



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:45 am BST

PDB ID : 5OVQ
Title : Crystal Structure of the peroxiredoxin (AhpC2) from the Hyperthermophilic bacteria Aquifex aeolicus VF
Authors : Warkentin, E.; Peng, G.
Deposited on : 2017-08-29
Resolution : 1.80 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 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

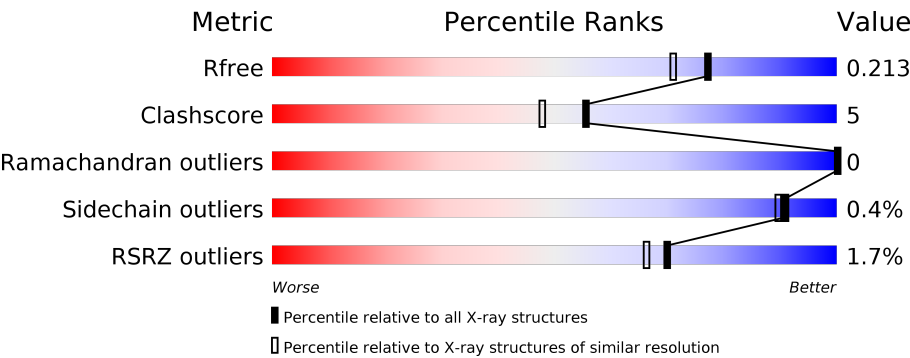
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	223	<div><div></div><div>91%7%•</div></div>
1	B	223	<div><div>%</div><div>90%9%•</div></div>
1	C	223	<div><div></div><div>88%10%•</div></div>
1	E	223	<div><div>%</div><div>89%9%•</div></div>
1	K	223	<div><div>4%</div><div>86%12%•</div></div>
2	D	222	<div><div>%</div><div>89%9%•</div></div>

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Mol	Chain	Length	Quality of chain
2	F	222	<div><div><div>%</div><div><div></div><div>88%</div><div>10%</div></div><div></div></div></div>
2	G	222	<div><div><div></div><div>92%</div><div>6%</div></div><div></div></div>
2	H	222	<div><div><div>2%</div><div><div></div><div>86%</div><div>12%</div></div><div></div></div></div>
2	I	222	<div><div><div>%</div><div><div></div><div>85%</div><div>14%</div></div><div></div></div></div>
2	J	222	<div><div><div>3%</div><div><div></div><div>88%</div><div>10%</div></div><div></div></div></div>
2	L	222	<div><div><div>4%</div><div><div></div><div>86%</div><div>12%</div></div><div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22777 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 Peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	1	0
			1767	1147	288	325	7			
1	B	221	Total	C	N	O	S	0	0	0
			1778	1155	290	326	7			
1	C	219	Total	C	N	O	S	0	0	0
			1764	1145	288	324	7			
1	E	219	Total	C	N	O	S	0	0	0
			1764	1145	288	324	7			
1	K	219	Total	C	N	O	S	0	0	0
			1764	1145	288	324	7			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ALA	-	expression tag	UNP O67024
B	223	ALA	-	expression tag	UNP O67024
C	223	ALA	-	expression tag	UNP O67024
E	223	ALA	-	expression tag	UNP O67024
K	223	ALA	-	expression tag	UNP O67024

- Molecule 2 is a protein called Peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	218	Total	C	N	O	S	0	0	0
			1759	1142	287	323	7			
2	F	218	Total	C	N	O	S	0	0	0
			1759	1142	287	323	7			
2	G	218	Total	C	N	O	S	0	0	0
			1758	1142	287	322	7			
2	H	218	Total	C	N	O	S	0	0	0
			1759	1142	287	323	7			
2	I	218	Total	C	N	O	S	0	0	0
			1759	1142	287	323	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	217	Total	C	N	O	S	0	0	0
			1753	1139	286	321	7			
2	L	220	Total	C	N	O	S	0	1	0
			1779	1156	289	327	7			

- Molecule 3 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			5	4	1		
3	J	1	Total	C	O	0	0
			5	4	1		
3	D	1	Total	C	O	0	0
			5	4	1		
3	K	1	Total	C	O	0	0
			5	4	1		
3	E	1	Total	C	O	0	0
			5	4	1		
3	H	1	Total	C	O	0	0
			5	4	1		
3	B	1	Total	C	O	0	0
			5	4	1		
3	I	1	Total	C	O	0	0
			5	4	1		
3	A	1	Total	C	O	0	0
			5	4	1		
3	L	1	Total	C	O	0	0
			5	4	1		
3	F	1	Total	C	O	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	191	Total	O	0	0
			191	191		
4	B	153	Total	O	0	0
			153	153		
4	C	128	Total	O	0	0
			128	128		
4	D	143	Total	O	0	0
			143	143		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	129	Total 129	O 129	0	0
4	F	113	Total 113	O 113	0	0
4	G	136	Total 136	O 136	0	0
4	H	117	Total 117	O 117	0	0
4	I	149	Total 149	O 149	0	0
4	J	106	Total 106	O 106	0	0
4	K	112	Total 112	O 112	0	0
4	L	82	Total 82	O 82	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

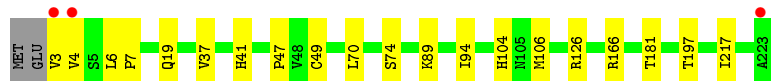
• Molecule 1: Peroxiredoxin

Chain A: 




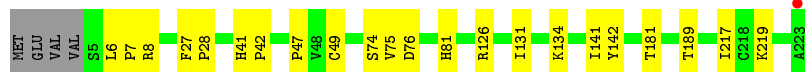
• Molecule 1: Peroxiredoxin

Chain B: 




• Molecule 1: Peroxiredoxin

Chain C: 




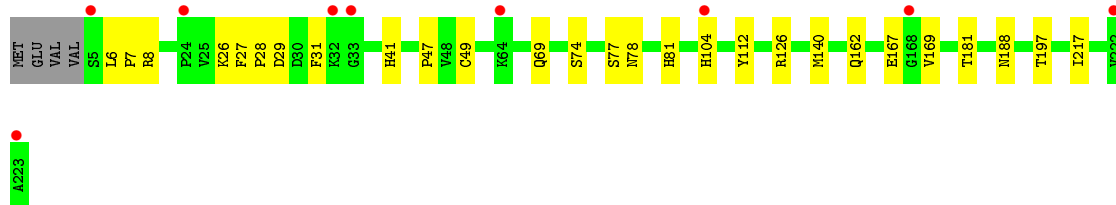
• Molecule 1: Peroxiredoxin

Chain E: 

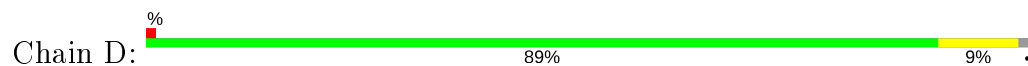


• Molecule 1: Peroxiredoxin

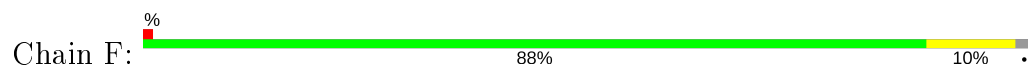
Chain K: 



- Molecule 2: Peroxiredoxin



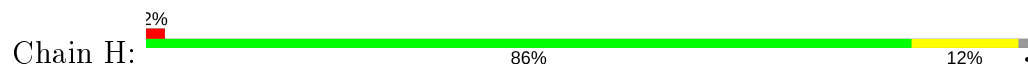
- Molecule 2: Peroxiredoxin



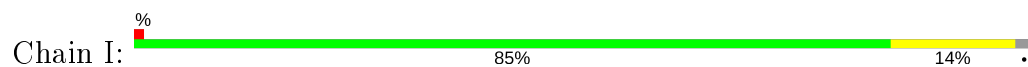
- Molecule 2: Peroxiredoxin



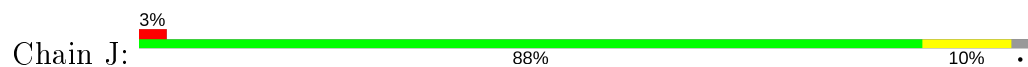
- Molecule 2: Peroxiredoxin



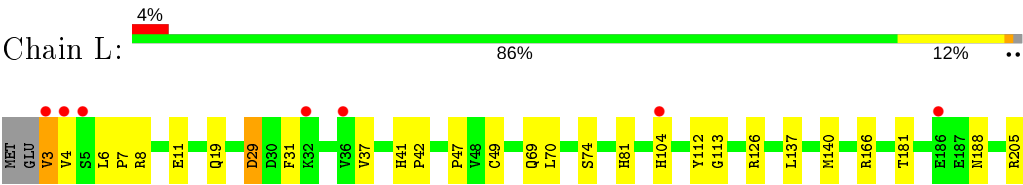
- Molecule 2: Peroxiredoxin



- Molecule 2: Peroxiredoxin



● Molecule 2: Peroxiredoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.10Å 141.50Å 143.00Å 61.00° 79.40° 80.90°	Depositor
Resolution (Å)	19.99 – 1.80 19.99 – 1.46	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.99-1.80) 84.1 (19.99-1.46)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.46Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.185 , 0.214 0.191 , 0.213	Depositor DCC
R_{free} test set	24911 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.044 for h,h-k,h-l 0.023 for -h,-h+l,-h+k 0.028 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22777	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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: OCS, UNL

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	0.41	0/1812	0.57	0/2468
1	B	0.42	0/1820	0.58	0/2480
1	C	0.37	0/1806	0.55	0/2460
1	E	0.36	0/1806	0.57	0/2460
1	K	0.35	0/1806	0.56	0/2460
2	D	0.37	0/1801	0.58	0/2453
2	F	0.35	0/1801	0.57	0/2453
2	G	0.38	0/1800	0.56	0/2452
2	H	0.36	0/1801	0.56	0/2453
2	I	0.36	0/1801	0.54	0/2453
2	J	0.38	0/1795	0.58	0/2445
2	L	0.35	0/1824	0.55	0/2486
All	All	0.37	0/21673	0.56	0/29523

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	146	THR	Peptide

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	1767	0	1739	16	0
1	B	1778	0	1752	19	0
1	C	1764	0	1734	22	0
1	E	1764	0	1734	19	0
1	K	1764	0	1734	25	0
2	D	1759	0	1729	19	0
2	F	1759	0	1729	19	0
2	G	1758	0	1726	10	0
2	H	1759	0	1728	20	0
2	I	1759	0	1729	25	0
2	J	1753	0	1724	18	0
2	L	1779	0	1753	27	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	1	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
4	A	191	0	0	4	1
4	B	153	0	0	7	0
4	C	128	0	0	5	0
4	D	143	0	0	2	0
4	E	129	0	0	6	0
4	F	113	0	0	5	0
4	G	136	0	0	0	1
4	H	117	0	0	4	1
4	I	149	0	0	7	0
4	J	106	0	0	4	0
4	K	112	0	0	4	0
4	L	82	0	0	7	1
All	All	22777	0	20811	215	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 5.

All (215) 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:A:6:LEU:HD13	1:B:6:LEU:HD13	1.42	1.01
2:H:77:SER:HA	2:H:104:HIS:NE2	1.79	0.97
1:C:6:LEU:HD13	2:D:6:LEU:HD13	1.48	0.95
2:I:178:GLU:OE2	4:I:401:HOH:O	1.86	0.92
2:F:219:LYS:NZ	4:F:401:HOH:O	2.02	0.91
2:I:194:PRO:O	4:I:402:HOH:O	1.90	0.87
2:L:19:GLN:OE1	4:L:401:HOH:O	1.93	0.86
1:E:19:GLN:NE2	4:E:402:HOH:O	2.09	0.86
2:D:166:ARG:NH1	4:D:401:HOH:O	2.07	0.83
1:B:104:HIS:O	4:B:401:HOH:O	1.97	0.82
1:C:189:THR:O	4:C:301:HOH:O	1.99	0.79
1:E:26:LYS:NZ	1:E:29:ASP:OD2	2.17	0.78
1:E:211:GLU:OE1	4:E:401:HOH:O	2.04	0.76
1:K:188:ASN:OD1	4:K:401:HOH:O	2.03	0.76
1:C:6:LEU:O	1:C:8:ARG:NH1	2.19	0.74
1:K:162:GLN:OE1	4:K:402:HOH:O	2.04	0.74
1:K:6:LEU:HD12	1:K:7:PRO:HD2	1.69	0.73
2:L:19:GLN:NE2	4:L:404:HOH:O	2.21	0.73
2:G:181:THR:HG23	2:H:181:THR:HG23	1.69	0.73
1:A:181:THR:HG23	1:B:181:THR:HG23	1.70	0.72
2:H:159:ASP:OD2	4:H:401:HOH:O	2.07	0.72
2:I:13:ALA:O	4:I:403:HOH:O	2.06	0.72
2:I:181:THR:HG23	2:J:181:THR:HG23	1.72	0.71
2:F:69:GLN:OE1	4:F:402:HOH:O	2.09	0.70
1:A:104:HIS:O	4:A:401:HOH:O	2.10	0.70
2:J:174:ASP:OD2	4:J:402:HOH:O	2.10	0.70
1:K:181:THR:HG23	2:L:181:THR:HG23	1.73	0.70
2:J:211:GLU:OE1	4:J:401:HOH:O	2.09	0.69
1:C:49:OCS:OD3	1:C:126:ARG:NH1	2.26	0.69
1:A:6:LEU:HD12	1:A:7:PRO:HD2	1.75	0.69
2:L:188:ASN:OD1	4:L:403:HOH:O	2.11	0.68
2:D:27:PHE:HZ	2:D:131:ILE:HD13	1.59	0.67
1:E:19:GLN:HG3	1:E:78:ASN:ND2	2.08	0.67
2:I:201:ASP:OD1	4:I:404:HOH:O	2.12	0.67
2:I:5:SER:N	4:I:407:HOH:O	2.28	0.67
2:L:49:OCS:OD3	2:L:126:ARG:NH1	2.26	0.67
1:K:49:OCS:OD3	1:K:126:ARG:NH1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:6:LEU:HD23	2:J:7:PRO:HD3	1.78	0.65
1:E:19:GLN:OE1	4:E:403:HOH:O	2.15	0.64
1:A:5:SER:N	4:A:404:HOH:O	2.30	0.63
1:C:28:PRO:HG3	4:C:390:HOH:O	1.96	0.63
2:J:6:LEU:HD21	2:J:113:GLY:HA3	1.81	0.63
2:G:49:OCS:OD3	2:G:126:ARG:NH1	2.32	0.62
2:D:137:LEU:HD21	2:D:140:MET:CE	2.30	0.62
2:I:49:OCS:OD2	2:I:126:ARG:NH1	2.31	0.62
2:L:8:ARG:HB2	2:L:11[B]:GLU:HG2	1.82	0.61
2:D:27:PHE:CZ	2:D:131:ILE:HD13	2.34	0.61
1:B:6:LEU:HD12	1:B:7:PRO:HD2	1.82	0.61
2:J:49:OCS:OD3	2:J:126:ARG:NH1	2.32	0.61
2:F:5:SER:HB3	4:F:426:HOH:O	1.99	0.60
1:C:181:THR:HG23	2:D:181:THR:HG23	1.83	0.60
2:G:6:LEU:HD12	2:G:7:PRO:HD2	1.84	0.60
2:H:49:OCS:OD2	2:H:126:ARG:NH1	2.35	0.60
2:D:6:LEU:HD12	2:D:7:PRO:HD2	1.84	0.59
1:E:49:OCS:OD3	1:E:126:ARG:NH1	2.32	0.59
2:H:90:GLU:OE2	4:H:403:HOH:O	2.17	0.59
1:E:141:ILE:HG12	2:F:141:ILE:HG12	1.85	0.59
1:E:219:LYS:NZ	4:E:408:HOH:O	2.35	0.59
2:L:47:PRO:HB3	2:L:217:ILE:HA	1.85	0.58
2:I:5:SER:N	4:I:410:HOH:O	2.35	0.58
1:B:19:GLN:NE2	4:B:402:HOH:O	2.11	0.58
2:D:17:GLU:OE2	2:D:26:LYS:NZ	2.33	0.58
2:L:137:LEU:HD21	2:L:140:MET:CE	2.31	0.58
1:B:197:THR:O	2:F:78:ASN:ND2	2.36	0.58
1:K:167:GLU:HB2	1:K:169:VAL:HG22	1.86	0.58
2:G:6:LEU:HD13	2:H:6:LEU:HD13	1.85	0.58
2:H:219:LYS:NZ	4:H:409:HOH:O	2.33	0.57
1:C:6:LEU:HD12	1:C:7:PRO:HD2	1.86	0.56
1:A:6:LEU:HB3	1:B:4:VAL:HG12	1.88	0.56
2:L:205:ARG:NH1	4:L:405:HOH:O	2.28	0.56
2:L:11[B]:GLU:HG3	4:L:433:HOH:O	2.04	0.56
2:D:41:HIS:CE1	2:D:74:SER:HB3	2.42	0.55
2:D:49:OCS:OD2	2:D:126:ARG:NH1	2.39	0.55
2:F:54:VAL:HG13	2:F:94:ILE:HD13	1.87	0.55
2:F:49:OCS:OD3	2:F:126:ARG:NH1	2.38	0.55
2:F:47:PRO:HB3	2:F:217:ILE:HA	1.89	0.55
1:K:6:LEU:HD13	2:L:6:LEU:HD13	1.87	0.55
2:J:219:LYS:NZ	4:J:405:HOH:O	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:143:TYR:HE1	2:H:141:ILE:HD11	1.70	0.54
1:K:6:LEU:O	1:K:8:ARG:NH1	2.39	0.54
1:E:6:LEU:HD12	1:E:7:PRO:HD2	1.89	0.54
2:J:41:HIS:HB2	2:J:49:OCS:OD3	2.08	0.54
2:H:102:ALA:HB1	2:H:104:HIS:CE1	2.43	0.54
2:L:29:ASP:N	2:L:29:ASP:OD1	2.41	0.54
1:C:134:LYS:HE3	4:C:306:HOH:O	2.07	0.54
2:G:167:GLU:HB2	2:G:169:VAL:HG22	1.90	0.54
2:H:77:SER:HA	2:H:104:HIS:CD2	2.43	0.54
1:B:104:HIS:NE2	4:B:408:HOH:O	2.34	0.53
1:B:166:ARG:NH1	4:B:404:HOH:O	2.26	0.53
2:I:26:LYS:HE3	2:I:29:ASP:OD2	2.08	0.53
1:A:49:OCS:OD3	1:A:126:ARG:NH1	2.41	0.53
2:J:6:LEU:HD21	2:J:113:GLY:CA	2.38	0.53
2:L:4:VAL:HG11	2:L:113:GLY:HA2	1.91	0.53
2:L:31:PHE:CE1	2:L:69:GLN:HG2	2.44	0.52
2:L:166:ARG:NH1	4:L:402:HOH:O	1.99	0.52
2:J:47:PRO:HB3	2:J:217:ILE:HA	1.90	0.52
1:B:41:HIS:HB2	1:B:49:OCS:OD2	2.10	0.52
1:K:31:PHE:CE1	1:K:69:GLN:HG2	2.44	0.52
2:H:47:PRO:HB3	2:H:217:ILE:HA	1.90	0.52
1:A:47:PRO:HB3	1:A:217:ILE:HA	1.91	0.51
2:F:29:ASP:OD1	2:F:29:ASP:N	2.43	0.51
1:B:3:VAL:HG22	4:B:453:HOH:O	2.10	0.51
1:A:89:LYS:NZ	4:A:405:HOH:O	2.38	0.50
1:A:41:HIS:HB2	1:A:49:OCS:OD3	2.12	0.50
2:J:26:LYS:NZ	4:J:410:HOH:O	2.44	0.50
1:B:49:OCS:OD2	1:B:126:ARG:NH1	2.45	0.49
1:A:29:ASP:OD1	1:A:29:ASP:N	2.46	0.49
2:H:26:LYS:NZ	2:H:29:ASP:OD2	2.34	0.49
1:B:37:VAL:HB	1:B:70:LEU:HD23	1.95	0.49
1:K:104:HIS:CE1	4:K:410:HOH:O	2.66	0.49
2:L:6:LEU:HD12	2:L:7:PRO:HD2	1.94	0.49
1:C:219:LYS:NZ	4:C:303:HOH:O	2.36	0.48
2:F:86:MET:O	2:F:90:GLU:HG3	2.13	0.48
1:K:26:LYS:HE3	1:K:29:ASP:OD2	2.13	0.48
1:C:41:HIS:CE1	1:C:74:SER:HB3	2.46	0.48
2:I:106:MET:CE	2:I:110:LYS:HE3	2.43	0.48
1:A:26:LYS:HE3	1:A:29:ASP:OD2	2.12	0.48
2:I:41:HIS:CE1	2:I:74:SER:HB3	2.48	0.48
2:J:197:THR:O	1:K:78:ASN:ND2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:47:PRO:HB3	2:G:217:ILE:HA	1.96	0.48
1:E:29:ASP:OD1	1:E:29:ASP:N	2.46	0.48
1:E:47:PRO:HB3	1:E:217:ILE:HA	1.96	0.48
2:G:62:GLU:O	2:G:65:LYS:HG2	2.14	0.47
1:K:41:HIS:CE1	1:K:74:SER:HB3	2.48	0.47
1:C:76:ASP:HB2	1:C:81:HIS:CE1	2.49	0.47
1:C:28:PRO:HB2	4:C:386:HOH:O	2.15	0.47
2:I:29:ASP:OD1	2:I:29:ASP:N	2.47	0.47
1:C:27:PHE:HZ	1:C:131:ILE:HD13	1.80	0.47
1:C:74:SER:OG	1:C:81:HIS:HE1	1.98	0.47
2:D:28:PRO:HB2	4:D:492:HOH:O	2.14	0.47
2:F:41:HIS:CE1	2:F:74:SER:HB3	2.50	0.47
2:I:6:LEU:HD12	2:I:7:PRO:HD2	1.97	0.47
2:G:41:HIS:HB2	2:G:49:OCS:OD3	2.15	0.46
2:I:128:LEU:HB3	2:I:141:ILE:HG12	1.96	0.46
1:K:47:PRO:HB3	1:K:217:ILE:HA	1.97	0.46
2:I:106:MET:HE3	2:I:115:ILE:HG13	1.98	0.46
2:J:8:ARG:HD3	2:J:11:GLU:OE2	2.16	0.45
2:L:41:HIS:CE1	2:L:74:SER:HB3	2.51	0.45
2:F:104:HIS:ND1	2:F:105:ASN:OD1	2.49	0.45
1:C:47:PRO:HB3	1:C:217:ILE:HA	1.98	0.45
2:H:41:HIS:CE1	2:H:74:SER:HB3	2.51	0.45
1:C:41:HIS:HB2	1:C:49:OCS:OD3	2.17	0.45
2:D:41:HIS:HB2	2:D:49:OCS:OD2	2.15	0.45
2:J:41:HIS:CE1	2:J:74:SER:HB3	2.52	0.45
2:L:4:VAL:CG1	2:L:113:GLY:HA2	2.47	0.45
1:A:41:HIS:CE1	1:A:74:SER:HB3	2.52	0.45
1:C:181:THR:OG1	2:D:183:GLU:OE1	2.35	0.45
1:E:61:GLU:HB2	4:E:451:HOH:O	2.17	0.45
1:E:181:THR:HG23	2:F:181:THR:HG23	1.99	0.44
1:K:104:HIS:NE2	4:K:410:HOH:O	2.36	0.44
2:J:78:ASN:ND2	1:K:197:THR:O	2.50	0.44
1:B:41:HIS:CE1	1:B:74:SER:HB3	2.52	0.44
2:I:91:LYS:NZ	4:I:418:HOH:O	2.51	0.44
2:D:47:PRO:HB3	2:D:217:ILE:HA	1.98	0.44
2:H:29:ASP:N	2:H:29:ASP:OD1	2.50	0.44
2:I:37:VAL:HB	2:I:70:LEU:HD23	1.98	0.44
1:B:89:LYS:NZ	4:B:417:HOH:O	2.49	0.44
2:F:27:PHE:CE1	2:F:36:VAL:HG11	2.53	0.44
1:K:74:SER:OG	1:K:81:HIS:HE1	2.01	0.44
2:I:42:PRO:HD2	2:I:49:OCS:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:3:VAL:HG12	2:L:4:VAL:HA	2.00	0.44
1:B:47:PRO:HB3	1:B:217:ILE:HA	2.00	0.44
2:F:27:PHE:HE1	2:F:36:VAL:HG11	1.83	0.44
2:H:204:LYS:HB3	2:H:204:LYS:NZ	2.32	0.44
2:J:29:ASP:N	2:J:29:ASP:OD1	2.50	0.44
1:K:8:ARG:NH2	2:L:4:VAL:H	2.16	0.44
2:H:37:VAL:HB	2:H:70:LEU:HD23	2.00	0.43
2:F:41:HIS:HB2	2:F:49:OCS:OD3	2.19	0.43
1:C:75:VAL:HB	2:L:104:HIS:NE2	2.33	0.43
2:I:41:HIS:HB2	2:I:49:OCS:OD2	2.19	0.43
1:C:42:PRO:HD2	1:C:49:OCS:OD3	2.19	0.43
1:E:183:GLU:OE1	2:F:181:THR:OG1	2.36	0.43
1:B:106:MET:HG3	4:B:401:HOH:O	2.18	0.43
1:E:41:HIS:CE1	1:E:74:SER:HB3	2.54	0.43
2:G:41:HIS:CE1	2:G:74:SER:HB3	2.54	0.43
2:I:106:MET:HE2	2:I:110:LYS:HE3	1.99	0.43
2:I:74:SER:OG	2:I:81:HIS:HE1	2.02	0.43
2:D:29:ASP:N	2:D:29:ASP:OD1	2.51	0.43
2:D:137:LEU:HD21	2:D:140:MET:HE1	2.01	0.42
1:C:141:ILE:HG22	2:D:141:ILE:HG12	2.01	0.42
1:A:19:GLN:NE2	4:A:407:HOH:O	2.43	0.42
1:A:8:ARG:NH2	1:B:4:VAL:H	2.16	0.42
2:H:74:SER:OG	2:H:81:HIS:HE1	2.02	0.42
1:E:41:HIS:HB2	1:E:49:OCS:OD3	2.19	0.42
1:K:77:SER:HA	1:K:104:HIS:NE2	2.35	0.42
2:F:178:GLU:OE2	4:F:403:HOH:O	2.21	0.42
2:I:145:LEU:HB3	3:I:301:UNL:C	2.50	0.42
1:K:29:ASP:OD1	1:K:29:ASP:N	2.53	0.42
2:L:7:PRO:HG3	2:L:112:TYR:HA	2.01	0.42
1:A:74:SER:OG	1:A:81:HIS:HE1	2.03	0.42
2:D:74:SER:OG	2:D:81:HIS:HE1	2.02	0.42
1:K:6:LEU:HD11	1:K:140:MET:HE3	2.02	0.41
2:L:42:PRO:HD2	2:L:49:OCS:OD3	2.20	0.41
1:C:27:PHE:CZ	1:C:131:ILE:HD13	2.55	0.41
2:L:166:ARG:HD3	4:L:402:HOH:O	2.20	0.41
1:C:142:TYR:HB2	2:D:140:MET:HG2	2.03	0.41
2:I:47:PRO:HB3	2:I:217:ILE:HA	2.02	0.41
2:L:74:SER:OG	2:L:81:HIS:HE1	2.03	0.41
1:B:6:LEU:HD12	1:B:7:PRO:CD	2.49	0.41
1:K:6:LEU:HD12	1:K:7:PRO:CD	2.47	0.41
1:E:215:TRP:NE1	4:E:404:HOH:O	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:PHE:CE1	1:E:69:GLN:HG2	2.56	0.41
2:H:105:ASN:HB2	4:H:477:HOH:O	2.21	0.41
2:H:196:PRO:HG2	2:H:202:ALA:HA	2.02	0.41
1:K:27:PHE:HA	1:K:28:PRO:HA	1.91	0.40
2:I:8:ARG:HD3	2:I:11:GLU:OE2	2.21	0.40
1:K:41:HIS:HB2	1:K:49:OCS:OD3	2.21	0.40
2:L:37:VAL:HB	2:L:70:LEU:HD23	2.03	0.40
2:L:3:VAL:HA	2:L:4:VAL:C	2.41	0.40
2:F:28:PRO:HB2	4:F:450:HOH:O	2.22	0.40
2:I:6:LEU:HB2	2:J:6:LEU:N	2.34	0.40
1:K:7:PRO:HG3	1:K:112:TYR:HA	2.03	0.40
1:E:19:GLN:HG3	1:E:78:ASN:HD21	1.82	0.40
2:H:31:PHE:CE1	2:H:69:GLN:HG2	2.56	0.40
2:J:205:ARG:HA	2:J:208:GLU:OE2	2.21	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)
4:A:563:HOH:O	4:G:444:HOH:O[1_565]	1.68	0.52
4:H:454:HOH:O	4:L:425:HOH:O[1_654]	1.97	0.23

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	217/223 (97%)	210 (97%)	7 (3%)	0	100	100
1	B	218/223 (98%)	212 (97%)	6 (3%)	0	100	100
1	C	216/223 (97%)	210 (97%)	6 (3%)	0	100	100
1	E	216/223 (97%)	210 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	216/223 (97%)	210 (97%)	6 (3%)	0	100	100
2	D	215/222 (97%)	209 (97%)	6 (3%)	0	100	100
2	F	215/222 (97%)	209 (97%)	6 (3%)	0	100	100
2	G	215/222 (97%)	210 (98%)	5 (2%)	0	100	100
2	H	215/222 (97%)	209 (97%)	6 (3%)	0	100	100
2	I	215/222 (97%)	209 (97%)	6 (3%)	0	100	100
2	J	214/222 (96%)	209 (98%)	5 (2%)	0	100	100
2	L	218/222 (98%)	212 (97%)	6 (3%)	0	100	100
All	All	2590/2669 (97%)	2519 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	190/193 (98%)	189 (100%)	1 (0%)	88	87
1	B	191/193 (99%)	190 (100%)	1 (0%)	88	87
1	C	189/193 (98%)	189 (100%)	0	100	100
1	E	189/193 (98%)	189 (100%)	0	100	100
1	K	189/193 (98%)	189 (100%)	0	100	100
2	D	189/193 (98%)	189 (100%)	0	100	100
2	F	189/193 (98%)	188 (100%)	1 (0%)	88	87
2	G	188/193 (97%)	188 (100%)	0	100	100
2	H	189/193 (98%)	186 (98%)	3 (2%)	62	54
2	I	189/193 (98%)	189 (100%)	0	100	100
2	J	188/193 (97%)	187 (100%)	1 (0%)	88	87
2	L	192/193 (100%)	190 (99%)	2 (1%)	76	71
All	All	2272/2316 (98%)	2263 (100%)	9 (0%)	91	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	B	94	ILE
2	F	29	ASP
2	H	178	GLU
2	H	204	LYS
2	H	222	VAL
2	J	94	ILE
2	L	3	VAL
2	L	29	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	OCS	C	49	1	7,8,9	0.94	0	6,11,13	1.53	1 (16%)
2	OCS	L	49	2	7,8,9	0.90	0	6,11,13	0.97	1 (16%)
2	OCS	J	49	2	7,8,9	0.80	0	6,11,13	1.20	1 (16%)
2	OCS	H	49	2	7,8,9	1.06	0	6,11,13	1.37	1 (16%)
1	OCS	E	49	1	7,8,9	0.86	0	6,11,13	1.18	0
1	OCS	K	49	1	7,8,9	0.90	0	6,11,13	1.83	1 (16%)
1	OCS	A	49	1	7,8,9	0.86	0	6,11,13	1.53	1 (16%)
2	OCS	G	49	2	7,8,9	1.01	0	6,11,13	1.70	1 (16%)
2	OCS	I	49	2	7,8,9	0.81	0	6,11,13	1.34	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OCS	F	49	2	7,8,9	1.09	0	6,11,13	1.18	0
2	OCS	D	49	2	7,8,9	0.99	0	6,11,13	1.12	1 (16%)
1	OCS	B	49	1	7,8,9	0.93	0	6,11,13	2.55	1 (16%)

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
1	OCS	C	49	1	-	0/4/7/9	-
2	OCS	L	49	2	-	0/4/7/9	-
2	OCS	J	49	2	-	0/4/7/9	-
2	OCS	H	49	2	-	0/4/7/9	-
1	OCS	E	49	1	-	0/4/7/9	-
1	OCS	K	49	1	-	0/4/7/9	-
1	OCS	A	49	1	-	0/4/7/9	-
2	OCS	G	49	2	-	0/4/7/9	-
2	OCS	I	49	2	-	0/4/7/9	-
2	OCS	F	49	2	-	0/4/7/9	-
2	OCS	D	49	2	-	0/4/7/9	-
1	OCS	B	49	1	-	0/4/7/9	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	OCS	OD3-SG-CB	5.35	113.30	106.94
1	K	49	OCS	OD2-SG-CB	4.05	112.20	105.74
2	G	49	OCS	OD1-SG-CB	3.78	111.43	106.94
1	C	49	OCS	OD2-SG-CB	3.49	111.31	105.74
2	I	49	OCS	OD3-SG-CB	2.71	110.16	106.94
2	H	49	OCS	OD3-SG-CB	2.62	110.06	106.94
2	J	49	OCS	OD1-SG-CB	2.55	109.97	106.94
1	A	49	OCS	OD1-SG-CB	2.26	109.62	106.94
2	D	49	OCS	OD3-SG-CB	2.17	109.52	106.94
2	L	49	OCS	OD2-SG-CB	2.09	109.07	105.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	49	OCS	3	0
2	L	49	OCS	2	0
2	J	49	OCS	2	0
2	H	49	OCS	1	0
1	E	49	OCS	2	0
1	K	49	OCS	2	0
1	A	49	OCS	2	0
2	G	49	OCS	2	0
2	I	49	OCS	3	0
2	F	49	OCS	2	0
2	D	49	OCS	2	0
1	B	49	OCS	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are unknown - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	218/223 (97%)	-0.39	0 100 100	19, 27, 43, 52	0
1	B	220/223 (98%)	-0.23	3 (1%) 75 72	20, 29, 48, 77	0
1	C	218/223 (97%)	-0.10	1 (0%) 91 89	28, 40, 57, 71	0
1	E	218/223 (97%)	-0.12	2 (0%) 84 82	32, 40, 59, 72	0
1	K	218/223 (97%)	0.10	9 (4%) 37 31	39, 46, 63, 83	0
2	D	217/222 (97%)	-0.28	2 (0%) 84 82	25, 34, 53, 62	0
2	F	217/222 (97%)	-0.13	3 (1%) 75 72	27, 38, 60, 70	0
2	G	217/222 (97%)	-0.24	1 (0%) 91 89	28, 37, 57, 68	0
2	H	217/222 (97%)	0.01	5 (2%) 60 56	31, 42, 64, 88	0
2	I	217/222 (97%)	-0.17	3 (1%) 75 72	27, 35, 54, 66	0
2	J	216/222 (97%)	-0.06	7 (3%) 47 41	30, 40, 61, 82	0
2	L	219/222 (98%)	0.21	9 (4%) 37 31	40, 48, 69, 97	0
All	All	2612/2669 (97%)	-0.12	45 (1%) 70 66	19, 39, 60, 97	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	4	VAL	12.0
1	B	3	VAL	6.8
2	L	3	VAL	6.8
1	B	223	ALA	6.6
1	K	223	ALA	6.2
2	J	222	VAL	5.9
2	H	222	VAL	5.7
2	I	222	VAL	5.0
2	L	222	VAL	4.4
1	C	223	ALA	4.0
2	H	104	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	222	VAL	3.8
1	B	4	VAL	3.8
1	K	5	SER	3.3
1	K	33	GLY	3.0
2	H	221	LYS	2.9
2	F	5	SER	2.8
1	E	222	VAL	2.8
1	K	222	VAL	2.8
1	K	32	LYS	2.8
2	I	32	LYS	2.8
1	E	223	ALA	2.7
1	K	24	PRO	2.7
2	F	6	LEU	2.5
2	L	221	LYS	2.5
1	K	104	HIS	2.5
2	I	5	SER	2.5
2	D	5	SER	2.5
2	H	209	GLY	2.4
2	J	221	LYS	2.4
2	J	209	GLY	2.4
2	J	207	GLN	2.4
2	L	104	HIS	2.4
1	K	64	LYS	2.4
2	L	32	LYS	2.3
2	G	32	LYS	2.3
2	F	28	PRO	2.3
2	L	36	VAL	2.2
2	J	24	PRO	2.2
2	L	5	SER	2.2
1	K	168	GLY	2.2
2	J	32	LYS	2.1
2	L	186	GLU	2.1
2	J	203	VAL	2.0
2	H	105	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	OCS	L	49	9/10	0.95	0.09	43,43,47,49	0
1	OCS	C	49	9/10	0.96	0.07	34,36,41,42	0
2	OCS	H	49	9/10	0.96	0.07	34,38,43,45	0
1	OCS	E	49	9/10	0.97	0.07	30,37,42,43	0
1	OCS	A	49	9/10	0.97	0.07	19,21,27,27	0
2	OCS	F	49	9/10	0.97	0.08	31,32,34,37	0
1	OCS	B	49	9/10	0.97	0.07	22,23,29,31	0
2	OCS	G	49	9/10	0.98	0.06	27,30,35,39	0
2	OCS	I	49	9/10	0.98	0.06	26,29,34,36	0
1	OCS	K	49	9/10	0.98	0.07	40,41,45,45	0
2	OCS	J	49	9/10	0.98	0.08	30,38,40,41	0
2	OCS	D	49	9/10	0.99	0.05	24,27,32,33	0

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, 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
3	UNL	D	301	5/-	0.87	0.17	31,36,52,53	0
3	UNL	J	301	5/-	0.90	0.13	44,52,54,54	0
3	UNL	G	301	5/-	0.91	0.21	43,52,60,63	0
3	UNL	K	301	5/-	0.92	0.16	42,45,50,58	0
3	UNL	E	301	5/-	0.93	0.17	46,50,53,54	0
3	UNL	H	301	5/-	0.93	0.15	55,55,59,59	0
3	UNL	F	301	5/-	0.93	0.12	44,47,49,50	0
3	UNL	I	301	5/-	0.94	0.12	33,41,46,51	0
3	UNL	B	301	5/-	0.94	0.14	31,41,43,46	0
3	UNL	A	301	5/-	0.95	0.18	44,51,53,53	0
3	UNL	L	301	5/-	0.95	0.09	44,46,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.