



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:10 AM UTC

PDB ID : 2ARH / pdb_00002arh
Title : Crystal Structure of a Protein of Unknown Function AQ1966 from Aquifex
aeolicus VF5
Authors : Qiu, Y.; Kim, Y.; Yang, X.; Collart, F.; Joachimiak, A.; Kossiakoff, A.; Mid-
west Center for Structural Genomics (MCSG)
Deposited on : 2005-08-19
Resolution : 2.46 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

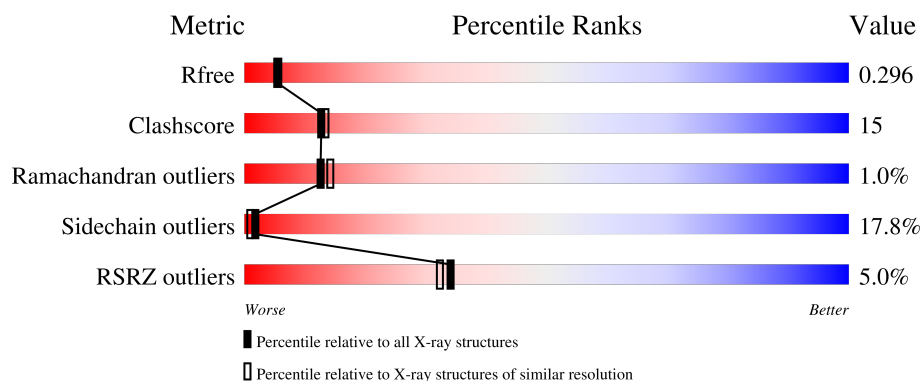
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	3% 61% 26% 11% .
1	B	203	2% 65% 21% 10% . .
1	C	203	8% 55% 29% 7% . 7%

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
4	SE	C	203	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5126 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 hypothetical protein aq_1966.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	Se	0	0	0
			1662	1082	274	303	1	2			
1	B	197	Total	C	N	O	S	Se	0	0	0
			1659	1081	275	300	1	2			
1	C	189	Total	C	N	O	S	Se	0	0	0
			1592	1041	264	286	1				

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	cloning artifact	UNP O67778
A	0	ALA	-	cloning artifact	UNP O67778
A	1	MSE	MET	modified residue	UNP O67778
A	138	PHE	TYR	engineered mutation	UNP O67778
A	144	MSE	MET	modified residue	UNP O67778
B	-1	ASP	-	cloning artifact	UNP O67778
B	0	ALA	-	cloning artifact	UNP O67778
B	1	MSE	MET	modified residue	UNP O67778
B	138	PHE	TYR	engineered mutation	UNP O67778
B	144	MSE	MET	modified residue	UNP O67778
C	-1	ASP	-	cloning artifact	UNP O67778
C	0	ALA	-	cloning artifact	UNP O67778
C	1	MSE	MET	modified residue	UNP O67778
C	138	PHE	TYR	engineered mutation	UNP O67778
C	144	MSE	MET	modified residue	UNP O67778

- 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		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SELENIUM ATOM (CCD ID: SE) (formula: Se).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Se	0	0
			2	2		

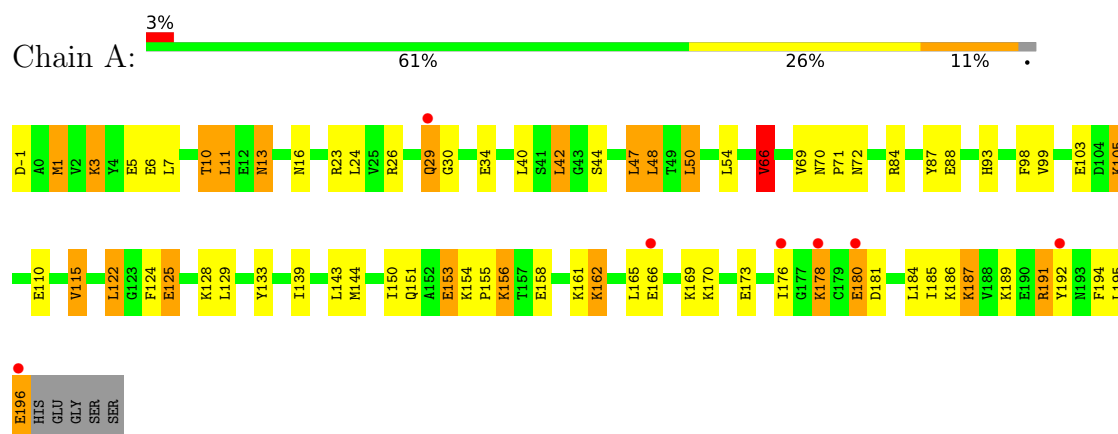
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	78	Total	O	0	0
			78	78		
5	B	76	Total	O	0	0
			76	76		
5	C	51	Total	O	0	0
			51	51		

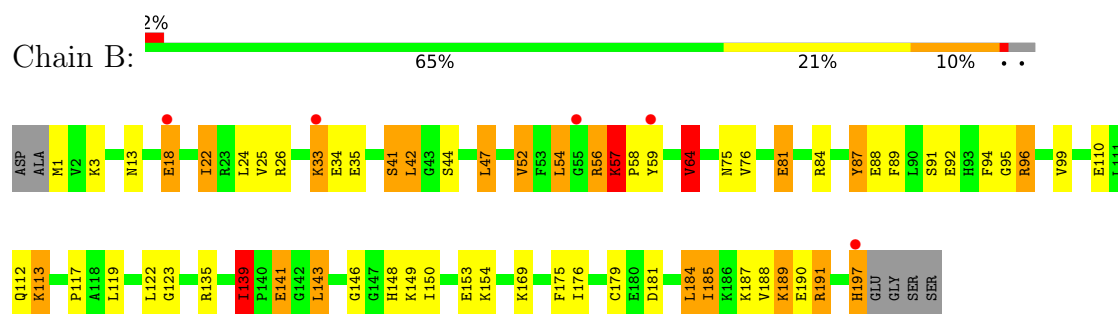
3 Residue-property plots [i](#)

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.

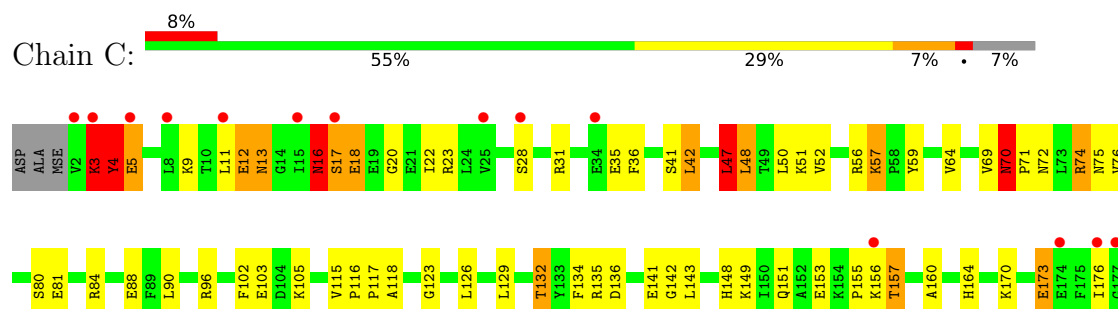
- Molecule 1: hypothetical protein aq_1966

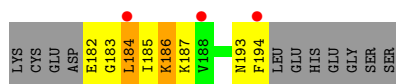


- Molecule 1: hypothetical protein aq_1966



- Molecule 1: hypothetical protein aq_1966





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.61Å 121.61Å 102.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.46 20.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.46) 99.5 (20.00-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.226 , 0.290 0.234 , 0.296	Depositor DCC
R_{free} test set	1458 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5126	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: CA, SE, 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	1.02	2/1701 (0.1%)	1.20	2/2276 (0.1%)
1	B	1.02	3/1700 (0.2%)	1.20	12/2276 (0.5%)
1	C	0.82	0/1631	1.14	8/2183 (0.4%)
All	All	0.96	5/5032 (0.1%)	1.18	22/6735 (0.3%)

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
1	C	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	ILE	CA-CB	7.91	1.64	1.54
1	A	66	VAL	CA-CB	6.01	1.61	1.54
1	B	188	VAL	CA-CB	5.55	1.61	1.54
1	B	76	VAL	CA-CB	5.26	1.61	1.54
1	A	1	MSE	SE-CE	5.05	2.10	1.95

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	LYS	CA-C-N	-11.73	106.76	119.19
1	C	57	LYS	C-N-CA	-11.73	106.76	119.19
1	B	141	GLU	N-CA-C	-9.85	96.61	110.50
1	A	115	VAL	N-CA-CB	7.64	117.86	109.99
1	C	4	TYR	N-CA-C	-7.51	100.42	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	VAL	CB-CA-C	-7.09	100.06	110.62
1	C	3	LYS	N-CA-C	6.79	120.02	107.60
1	B	57	LYS	CA-C-N	-6.54	111.86	119.32
1	B	57	LYS	C-N-CA	-6.54	111.86	119.32
1	C	57	LYS	N-CA-C	5.92	122.90	109.81
1	B	176	ILE	N-CA-C	-5.84	101.48	109.37
1	C	70	ASN	CA-C-N	5.72	125.43	119.82
1	C	70	ASN	C-N-CA	5.72	125.43	119.82
1	A	191	ARG	CB-CG-CD	5.45	123.83	111.30
1	B	57	LYS	N-CA-C	5.44	121.84	109.81
1	B	87	TYR	CA-C-N	5.15	127.14	120.44
1	B	87	TYR	C-N-CA	5.15	127.14	120.44
1	B	176	ILE	CA-C-N	-5.08	111.44	121.41
1	B	176	ILE	C-N-CA	-5.08	111.44	121.41
1	C	173	GLU	N-CA-C	5.04	116.78	111.28
1	B	141	GLU	CA-C-N	-5.02	111.58	121.41
1	B	141	GLU	C-N-CA	-5.02	111.58	121.41

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	12	GLU	Peptide
1	C	193	ASN	Peptide
1	C	3	LYS	Peptide
1	C	47	LEU	Peptide
1	C	56	ARG	Peptide

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	1662	0	1653	53	1
1	B	1659	0	1651	52	0
1	C	1592	0	1586	52	0
2	A	5	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	2	0	0	3	0
5	A	78	0	0	4	8
5	B	76	0	0	9	7
5	C	51	0	0	2	6
All	All	5126	0	4890	149	12

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 15.

All (149) 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:47:LEU:HD13	1:A:48:LEU:HD13	1.40	1.04
1:A:156:LYS:H	1:A:156:LYS:HZ2	1.06	1.01
1:B:197:HIS:NE2	5:B:245:HOH:O	1.97	0.95
1:A:158:GLU:OE2	1:A:162:LYS:HE3	1.66	0.94
1:B:56:ARG:HD3	5:B:223:HOH:O	1.70	0.91
1:A:23:ARG:NH1	5:A:252:HOH:O	2.02	0.91
1:A:133:TYR:HB2	1:A:153:GLU:HG2	1.54	0.88
1:B:75:ASN:OD1	5:B:225:HOH:O	1.92	0.88
1:C:4:TYR:O	1:C:5:GLU:HB2	1.75	0.84
1:C:4:TYR:CD1	4:C:203:SE:SE	2.81	0.84
1:B:33:LYS:HD3	1:C:74:ARG:NH2	1.93	0.83
1:B:141:GLU:O	5:B:212:HOH:O	1.97	0.82
1:B:146:GLY:O	1:B:149:LYS:HE2	1.80	0.82
1:B:33:LYS:HD3	1:C:74:ARG:HH21	1.46	0.80
1:C:70:ASN:HD22	1:C:72:ASN:H	1.30	0.79
1:C:132:THR:HG23	1:C:164:HIS:ND1	1.99	0.78
1:A:170:LYS:HE2	5:A:275:HOH:O	1.83	0.77
1:C:84:ARG:O	1:C:88:GLU:HB2	1.84	0.77
1:B:57:LYS:O	1:B:58:PRO:C	2.29	0.75
1:B:139:ILE:HD11	1:B:143:LEU:HD12	1.66	0.74
1:A:42:LEU:HB2	1:A:47:LEU:HG	1.70	0.72
1:B:139:ILE:CD1	1:B:143:LEU:HD12	2.19	0.72
1:C:4:TYR:O	1:C:5:GLU:CB	2.38	0.71
1:B:42:LEU:HB2	1:B:47:LEU:HG	1.70	0.71
1:C:132:THR:CG2	1:C:155:PRO:HD3	2.22	0.69
1:C:132:THR:HG22	1:C:155:PRO:HD3	1.75	0.67
1:A:178:LYS:O	1:A:178:LYS:HG2	1.95	0.67
1:C:16:ASN:HA	5:C:211:HOH:O	1.94	0.66
1:C:141:GLU:OE2	1:C:148:HIS:HD2	1.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:HD23	1:B:150:ILE:HD12	1.78	0.65
1:A:194:PHE:O	1:A:196:GLU:N	2.30	0.64
1:B:18:GLU:HB2	1:B:81:GLU:OE1	1.97	0.64
1:A:13:ASN:HD22	1:A:13:ASN:C	2.06	0.64
1:A:13:ASN:C	1:A:13:ASN:ND2	2.55	0.63
1:B:96:ARG:HD2	1:B:153:GLU:OE1	1.97	0.63
1:B:89:PHE:O	1:B:92:GLU:HG2	1.99	0.63
1:A:194:PHE:C	1:A:196:GLU:H	2.07	0.63
1:A:170:LYS:CE	5:A:275:HOH:O	2.45	0.62
1:A:169:LYS:HG3	1:A:192:TYR:OH	2.00	0.62
1:A:139:ILE:HG21	1:A:144:MSE:HE3	1.83	0.61
1:B:33:LYS:HE2	1:C:102:PHE:HE2	1.65	0.61
1:C:132:THR:CG2	1:C:164:HIS:ND1	2.64	0.60
1:B:1:MSE:N	5:B:260:HOH:O	2.34	0.60
1:A:70:ASN:C	1:A:70:ASN:HD22	2.10	0.60
1:A:29:GLN:NE2	1:A:30:GLY:O	2.35	0.59
1:A:34:GLU:HB3	1:A:54:LEU:HB2	1.85	0.59
1:C:17:SER:OG	1:C:20:GLY:O	2.21	0.59
1:C:4:TYR:CE1	4:C:203:SE:SE	3.06	0.59
1:A:40:LEU:HD11	1:A:50:LEU:HD22	1.86	0.58
1:A:176:ILE:CD1	1:A:185:ILE:HG23	2.33	0.58
1:C:70:ASN:ND2	1:C:72:ASN:H	1.99	0.58
1:C:157:THR:HG22	1:C:160:ALA:H	1.68	0.58
1:C:9:LYS:O	1:C:13:ASN:ND2	2.38	0.57
1:B:58:PRO:HD2	5:B:252:HOH:O	2.04	0.57
1:C:75:ASN:HD22	1:C:105:LYS:NZ	2.02	0.56
1:B:64:VAL:HG22	1:B:94:PHE:CG	2.42	0.55
1:B:141:GLU:OE2	1:B:148:HIS:HD2	1.89	0.55
1:C:4:TYR:CD1	1:C:4:TYR:C	2.85	0.55
1:B:139:ILE:HD11	1:B:143:LEU:CD1	2.38	0.54
1:C:4:TYR:C	1:C:4:TYR:HD1	2.16	0.54
1:B:33:LYS:HG2	1:C:103:GLU:OE2	2.08	0.54
1:A:178:LYS:O	1:A:178:LYS:CG	2.56	0.53
1:B:181:ASP:HB3	5:B:249:HOH:O	2.07	0.53
1:B:57:LYS:O	1:B:59:TYR:N	2.41	0.53
1:A:11:LEU:HB3	1:A:24:LEU:HB2	1.90	0.52
1:A:176:ILE:HD12	1:A:185:ILE:HG23	1.90	0.52
1:A:110:GLU:CD	1:A:191:ARG:HH22	2.18	0.52
1:B:22:ILE:HA	1:B:41:SER:O	2.09	0.52
1:B:179:CYS:SG	1:B:185:ILE:HG12	2.50	0.52
1:A:122:LEU:HD13	1:A:150:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LEU:HB2	1:C:47:LEU:HG	1.92	0.51
1:C:135:ARG:HB2	1:C:151:GLN:HB3	1.92	0.51
1:B:88:GLU:CD	5:B:209:HOH:O	2.52	0.51
1:A:156:LYS:HZ2	1:A:156:LYS:N	1.90	0.51
1:A:170:LYS:NZ	5:A:275:HOH:O	2.43	0.50
1:A:162:LYS:O	1:A:166:GLU:HG2	2.12	0.50
1:C:118:ALA:HB2	1:C:134:PHE:CD1	2.46	0.50
1:C:75:ASN:HD22	1:C:105:LYS:HZ3	1.58	0.50
1:A:66:VAL:HG13	1:A:99:VAL:HG22	1.93	0.49
1:B:99:VAL:HB	1:B:122:LEU:HD21	1.94	0.49
1:C:76:VAL:O	1:C:80:SER:HB3	2.13	0.49
1:B:33:LYS:HG3	1:B:33:LYS:O	2.12	0.49
1:C:18:GLU:O	1:C:18:GLU:HG3	2.12	0.48
1:C:48:LEU:HD12	1:C:69:VAL:HG22	1.96	0.48
1:B:117:PRO:O	1:B:123:GLY:HA3	2.14	0.48
1:B:87:TYR:O	1:B:91:SER:HB2	2.14	0.48
1:C:22:ILE:HA	1:C:41:SER:O	2.13	0.48
1:C:71:PRO:O	1:C:74:ARG:HG3	2.14	0.48
1:A:70:ASN:HD22	1:A:71:PRO:N	2.12	0.47
1:C:36:PHE:CZ	4:C:202:SE:SE	3.17	0.47
1:A:169:LYS:CG	1:A:192:TYR:OH	2.62	0.47
1:B:110:GLU:OE2	1:B:191:ARG:NH2	2.46	0.47
1:B:33:LYS:O	1:B:34:GLU:HB2	2.15	0.46
1:A:122:LEU:O	1:A:125:GLU:HB3	2.16	0.46
1:C:28:SER:O	1:C:36:PHE:HD2	1.99	0.46
1:A:87:TYR:HD2	1:A:125:GLU:HG2	1.81	0.46
1:B:185:ILE:O	1:B:189:LYS:HG2	2.16	0.46
1:C:117:PRO:O	1:C:123:GLY:HA3	2.16	0.46
1:C:28:SER:O	1:C:36:PHE:CD2	2.70	0.45
1:A:155:PRO:HG3	1:A:161:LYS:HB2	1.97	0.45
1:A:133:TYR:OH	1:A:156:LYS:NZ	2.38	0.45
1:C:35:GLU:OE2	1:C:51:LYS:HD3	2.15	0.45
1:A:185:ILE:O	1:A:189:LYS:HB2	2.17	0.45
1:B:112:GLN:NE2	5:B:217:HOH:O	2.49	0.45
1:B:175:PHE:HZ	1:B:184:LEU:HD13	1.81	0.45
1:B:34:GLU:HB3	1:B:54:LEU:HB2	1.98	0.45
1:C:183:GLY:O	1:C:186:LYS:HD3	2.17	0.45
1:A:1:MSE:HE1	1:A:5:GLU:OE1	2.17	0.44
1:B:33:LYS:CD	1:C:74:ARG:HH21	2.23	0.44
1:B:113:LYS:HZ3	1:B:113:LYS:HG3	1.55	0.44
1:A:3:LYS:O	1:A:7:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:PRO:HG3	1:C:136:ASP:HB2	1.99	0.44
1:A:3:LYS:HD2	1:A:93:HIS:HB3	2.01	0.43
1:B:149:LYS:HE3	1:C:142:GLY:O	2.18	0.43
1:A:180:GLU:O	1:A:181:ASP:HB3	2.18	0.43
1:B:95:GLY:HA2	1:B:154:LYS:HG3	1.99	0.43
1:A:6:GLU:O	1:A:10:THR:HG23	2.19	0.43
1:A:7:LEU:O	1:A:11:LEU:HB2	2.18	0.43
1:B:22:ILE:HG22	1:B:41:SER:O	2.19	0.43
1:C:5:GLU:O	1:C:9:LYS:HB2	2.18	0.43
1:A:162:LYS:HA	1:A:162:LYS:HE2	2.01	0.43
1:B:187:LYS:O	1:B:191:ARG:HG3	2.19	0.43
1:B:33:LYS:HE2	1:C:102:PHE:CE2	2.51	0.42
1:C:135:ARG:HE	1:C:135:ARG:HB3	1.62	0.42
1:A:162:LYS:HE2	1:A:162:LYS:CA	2.48	0.42
1:A:187:LYS:O	1:A:191:ARG:HG3	2.20	0.42
1:A:124:PHE:CE2	1:A:128:LYS:HD2	2.55	0.42
1:A:194:PHE:C	1:A:196:GLU:N	2.71	0.42
1:A:180:GLU:O	1:A:181:ASP:CB	2.66	0.42
1:B:33:LYS:O	1:B:33:LYS:CG	2.67	0.42
1:C:70:ASN:HA	1:C:71:PRO:HD3	1.91	0.42
1:C:117:PRO:HB2	1:C:134:PHE:HB3	2.02	0.42
1:B:84:ARG:O	1:B:88:GLU:HB2	2.20	0.42
1:A:98:PHE:CE2	1:A:151:GLN:HG3	2.54	0.42
1:B:3:LYS:HD2	1:B:54:LEU:HD12	2.02	0.42
1:A:84:ARG:O	1:A:88:GLU:HB2	2.20	0.42
1:B:25:VAL:HG23	1:B:41:SER:HB2	2.00	0.42
1:B:22:ILE:CG2	1:B:47:LEU:HD12	2.50	0.41
1:C:185:ILE:HD11	5:C:232:HOH:O	2.20	0.41
1:A:105:LYS:HB2	1:C:59:TYR:CE2	2.56	0.41
1:B:35:GLU:HA	1:B:52:VAL:O	2.20	0.41
1:A:70:ASN:C	1:A:70:ASN:ND2	2.78	0.41
1:C:64:VAL:HG21	1:C:90:LEU:HD22	2.03	0.41
1:C:70:ASN:HD21	1:C:72:ASN:HD22	1.67	0.41
1:B:22:ILE:HD13	1:B:22:ILE:HG21	1.74	0.41
1:B:64:VAL:HG22	1:B:94:PHE:CD1	2.55	0.41
1:A:69:VAL:O	1:A:103:GLU:OE2	2.40	0.40
1:C:115:VAL:HA	1:C:116:PRO:HD3	1.94	0.40
1:C:184:LEU:O	1:C:187:LYS:HB3	2.21	0.40

All (12) 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)
5:A:205:HOH:O	5:B:232:HOH:O[4_556]	1.26	0.94
5:A:204:HOH:O	5:B:226:HOH:O[4_556]	1.59	0.61
5:A:242:HOH:O	5:B:235:HOH:O[6_656]	1.65	0.55
5:A:239:HOH:O	5:B:221:HOH:O[6_656]	1.74	0.46
5:B:205:HOH:O	5:B:230:HOH:O[4_556]	1.75	0.45
5:A:237:HOH:O	5:C:220:HOH:O[2_655]	1.90	0.30
5:A:277:HOH:O	5:C:235:HOH:O[2_655]	2.01	0.19
1:A:186:LYS:NZ	5:C:249:HOH:O[3_664]	2.04	0.16
5:B:270:HOH:O	5:C:248:HOH:O[2_655]	2.14	0.06
5:A:269:HOH:O	5:C:251:HOH:O[2_655]	2.15	0.05
5:B:263:HOH:O	5:B:264:HOH:O[4_556]	2.15	0.05
5:A:245:HOH:O	5:C:220:HOH:O[2_655]	2.19	0.01

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	196/203 (97%)	188 (96%)	7 (4%)	1 (0%)	24	32
1	B	195/203 (96%)	183 (94%)	11 (6%)	1 (0%)	24	32
1	C	185/203 (91%)	169 (91%)	12 (6%)	4 (2%)	5	3
All	All	576/609 (95%)	540 (94%)	30 (5%)	6 (1%)	12	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	LEU
1	B	57	LYS
1	C	5	GLU
1	C	16	ASN
1	C	17	SER
1	C	48	LEU

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	177/179 (99%)	145 (82%)	32 (18%)	2	1
1	B	177/179 (99%)	149 (84%)	28 (16%)	2	1
1	C	169/179 (94%)	136 (80%)	33 (20%)	1	0
All	All	523/537 (97%)	430 (82%)	93 (18%)	2	1

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASP
1	A	3	LYS
1	A	10	THR
1	A	11	LEU
1	A	13	ASN
1	A	16	ASN
1	A	26	ARG
1	A	29	GLN
1	A	42	LEU
1	A	44	SER
1	A	47	LEU
1	A	48	LEU
1	A	50	LEU
1	A	66	VAL
1	A	72	ASN
1	A	105	LYS
1	A	115	VAL
1	A	122	LEU
1	A	125	GLU
1	A	129	LEU
1	A	143	LEU
1	A	153	GLU
1	A	154	LYS
1	A	156	LYS
1	A	162	LYS
1	A	165	LEU

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Mol	Chain	Res	Type
1	A	173	GLU
1	A	178	LYS
1	A	180	GLU
1	A	184	LEU
1	A	187	LYS
1	A	196	GLU
1	B	13	ASN
1	B	18	GLU
1	B	22	ILE
1	B	24	LEU
1	B	26	ARG
1	B	33	LYS
1	B	41	SER
1	B	42	LEU
1	B	44	SER
1	B	47	LEU
1	B	52	VAL
1	B	54	LEU
1	B	56	ARG
1	B	64	VAL
1	B	81	GLU
1	B	96	ARG
1	B	113	LYS
1	B	119	LEU
1	B	135	ARG
1	B	139	ILE
1	B	143	LEU
1	B	169	LYS
1	B	184	LEU
1	B	185	ILE
1	B	189	LYS
1	B	190	GLU
1	B	191	ARG
1	B	197	HIS
1	C	3	LYS
1	C	4	TYR
1	C	11	LEU
1	C	12	GLU
1	C	13	ASN
1	C	16	ASN
1	C	18	GLU
1	C	23	ARG

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Mol	Chain	Res	Type
1	C	31	ARG
1	C	42	LEU
1	C	47	LEU
1	C	50	LEU
1	C	52	VAL
1	C	57	LYS
1	C	70	ASN
1	C	74	ARG
1	C	81	GLU
1	C	96	ARG
1	C	126	LEU
1	C	129	LEU
1	C	132	THR
1	C	143	LEU
1	C	149	LYS
1	C	153	GLU
1	C	156	LYS
1	C	157	THR
1	C	170	LYS
1	C	173	GLU
1	C	176	ILE
1	C	182	GLU
1	C	184	LEU
1	C	186	LYS
1	C	194	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	16	ASN
1	A	29	GLN
1	A	70	ASN
1	A	75	ASN
1	A	164	HIS
1	B	13	ASN
1	B	72	ASN
1	B	75	ASN
1	B	112	GLN
1	B	148	HIS
1	C	37	ASN
1	C	61	GLN

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Mol	Chain	Res	Type
1	C	70	ASN
1	C	75	ASN
1	C	148	HIS
1	C	167	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	A	202	-	4,4,4	0.24	0	6,6,6	0.45	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.

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	196/203 (96%)	0.65	7 (3%) 46 46	28, 39, 53, 61	0
1	B	195/203 (96%)	0.13	5 (2%) 57 58	29, 42, 58, 63	0
1	C	188/203 (92%)	0.85	17 (9%) 15 13	35, 55, 78, 82	0
All	All	579/609 (95%)	0.54	29 (5%) 34 32	28, 44, 71, 82	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	VAL	5.6
1	C	184	LEU	3.7
1	C	17	SER	3.6
1	C	11	LEU	3.3
1	A	196	GLU	3.3
1	C	177	GLY	3.1
1	A	176	ILE	2.9
1	A	166	GLU	2.8
1	C	34	GLU	2.8
1	B	33	LYS	2.7
1	A	192	TYR	2.7
1	C	8	LEU	2.7
1	C	25	VAL	2.6
1	A	180	GLU	2.6
1	B	197	HIS	2.6
1	C	188	VAL	2.4
1	C	194	PHE	2.4
1	C	5	GLU	2.4
1	A	29	GLN	2.2
1	C	176	ILE	2.2
1	C	3	LYS	2.2
1	C	174	GLU	2.2
1	C	15	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	28	SER	2.1
1	B	55	GLY	2.1
1	A	178	LYS	2.0
1	B	18	GLU	2.0
1	C	156	LYS	2.0
1	B	59	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
4	SE	C	202	1/1	0.86	0.42	157,157,157,157	1
4	SE	C	203	1/1	0.94	0.09	78,78,78,78	1
3	CA	A	203	1/1	0.97	0.15	55,55,55,55	0
2	SO4	A	202	5/5	0.98	0.07	37,38,39,41	5

6.5 Other polymers [i](#)

There are no such residues in this entry.