecules in this entry. The entry contains 8120 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 protein ArtP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	242	Total 1896	C 1205	N 326	O 351	S 14	0	0	0
1	B	241	Total 1888	C 1199	N 325	O 350	S 14	0	0	0
1	C	242	Total 1896	C 1205	N 326	O 351	S 14	0	0	0
1	D	241	Total 1888	C 1199	N 325	O 350	S 14	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	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		

- Molecule 3 is water.

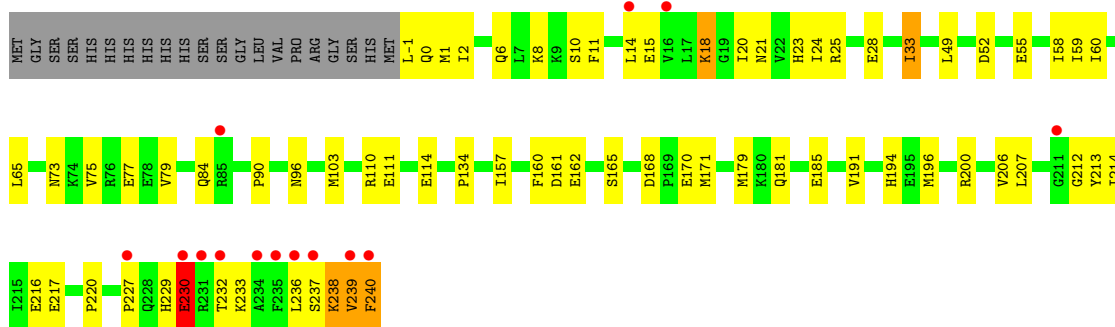
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total	O	0	0
			123	123		
3	B	139	Total	O	0	0
			139	139		
3	C	109	Total	O	0	0
			109	109		
3	D	151	Total	O	0	0
			151	151		

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.

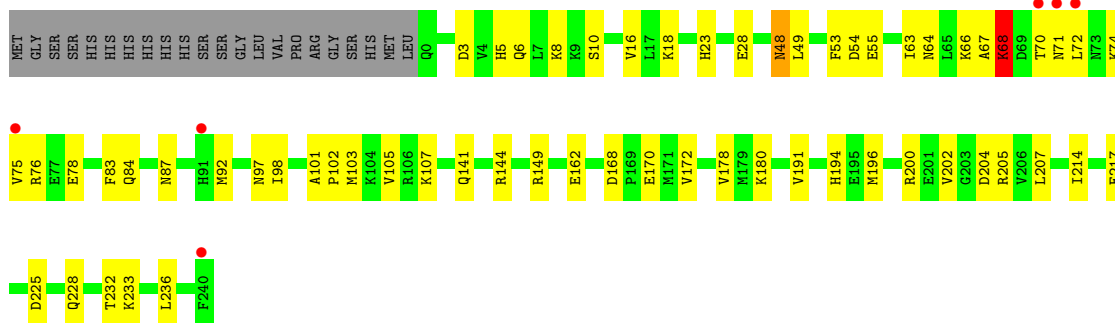
- Molecule 1: protein ArtP

Chain A: 



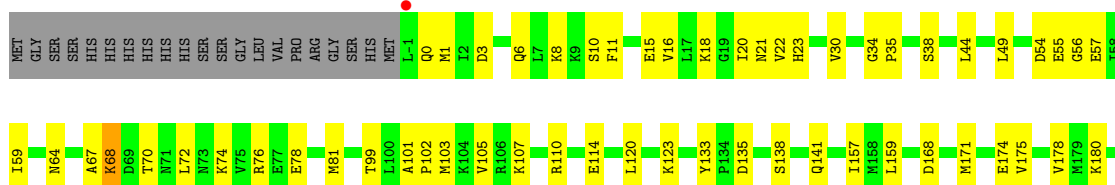
- Molecule 1: protein ArtP

Chain B: 



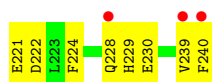
- Molecule 1: protein ArtP

Chain C: 





• Molecule 1: protein ArtP



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.16Å 80.63Å 95.58Å 90.00° 104.23° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 50.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	88.2 (50.00-2.15) 88.2 (50.00-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.16Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.255 0.209 , 0.253	Depositor DCC
R_{free} test set	2795 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtrriage
Anisotropy	0.072	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8120	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2484e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/1927	0.93	4/2589 (0.2%)
1	B	0.41	0/1919	0.95	8/2578 (0.3%)
1	C	0.38	0/1927	0.91	5/2589 (0.2%)
1	D	0.40	0/1919	0.92	6/2578 (0.2%)
All	All	0.40	0/7692	0.93	23/10334 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	VAL	N-CA-C	6.92	117.06	110.42
1	D	202	VAL	N-CA-C	6.79	118.62	112.17
1	D	215	ILE	N-CA-C	6.44	117.22	110.72
1	B	98	ILE	N-CA-C	6.33	117.11	110.72
1	C	105	VAL	N-CA-C	6.15	116.34	110.74
1	B	214	ILE	N-CA-C	-6.08	98.45	107.51
1	C	191	VAL	N-CA-C	5.78	116.47	107.28
1	B	204	ASP	N-CA-C	-5.71	105.42	112.90
1	A	238	LYS	N-CA-C	-5.68	106.43	113.19
1	B	18	LYS	N-CA-C	5.53	118.82	112.57
1	A	79	VAL	N-CA-C	5.52	116.43	108.48
1	B	228	GLN	N-CA-C	5.50	118.12	111.40
1	A	191	VAL	N-CA-C	5.36	115.57	107.75
1	B	191	VAL	N-CA-C	5.35	115.57	107.75
1	D	98	ILE	N-CA-C	5.31	116.08	110.72
1	B	105	VAL	N-CA-C	5.29	115.50	110.53
1	D	192	VAL	N-CA-C	-5.26	100.84	108.36
1	C	34	GLY	CA-C-N	5.23	125.21	120.03
1	C	34	GLY	C-N-CA	5.23	125.21	120.03
1	C	228	GLN	N-CA-C	5.21	118.09	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	THR	N-CA-C	-5.09	105.19	111.40
1	D	63	ILE	N-CA-C	5.08	115.41	107.99
1	D	156	LYS	N-CA-C	-5.01	107.34	113.50

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	1896	0	1941	58	0
1	B	1888	0	1930	47	0
1	C	1896	0	1941	65	0
1	D	1888	0	1930	52	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	1	0
3	A	123	0	0	8	0
3	B	139	0	0	5	0
3	C	109	0	0	4	0
3	D	151	0	0	9	0
All	All	8120	0	7742	219	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (219) 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:C:68:LYS:HE2	1:C:68:LYS:H	1.24	1.00
1:B:83:PHE:H	1:B:87:ASN:HD21	1.04	1.00
1:B:63:ILE:HD11	1:B:74:LYS:HE2	1.42	0.98
1:D:63:ILE:HD11	1:D:74:LYS:HD3	1.44	0.96
1:A:6:GLN:HE21	1:A:21:ASN:HD21	1.14	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:PHE:H	1:D:87:ASN:HD21	1.07	0.93
1:A:168:ASP:HB3	3:A:9117:HOH:O	1.74	0.87
1:C:68:LYS:H	1:C:68:LYS:CE	1.86	0.87
1:B:68:LYS:H	1:B:68:LYS:HD2	1.40	0.86
1:A:239:VAL:HG13	1:A:240:PHE:H	1.41	0.85
1:D:228:GLN:HG2	3:D:9060:HOH:O	1.79	0.81
1:A:6:GLN:NE2	1:A:21:ASN:HD21	1.81	0.78
1:B:68:LYS:HD2	1:B:68:LYS:N	1.99	0.77
1:D:1:MET:HE2	1:D:26:GLU:HB2	1.66	0.77
1:B:168:ASP:HB3	1:B:170:GLU:OE2	1.85	0.76
1:D:1:MET:HG3	1:D:157:ILE:HD11	1.68	0.75
1:A:1:MET:HG3	1:A:157:ILE:HD11	1.68	0.74
1:D:171:MET:HE3	3:D:9059:HOH:O	1.89	0.72
1:A:168:ASP:HB2	1:A:171:MET:HE3	1.70	0.72
1:C:6:GLN:HE21	1:C:21:ASN:HD21	1.34	0.72
1:A:15:GLU:HG2	1:A:18:LYS:HG2	1.72	0.71
1:B:8:LYS:HB2	1:B:55:GLU:HG2	1.73	0.70
1:A:230:GLU:CD	1:A:230:GLU:H	1.98	0.69
1:B:48:ASN:O	1:B:49:LEU:HB2	1.92	0.69
1:A:8:LYS:HB2	1:A:55:GLU:HB2	1.75	0.69
1:A:20:ILE:HD12	1:A:214:ILE:HG13	1.73	0.69
1:B:207:LEU:HD23	1:B:217:GLU:HG3	1.74	0.69
1:B:74:LYS:O	1:B:78:GLU:HG3	1.94	0.67
1:A:0:GLN:HE22	1:A:23:HIS:CD2	2.13	0.67
1:B:72:LEU:O	1:B:75:VAL:HG22	1.95	0.67
1:A:1:MET:HG3	1:A:157:ILE:CD1	2.25	0.66
1:A:239:VAL:HG13	1:A:240:PHE:N	2.11	0.65
1:A:181:GLN:O	1:A:185:GLU:HG3	1.97	0.65
1:B:63:ILE:CD1	1:B:74:LYS:HE2	2.25	0.64
1:A:239:VAL:HG22	1:A:240:PHE:N	2.13	0.63
1:C:168:ASP:HB3	3:C:9109:HOH:O	1.98	0.63
1:D:196:MET:HE3	1:D:224:PHE:CE1	2.34	0.62
1:C:64:ASN:HB3	1:C:67:ALA:HB2	1.82	0.61
1:B:67:ALA:O	1:B:70:THR:HG22	2.01	0.61
1:B:28:GLU:OE2	1:B:205:ARG:HD3	2.01	0.61
1:C:223:LEU:HD23	1:C:223:LEU:O	2.01	0.60
1:A:0:GLN:HE22	1:A:23:HIS:HD2	1.48	0.60
1:D:196:MET:HE3	1:D:224:PHE:HE1	1.66	0.60
1:B:170:GLU:CD	1:B:170:GLU:H	2.10	0.59
1:D:221:GLU:HG2	1:D:222:ASP:N	2.16	0.59
1:D:221:GLU:HG2	1:D:222:ASP:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:HD21	3:A:9114:HOH:O	2.03	0.59
1:D:180:LYS:HG2	1:D:202:VAL:HG11	1.85	0.59
1:C:196:MET:HG3	1:C:224:PHE:CE1	2.38	0.58
1:C:215:ILE:HD12	1:C:215:ILE:N	2.19	0.58
1:C:57:GLU:HG3	3:C:9097:HOH:O	2.03	0.58
1:D:33:ILE:HG21	1:D:196:MET:HE1	1.86	0.58
1:B:144:ARG:HG2	1:B:178:VAL:HG21	1.85	0.58
1:B:101:ALA:HB3	1:B:102:PRO:HD3	1.86	0.58
1:B:68:LYS:H	1:B:68:LYS:CD	2.11	0.57
1:A:110:ARG:O	1:A:114:GLU:HG3	2.04	0.57
1:A:216:GLU:HG3	1:A:229:HIS:HD2	1.70	0.57
1:D:83:PHE:N	1:D:87:ASN:HD21	1.90	0.57
1:B:67:ALA:HB3	1:B:70:THR:HB	1.87	0.56
1:D:74:LYS:O	1:D:78:GLU:HG3	2.06	0.56
1:D:48:ASN:HB3	1:D:79:VAL:HG11	1.88	0.56
1:C:1:MET:HG3	1:C:157:ILE:HD11	1.88	0.55
1:C:15:GLU:HG2	1:C:18:LYS:HG2	1.89	0.55
1:A:58:ILE:C	1:A:59:ILE:HD12	2.31	0.55
1:A:236:LEU:O	1:A:239:VAL:HB	2.07	0.55
1:C:35:PRO:HD3	1:C:235:PHE:CE2	2.42	0.54
1:C:238:LYS:O	1:C:239:VAL:HG13	2.07	0.54
1:C:44:LEU:HB3	1:C:81:MET:HE1	1.90	0.54
1:D:81:MET:HE3	1:D:159:LEU:HD12	1.90	0.54
1:C:171:MET:O	1:C:174:GLU:HG2	2.07	0.54
1:C:237:SER:O	1:C:238:LYS:HG2	2.07	0.54
1:C:135:ASP:HB2	1:D:85:ARG:H	1.73	0.54
1:A:237:SER:C	1:A:239:VAL:H	2.14	0.54
1:C:234:ALA:HA	1:C:238:LYS:CG	2.38	0.54
1:C:68:LYS:CE	1:C:68:LYS:N	2.66	0.54
1:B:101:ALA:HB3	3:B:9048:HOH:O	2.08	0.53
1:C:200:ARG:HH22	1:C:225:ASP:CG	2.16	0.53
1:C:38:SER:HB2	1:C:210:ASP:HA	1.89	0.53
1:B:194:HIS:C	1:B:196:MET:HE2	2.34	0.53
1:D:180:LYS:HG2	1:D:202:VAL:CG1	2.39	0.53
1:D:101:ALA:HB3	1:D:102:PRO:HD3	1.90	0.53
1:A:200:ARG:HD2	3:A:9073:HOH:O	2.09	0.53
1:C:20:ILE:CD1	1:C:213:TYR:HA	2.40	0.52
1:D:49:LEU:HD13	1:D:76:ARG:NH1	2.25	0.52
1:C:231:ARG:HA	1:C:234:ALA:HB3	1.92	0.52
1:C:175:VAL:O	1:C:178:VAL:HG22	2.10	0.51
1:B:194:HIS:HE1	3:B:9017:HOH:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LYS:HD2	1:C:55:GLU:OE2	2.10	0.51
1:C:49:LEU:N	1:C:49:LEU:HD12	2.25	0.51
1:C:67:ALA:HB3	1:C:70:THR:OG1	2.09	0.51
1:C:123:LYS:HE3	1:C:185:GLU:OE2	2.10	0.51
1:A:59:ILE:HD12	1:A:59:ILE:N	2.24	0.51
1:A:60:ILE:HG13	3:A:9114:HOH:O	2.11	0.51
1:C:11:PHE:CD2	1:C:16:VAL:HG11	2.46	0.51
1:D:40:LYS:HD2	1:D:192:VAL:HG13	1.92	0.51
1:B:83:PHE:N	1:B:87:ASN:HD21	1.89	0.51
1:D:201:GLU:HB2	3:D:9152:HOH:O	2.10	0.51
1:C:81:MET:HE3	1:C:159:LEU:CB	2.40	0.51
1:B:10:SER:N	1:B:54:ASP:OD2	2.43	0.51
1:C:81:MET:HE3	1:C:159:LEU:HB2	1.93	0.50
1:A:18:LYS:NZ	1:A:213:TYR:CE2	2.79	0.50
1:A:237:SER:C	1:A:239:VAL:N	2.69	0.50
1:D:67:ALA:HB3	1:D:70:THR:HB	1.94	0.49
1:D:84:GLN:HG3	1:D:162:GLU:O	2.12	0.49
1:C:0:GLN:OE1	1:C:23:HIS:HD2	1.95	0.49
1:A:227:PRO:HG2	1:A:233:LYS:HG2	1.93	0.49
1:A:212:GLY:N	3:A:9095:HOH:O	2.46	0.49
1:B:5:HIS:CE1	1:B:6:GLN:HG3	2.47	0.49
1:D:76:ARG:HG2	3:D:9051:HOH:O	2.13	0.49
1:C:10:SER:N	1:C:54:ASP:OD2	2.45	0.49
1:B:3:ASP:OD1	1:B:23:HIS:HD2	1.95	0.48
1:A:207:LEU:CD2	1:A:217:GLU:HG2	2.44	0.48
1:C:135:ASP:O	1:D:84:GLN:HB3	2.13	0.48
1:A:1:MET:HG3	1:A:157:ILE:CG1	2.44	0.48
1:C:234:ALA:HA	1:C:238:LYS:HG3	1.95	0.48
1:B:84:GLN:HG3	1:B:162:GLU:O	2.13	0.48
1:C:3:ASP:HB3	1:C:59:ILE:HB	1.96	0.48
1:B:103:MET:O	1:B:107:LYS:HA	2.14	0.48
1:A:6:GLN:HE21	1:A:21:ASN:ND2	1.97	0.48
1:A:206:VAL:HG23	1:A:220:PRO:HG3	1.96	0.48
1:B:75:VAL:HG23	1:B:76:ARG:N	2.28	0.48
1:A:10:SER:HA	1:A:15:GLU:HA	1.95	0.47
1:B:141:GLN:HG2	1:B:144:ARG:NH2	2.29	0.47
1:C:8:LYS:HB2	1:C:55:GLU:HB2	1.95	0.47
1:D:94:VAL:O	1:D:98:ILE:HG13	2.14	0.47
1:C:99:THR:C	1:C:102:PRO:HD2	2.40	0.47
1:C:20:ILE:HG22	1:C:22:VAL:HG23	1.97	0.47
1:C:0:GLN:OE1	1:C:23:HIS:CD2	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:VAL:O	1:D:240:PHE:HB2	2.15	0.47
1:C:101:ALA:HB3	1:C:102:PRO:HD3	1.97	0.47
1:D:57:GLU:HB2	3:D:9153:HOH:O	2.14	0.47
1:D:205:ARG:HD2	3:D:9043:HOH:O	2.13	0.47
1:C:234:ALA:O	1:C:238:LYS:HB2	2.14	0.46
1:A:-1:LEU:HD23	1:A:-1:LEU:N	2.31	0.46
1:A:240:PHE:CD2	1:A:240:PHE:C	2.94	0.46
1:D:0:GLN:HE21	1:D:3:ASP:HB2	1.81	0.46
1:C:72:LEU:O	1:C:76:ARG:HG3	2.16	0.46
1:D:0:GLN:HE22	1:D:23:HIS:CG	2.33	0.46
1:C:171:MET:HG2	3:C:9100:HOH:O	2.15	0.46
1:C:110:ARG:O	1:C:114:GLU:HG3	2.16	0.46
1:C:234:ALA:CA	1:C:238:LYS:HG3	2.46	0.46
1:D:8:LYS:HB2	1:D:55:GLU:HB2	1.98	0.46
1:D:63:ILE:HD13	1:D:71:ASN:O	2.16	0.45
1:B:180:LYS:HG3	1:B:202:VAL:HG22	1.98	0.45
1:A:73:ASN:O	1:A:77:GLU:HG3	2.17	0.45
1:A:194:HIS:C	1:A:196:MET:HE3	2.41	0.45
1:B:180:LYS:HD2	3:B:9127:HOH:O	2.16	0.45
1:D:64:ASN:HB3	1:D:67:ALA:HB2	1.98	0.45
1:D:187:MET:O	1:D:189:MET:HG3	2.16	0.45
1:D:169:PRO:HG3	3:D:9117:HOH:O	2.17	0.45
1:A:49:LEU:HG	1:A:75:VAL:HG21	1.98	0.45
1:B:232:THR:O	1:B:236:LEU:HG	2.16	0.45
1:C:120:LEU:O	1:C:123:LYS:HB3	2.17	0.45
1:C:20:ILE:HD11	1:C:213:TYR:HA	1.99	0.45
1:C:200:ARG:NH2	1:C:225:ASP:OD2	2.50	0.45
1:B:63:ILE:HD13	1:B:71:ASN:O	2.17	0.44
1:D:6:GLN:HG3	3:D:9112:HOH:O	2.17	0.44
1:D:52:ASP:HB2	3:D:9048:HOH:O	2.16	0.44
1:A:90:PRO:HA	1:A:134:PRO:HD2	1.98	0.44
1:A:103:MET:HE1	1:A:110:ARG:HE	1.82	0.44
1:D:210:ASP:HB3	1:D:215:ILE:HG13	1.99	0.44
1:A:84:GLN:HG3	1:A:165:SER:OG	2.17	0.44
1:B:207:LEU:CD2	1:B:217:GLU:HG3	2.45	0.44
1:C:6:GLN:NE2	1:C:21:ASN:HD21	2.08	0.44
1:C:103:MET:O	1:C:107:LYS:HA	2.17	0.44
1:D:48:ASN:O	1:D:49:LEU:HB2	2.18	0.44
1:A:33:ILE:HD13	1:A:33:ILE:H	1.81	0.44
1:B:75:VAL:CG2	1:B:76:ARG:N	2.81	0.44
1:A:1:MET:HG3	1:A:157:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASP:HB2	3:A:9109:HOH:O	2.17	0.44
1:B:64:ASN:HB3	1:B:67:ALA:HB2	2.00	0.44
1:B:149:ARG:NH1	1:B:149:ARG:HG2	2.33	0.43
1:D:219:LYS:HE2	1:D:221:GLU:OE2	2.18	0.43
1:B:149:ARG:HG2	1:B:149:ARG:HH11	1.83	0.43
1:D:120:LEU:HD12	1:D:120:LEU:HA	1.88	0.43
1:C:138:SER:OG	1:C:141:GLN:HG3	2.18	0.43
1:B:200:ARG:HH22	1:B:225:ASP:CG	2.26	0.43
1:C:196:MET:HG3	1:C:224:PHE:CZ	2.54	0.43
1:D:83:PHE:H	1:D:87:ASN:ND2	1.92	0.43
1:B:92:MET:HG3	1:B:97:ASN:ND2	2.34	0.43
1:A:33:ILE:HD12	1:A:206:VAL:CG1	2.49	0.42
1:B:53:PHE:CE1	1:B:66:LYS:HE2	2.54	0.42
1:A:230:GLU:CD	1:A:230:GLU:N	2.73	0.42
1:B:170:GLU:HG2	3:B:9066:HOH:O	2.19	0.42
1:D:0:GLN:HE21	1:D:3:ASP:CB	2.32	0.42
1:C:74:LYS:O	1:C:78:GLU:HG3	2.19	0.42
1:C:138:SER:HG	1:C:141:GLN:HG3	1.84	0.42
1:C:76:ARG:NH2	3:C:9041:HOH:O	2.51	0.42
1:D:229:HIS:HB3	2:D:9005:SO4:O1	2.20	0.42
1:A:181:GLN:HG3	3:A:9106:HOH:O	2.20	0.42
1:B:67:ALA:O	1:B:68:LYS:C	2.63	0.42
1:A:160:PHE:CD1	1:A:179:MET:HE3	2.54	0.42
1:C:234:ALA:HA	1:C:238:LYS:HG2	2.02	0.42
1:A:11:PHE:N	1:A:14:LEU:O	2.42	0.41
1:C:205:ARG:HG2	1:C:205:ARG:HH11	1.85	0.41
1:C:203:GLY:O	1:C:220:PRO:HG2	2.20	0.41
1:A:25:ARG:HG2	1:A:25:ARG:HH11	1.86	0.41
1:D:71:ASN:HD21	1:D:74:LYS:HB2	1.86	0.41
1:A:25:ARG:O	1:A:28:GLU:HB2	2.21	0.41
1:C:30:VAL:HG13	1:C:207:LEU:HD13	2.03	0.41
1:C:133:TYR:OH	1:D:51:GLU:HG3	2.21	0.41
1:D:221:GLU:OE1	1:D:221:GLU:N	2.49	0.41
1:A:2:ILE:HB	1:A:24:ILE:HB	2.03	0.41
1:D:53:PHE:CE2	1:D:58:ILE:HD12	2.56	0.41
1:A:96:ASN:ND2	3:A:9091:HOH:O	2.54	0.41
1:B:83:PHE:H	1:B:87:ASN:ND2	1.89	0.41
1:C:180:LYS:HB3	1:C:180:LYS:HE2	1.93	0.41
1:D:20:ILE:HG22	1:D:22:VAL:HG23	2.03	0.41
1:A:239:VAL:CG1	1:A:240:PHE:H	2.15	0.41
1:B:233:LYS:HD2	3:B:9101:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASP:O	1:A:162:GLU:C	2.64	0.40
1:B:67:ALA:O	1:B:68:LYS:O	2.39	0.40
1:C:200:ARG:HA	1:C:220:PRO:HB3	2.03	0.40
1:A:6:GLN:NE2	1:A:21:ASN:ND2	2.59	0.40
1:A:111:GLU:H	1:A:111:GLU:CD	2.30	0.40
1:C:6:GLN:O	1:C:56:GLY:HA3	2.21	0.40
1:C:229:HIS:CD2	1:C:229:HIS:N	2.89	0.40
1:B:194:HIS:HA	1:B:196:MET:CE	2.52	0.40
1:D:71:ASN:ND2	1:D:74:LYS:HB2	2.36	0.40

There are no symmetry-related clashes.

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	240/263 (91%)	232 (97%)	6 (2%)	2 (1%)	16	10
1	B	239/263 (91%)	232 (97%)	6 (2%)	1 (0%)	30	26
1	C	240/263 (91%)	226 (94%)	12 (5%)	2 (1%)	16	10
1	D	239/263 (91%)	232 (97%)	7 (3%)	0	100	100
All	All	958/1052 (91%)	922 (96%)	31 (3%)	5 (0%)	24	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	VAL
1	B	68	LYS
1	C	239	VAL
1	A	230	GLU
1	C	238	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	207/225 (92%)	201 (97%)	6 (3%)	37	39
1	B	206/225 (92%)	203 (98%)	3 (2%)	57	64
1	C	207/225 (92%)	203 (98%)	4 (2%)	50	56
1	D	206/225 (92%)	203 (98%)	3 (2%)	57	64
All	All	826/900 (92%)	810 (98%)	16 (2%)	50	56

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	33	ILE
1	A	170	GLU
1	A	230	GLU
1	A	238	LYS
1	A	240	PHE
1	B	16	VAL
1	B	48	ASN
1	B	68	LYS
1	C	68	LYS
1	C	196	MET
1	C	205	ARG
1	C	239	VAL
1	D	120	LEU
1	D	171	MET
1	D	230	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	GLN
1	A	6	GLN
1	A	23	HIS

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Mol	Chain	Res	Type
1	A	73	ASN
1	A	96	ASN
1	A	131	HIS
1	A	181	GLN
1	A	229	HIS
1	B	0	GLN
1	B	23	HIS
1	B	48	ASN
1	B	87	ASN
1	B	181	GLN
1	B	194	HIS
1	C	6	GLN
1	C	23	HIS
1	C	96	ASN
1	C	181	GLN
1	D	0	GLN
1	D	5	HIS
1	D	87	ASN
1	D	131	HIS
1	D	194	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	D	9005	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	B	9001	-	4,4,4	0.39	0	6,6,6	0.14	0
2	SO4	D	9002	-	4,4,4	0.34	0	6,6,6	0.25	0
2	SO4	B	9006	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	A	9003	-	4,4,4	0.33	0	6,6,6	0.13	0
2	SO4	C	9004	-	4,4,4	0.40	0	6,6,6	0.13	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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	9005	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	242/263 (92%)	0.21	14 (5%) 29 32	15, 29, 54, 104	0
1	B	241/263 (91%)	-0.02	6 (2%) 58 62	14, 27, 49, 80	0
1	C	242/263 (92%)	0.32	15 (6%) 26 30	15, 33, 61, 99	0
1	D	241/263 (91%)	0.05	4 (1%) 69 73	16, 30, 48, 69	0
All	All	966/1052 (91%)	0.14	39 (4%) 42 47	14, 30, 54, 104	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	VAL	6.6
1	C	236	LEU	5.6
1	D	240	PHE	5.0
1	C	239	VAL	5.0
1	A	236	LEU	4.7
1	A	240	PHE	4.6
1	C	235	PHE	4.4
1	C	234	ALA	4.0
1	C	232	THR	3.9
1	C	237	SER	3.7
1	B	240	PHE	3.6
1	A	235	PHE	3.6
1	C	238	LYS	3.6
1	C	240	PHE	3.5
1	C	230	GLU	3.2
1	A	211	GLY	2.9
1	B	72	LEU	2.9
1	D	228	GLN	2.8
1	C	233	LYS	2.7
1	A	234	ALA	2.6
1	C	227	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	231	ARG	2.6
1	A	237	SER	2.6
1	A	227	PRO	2.5
1	A	16	VAL	2.4
1	D	239	VAL	2.4
1	C	223	LEU	2.4
1	B	70	THR	2.4
1	A	14	LEU	2.4
1	B	91	HIS	2.4
1	A	85	ARG	2.3
1	B	71	ASN	2.2
1	A	231	ARG	2.2
1	C	-1	LEU	2.1
1	C	224	PHE	2.1
1	B	75	VAL	2.1
1	A	232	THR	2.1
1	A	230	GLU	2.1
1	D	91	HIS	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(\AA^2)	Q<0.9
2	SO4	C	9004	5/5	0.86	0.14	47,48,51,51	0
2	SO4	A	9003	5/5	0.93	0.10	40,40,43,43	0
2	SO4	D	9005	5/5	0.93	0.09	46,46,47,47	0
2	SO4	B	9006	5/5	0.97	0.05	39,40,40,42	0
2	SO4	D	9002	5/5	0.98	0.04	13,14,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	B	9001	5/5	0.99	0.04	21,21,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.