Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 09:25 PM JST

PDB ID	:	7W7R
Title	:	High resolution structure of a fish aquaporin reveals a novel extracellular fold.
Authors	:	Zeng, J.; Schmitz, F.; Isaksson, S.; Glas, J.; Arbab, O.; Andersson, M.; Sundell, K.; Eriksson, L.; Swaminathan, K.; Tornroth-Horsefield, S.; Hedfalk, K.
Deposited on	:	2021-12-06
Resolution	:	3.46 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:

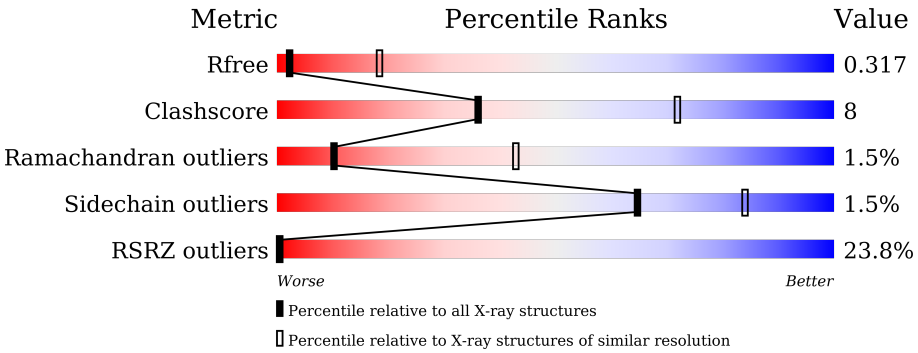
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.46 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}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 <=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	244	22% 73% 16% 10%
1	B	244	17% 73% 16% • 11%
1	C	244	23% 73% 17% • 8%
1	D	244	25% 74% 16% • 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6438 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 Aquaporin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1595	1033	266	286	10			
1	B	218	Total	C	N	O	S	0	0	0
			1581	1025	264	282	10			
1	C	224	Total	C	N	O	S	0	0	0
			1629	1054	273	292	10			
1	D	225	Total	C	N	O	S	0	0	0
			1633	1056	275	292	10			

There are 8 discrepancies between the modelled and reference sequences:

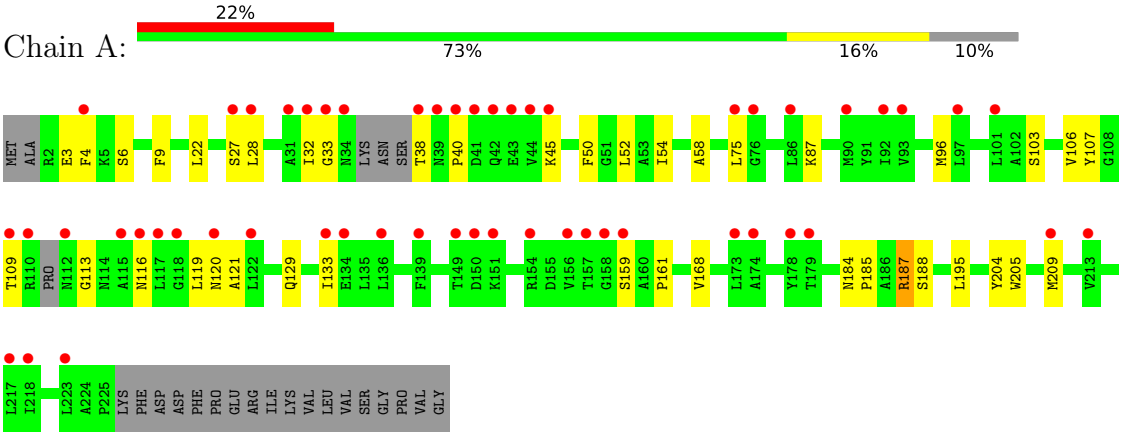
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP M1K561
A	1	ALA	-	expression tag	UNP M1K561
B	0	MET	-	initiating methionine	UNP M1K561
B	1	ALA	-	expression tag	UNP M1K561
C	0	MET	-	initiating methionine	UNP M1K561
C	1	ALA	-	expression tag	UNP M1K561
D	0	MET	-	initiating methionine	UNP M1K561
D	1	ALA	-	expression tag	UNP M1K561

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.

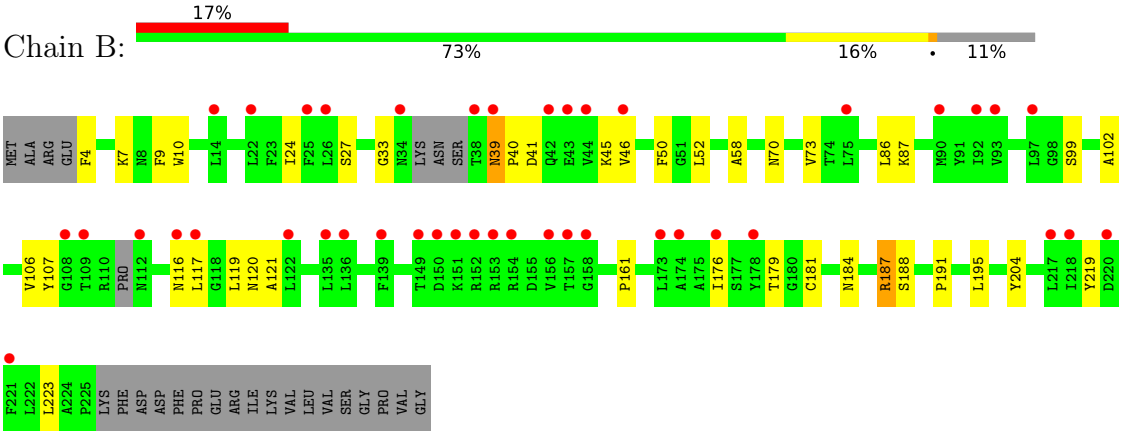
• Molecule 1: Aquaporin 1

Chain A:



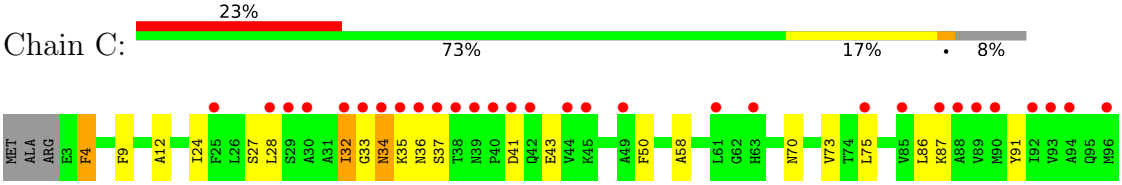
• Molecule 1: Aquaporin 1

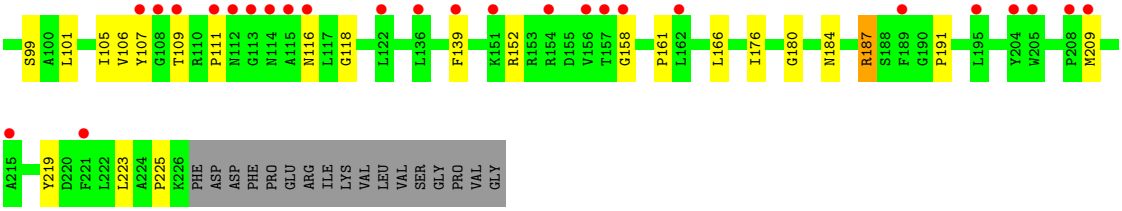
Chain B:



• Molecule 1: Aquaporin 1

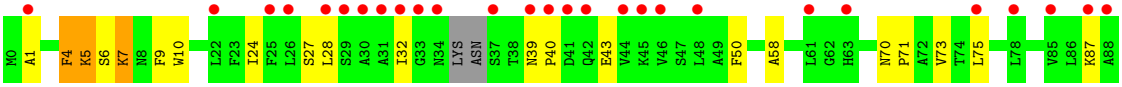
Chain C:

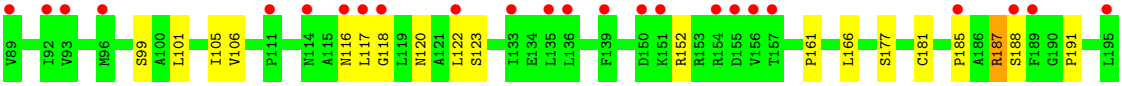


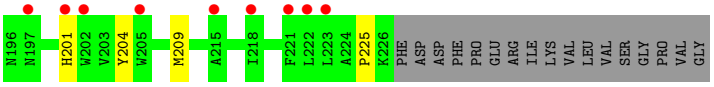


• Molecule 1: Aquaporin 1

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	113.67Å 178.10Å 177.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.36 – 3.46 95.82 – 3.46	Depositor EDS
% Data completeness (in resolution range)	88.4 (84.36-3.46) 98.5 (95.82-3.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.271 , 0.299 0.290 , 0.317	Depositor DCC
R_{free} test set	1182 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	87.6	Xtriage
Anisotropy	1.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 69.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	6438	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.15 % 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 1.3773e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.28	0/1624	0.45	0/2211
1	B	0.28	0/1610	0.45	0/2192
1	C	0.28	0/1661	0.47	0/2263
1	D	0.28	0/1664	0.46	0/2266
All	All	0.28	0/6559	0.46	0/8932

There are no bond length outliers.

There are no bond angle outliers.

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	1595	0	1633	23	0
1	B	1581	0	1625	27	0
1	C	1629	0	1677	28	0
1	D	1633	0	1680	34	0
All	All	6438	0	6615	105	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 8.

All (105) 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:188:SER:O	1:D:201:HIS:CE1	2.17	0.98
1:D:188:SER:O	1:D:201:HIS:HE1	1.48	0.95
1:B:45:LYS:NZ	1:D:43:GLU:OE1	2.15	0.74
1:B:121:ALA:O	1:B:204:TYR:OH	2.09	0.71
1:D:187:ARG:HH11	1:D:187:ARG:HG2	1.56	0.68
1:D:188:SER:C	1:D:201:HIS:HE1	1.99	0.67
1:B:46:VAL:HG21	1:B:117:LEU:HD22	1.77	0.65
1:B:9:PHE:HE1	1:B:87:LYS:HA	1.62	0.64
1:C:152:ARG:NH1	1:C:225:PRO:O	2.30	0.63
1:D:7:LYS:H	1:D:7:LYS:HD2	1.64	0.62
1:C:28:LEU:HB3	1:C:106:VAL:HG11	1.81	0.62
1:B:120:ASN:ND2	1:B:188:SER:OG	2.33	0.62
1:D:28:LEU:HD11	1:D:191:PRO:HG3	1.83	0.60
1:A:45:LYS:NZ	1:C:43:GLU:OE1	2.29	0.59
1:D:187:ARG:HG2	1:D:187:ARG:NH1	2.18	0.59
1:A:58:ALA:HB3	1:A:161:PRO:HB3	1.86	0.58
1:B:102:ALA:O	1:B:106:VAL:HG23	2.04	0.58
1:A:120:ASN:HB3	1:A:204:TYR:CZ	2.39	0.57
1:B:58:ALA:HB3	1:B:161:PRO:HB3	1.85	0.57
1:C:34:ASN:O	1:C:36:ASN:N	2.39	0.56
1:A:120:ASN:ND2	1:A:188:SER:OG	2.39	0.56
1:D:1:ALA:HB3	1:D:87:LYS:HD2	1.87	0.56
1:D:120:ASN:HB3	1:D:204:TYR:CZ	2.41	0.55
1:D:123:SER:OG	1:D:177:SER:O	2.24	0.55
1:C:219:TYR:HA	1:C:223:LEU:HB2	1.90	0.53
1:A:27:SER:HB3	1:A:50:PHE:CZ	2.43	0.53
1:A:184:ASN:HB3	1:A:187:ARG:HB3	1.90	0.53
1:C:4:PHE:HE1	1:C:86:LEU:HD11	1.74	0.53
1:D:27:SER:HB3	1:D:50:PHE:CZ	2.44	0.53
1:C:9:PHE:HE1	1:C:87:LYS:HA	1.73	0.52
1:B:4:PHE:O	1:B:10:TRP:NE1	2.41	0.52
1:A:119:LEU:HD22	1:A:195:LEU:HD12	1.91	0.52
1:B:27:SER:HB3	1:B:50:PHE:CE1	2.44	0.52
1:D:58:ALA:HB3	1:D:161:PRO:HB3	1.92	0.52
1:B:4:PHE:HD1	1:B:86:LEU:HD21	1.74	0.51
1:B:117:LEU:HD21	1:B:176:ILE:HD11	1.92	0.51
1:A:121:ALA:O	1:A:204:TYR:OH	2.28	0.51
1:D:39:ASN:N	1:D:40:PRO:HD2	2.24	0.51
1:B:41:ASP:N	1:B:41:ASP:OD1	2.43	0.50
1:B:119:LEU:HD22	1:B:195:LEU:HD12	1.94	0.50
1:C:41:ASP:OD1	1:C:41:ASP:N	2.45	0.50
1:D:32:ILE:HG12	1:D:116:ASN:HB2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:TYR:CE2	1:B:195:LEU:HG	2.47	0.49
1:C:75:LEU:HD12	1:C:209:MET:SD	2.53	0.49
1:B:184:ASN:HB3	1:B:187:ARG:HB3	1.94	0.49
1:C:184:ASN:HB3	1:C:187:ARG:HB3	1.94	0.48
1:D:118:GLY:HA2	1:D:187:ARG:HH22	1.78	0.48
1:B:187:ARG:C	1:B:187:ARG:HD3	2.34	0.48
1:A:9:PHE:HE1	1:A:87:LYS:HA	1.79	0.47
1:C:24:ILE:HG13	1:C:99:SER:HA	1.96	0.47
1:D:4:PHE:C	1:D:6:SER:H	2.17	0.47
1:D:71:PRO:HD2	1:D:185:PRO:HD2	1.96	0.47
1:A:54:ILE:HG13	1:A:168:VAL:HG21	1.97	0.47
1:C:70:ASN:HB3	1:C:73:VAL:HB	1.97	0.47
1:B:52:LEU:HD22	1:D:166:LEU:HB3	1.96	0.46
1:C:28:LEU:HD11	1:C:191:PRO:HG3	1.97	0.45
1:B:107:TYR:OH	1:B:191:PRO:HB3	2.17	0.45
1:A:159:SER:HB2	1:C:158:GLY:HA3	1.99	0.45
1:D:24:ILE:HG13	1:D:99:SER:HA	1.98	0.45
1:D:101:LEU:O	1:D:105:ILE:HG13	2.16	0.45
1:A:52:LEU:HD22	1:C:166:LEU:HB3	1.99	0.45
1:D:7:LYS:H	1:D:7:LYS:CD	2.26	0.45
1:D:27:SER:HB3	1:D:50:PHE:CE1	2.52	0.45
1:A:32:ILE:HD11	1:A:107:TYR:HE1	1.82	0.44
1:C:27:SER:HB3	1:C:50:PHE:CZ	2.51	0.44
1:C:107:TYR:OH	1:C:116:ASN:OD1	2.25	0.44
1:D:5:LYS:O	1:D:5:LYS:HG2	2.17	0.44
1:C:34:ASN:OD1	1:C:34:ASN:N	2.51	0.44
1:C:101:LEU:O	1:C:105:ILE:HG13	2.17	0.44
1:D:75:LEU:HD12	1:D:209:MET:SD	2.58	0.44
1:D:116:ASN:O	1:D:118:GLY:N	2.51	0.44
1:B:39:ASN:N	1:B:40:PRO:CD	2.81	0.44
1:D:9:PHE:HE1	1:D:87:LYS:HA	1.83	0.44
1:A:129:GLN:O	1:A:133:ILE:HG12	2.18	0.44
1:B:70:ASN:HB3	1:B:73:VAL:HB	2.00	0.43
1:A:106:VAL:O	1:A:109:THR:HG22	2.18	0.43
1:B:219:TYR:HA	1:B:223:LEU:HB2	2.01	0.43
1:A:28:LEU:HD12	1:A:106:VAL:HG21	2.00	0.43
1:A:96:MET:HE3	1:A:96:MET:HB3	1.87	0.43
1:A:185:PRO:HB3	1:A:205:TRP:CD2	2.54	0.43
1:A:75:LEU:HD12	1:A:209:MET:SD	2.59	0.43
1:B:24:ILE:HG13	1:B:99:SER:HA	2.00	0.43
1:D:70:ASN:HB3	1:D:73:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:SER:HA	1:A:106:VAL:HG22	2.01	0.42
1:D:28:LEU:HB3	1:D:106:VAL:HG11	2.01	0.42
1:B:7:LYS:HD3	1:B:7:LYS:HA	1.78	0.42
1:B:120:ASN:HD22	1:B:188:SER:CB	2.32	0.42
1:C:105:ILE:O	1:C:109:THR:HG23	2.20	0.42
1:D:4:PHE:CE2	1:D:10:TRP:HZ2	2.38	0.42
1:B:120:ASN:HB3	1:B:204:TYR:CZ	2.55	0.42
1:C:28:LEU:HB2	1:C:106:VAL:HG21	2.01	0.42
1:B:179:THR:O	1:B:204:TYR:OH	2.28	0.41
1:D:32:ILE:HG22	1:D:32:ILE:O	2.19	0.41
1:D:152:ARG:NH1	1:D:225:PRO:O	2.43	0.41
1:C:12:ALA:HB1	1:C:91:TYR:OH	2.20	0.41
1:C:116:ASN:C	1:C:118:GLY:H	2.24	0.41
1:C:4:PHE:HD1	1:C:86:LEU:HD21	1.84	0.41
1:C:58:ALA:HB3	1:C:161:PRO:HB3	2.03	0.41
1:C:176:ILE:HA	1:C:180:GLY:C	2.41	0.41
1:B:33:GLY:HA3	1:D:177:SER:OG	2.20	0.41
1:D:122:LEU:H	1:D:122:LEU:HD23	1.85	0.41
1:A:3:GLU:O	1:A:3:GLU:HG2	2.21	0.41
1:A:38:THR:OG1	1:A:40:PRO:HD2	2.21	0.41
1:C:32:ILE:HG22	1:C:33:GLY:N	2.35	0.40
1:A:22:LEU:HD11	1:C:139:PHE:CE1	2.57	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	214/244 (88%)	193 (90%)	17 (8%)	4 (2%)	8 38
1	B	212/244 (87%)	197 (93%)	12 (6%)	3 (1%)	11 44
1	C	222/244 (91%)	197 (89%)	21 (10%)	4 (2%)	8 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	221/244 (91%)	199 (90%)	20 (9%)	2 (1%)	17 54
All	All	869/976 (89%)	786 (90%)	70 (8%)	13 (2%)	10 43

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	116	ASN
1	C	35	LYS
1	D	117	LEU
1	A	113	GLY
1	C	32	ILE
1	A	6	SER
1	A	116	ASN
1	C	37	SER
1	C	111	PRO
1	B	39	ASN
1	B	181	CYS
1	D	181	CYS
1	A	33	GLY

5.3.2 Protein sidechains (i)

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	165/189 (87%)	163 (99%)	2 (1%)	71 87
1	B	164/189 (87%)	163 (99%)	1 (1%)	86 95
1	C	170/189 (90%)	167 (98%)	3 (2%)	59 81
1	D	169/189 (89%)	165 (98%)	4 (2%)	49 76
All	All	668/756 (88%)	658 (98%)	10 (2%)	65 84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE

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Mol	Chain	Res	Type
1	A	187	ARG
1	B	187	ARG
1	C	4	PHE
1	C	34	ASN
1	C	187	ARG
1	D	4	PHE
1	D	5	LYS
1	D	7	LYS
1	D	187	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	B	120	ASN
1	D	201	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	220/244 (90%)	1.37	53 (24%)	0	0	71, 110, 178, 243	0
1	B	218/244 (89%)	1.14	42 (19%)	1	1	73, 112, 171, 225	0
1	C	224/244 (91%)	1.54	56 (25%)	0	0	76, 113, 185, 252	0
1	D	225/244 (92%)	1.38	60 (26%)	0	0	69, 113, 171, 204	0
All	All	887/976 (90%)	1.36	211 (23%)	0	0	69, 113, 177, 252	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	34	ASN	23.4
1	A	34	ASN	21.1
1	D	34	ASN	19.3
1	C	35	LYS	16.2
1	B	34	ASN	13.0
1	C	36	ASN	12.8
1	C	41	ASP	11.3
1	C	40	PRO	9.0
1	C	111	PRO	7.7
1	A	42	GLN	7.6
1	D	37	SER	7.5
1	A	158	GLY	6.7
1	A	150	ASP	6.6
1	C	157	THR	6.0
1	B	117	LEU	5.9
1	A	178	TYR	5.9
1	B	150	ASP	5.8
1	D	154	ARG	5.7
1	A	39	ASN	5.5
1	C	112	ASN	5.5
1	B	112	ASN	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	114	ASN	5.4
1	D	117	LEU	5.4
1	C	33	GLY	5.4
1	B	42	GLN	5.3
1	D	32	ILE	5.2
1	C	109	THR	5.2
1	C	42	GLN	5.0
1	A	40	PRO	5.0
1	D	33	GLY	4.9
1	A	156	VAL	4.9
1	C	38	THR	4.8
1	D	41	ASP	4.7
1	C	39	ASN	4.6
1	A	112	ASN	4.5
1	B	136	LEU	4.5
1	A	41	ASP	4.5
1	D	118	GLY	4.4
1	A	116	ASN	4.4
1	C	37	SER	4.3
1	C	115	ALA	4.3
1	C	45	LYS	4.3
1	A	27	SER	4.3
1	B	43	GLU	4.2
1	C	154	ARG	4.2
1	C	89	VAL	4.2
1	A	4	PHE	4.2
1	A	31	ALA	4.0
1	A	136	LEU	4.0
1	A	149	THR	4.0
1	B	178	TYR	3.9
1	D	29	SER	3.9
1	D	111	PRO	3.8
1	C	116	ASN	3.8
1	A	117	LEU	3.8
1	D	89	VAL	3.8
1	D	136	LEU	3.8
1	A	38	THR	3.7
1	A	90	MET	3.7
1	B	158	GLY	3.7
1	A	97	LEU	3.7
1	D	31	ALA	3.7
1	A	109	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	92	ILE	3.6
1	D	45	LYS	3.6
1	D	205	TRP	3.6
1	C	32	ILE	3.6
1	B	151	LYS	3.6
1	B	44	VAL	3.6
1	A	93	VAL	3.6
1	C	158	GLY	3.6
1	D	222	LEU	3.6
1	D	87	LYS	3.5
1	A	157	THR	3.5
1	D	96	MET	3.5
1	A	120	ASN	3.4
1	B	109	THR	3.4
1	A	174	ALA	3.4
1	C	93	VAL	3.4
1	D	157	THR	3.4
1	D	42	GLN	3.4
1	A	33	GLY	3.4
1	D	151	LYS	3.3
1	C	85	VAL	3.3
1	C	204	TYR	3.3
1	A	173	LEU	3.3
1	A	115	ALA	3.3
1	A	75	LEU	3.3
1	C	205	TRP	3.3
1	A	217	LEU	3.2
1	B	156	VAL	3.1
1	A	122	LEU	3.1
1	D	201	HIS	3.1
1	D	85	VAL	3.1
1	B	90	MET	3.1
1	B	97	LEU	3.0
1	D	139	PHE	3.0
1	B	221	PHE	3.0
1	B	173	LEU	3.0
1	D	22	LEU	3.0
1	B	157	THR	3.0
1	A	154	ARG	3.0
1	A	151	LYS	2.9
1	B	153	ARG	2.9
1	B	25	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	223	LEU	2.9
1	D	25	PHE	2.9
1	B	174	ALA	2.9
1	C	215	ALA	2.9
1	D	39	ASN	2.9
1	B	93	VAL	2.8
1	D	40	PRO	2.8
1	D	63	HIS	2.8
1	B	22	LEU	2.8
1	D	188	SER	2.8
1	C	28	LEU	2.8
1	C	44	VAL	2.8
1	D	30	ALA	2.7
1	D	215	ALA	2.7
1	B	154	ARG	2.7
1	A	28	LEU	2.7
1	B	217	LEU	2.7
1	D	44	VAL	2.6
1	D	93	VAL	2.6
1	B	116	ASN	2.6
1	C	189	PHE	2.6
1	D	195	LEU	2.6
1	D	156	VAL	2.6
1	C	92	ILE	2.5
1	C	209	MET	2.5
1	C	75	LEU	2.5
1	D	61	LEU	2.5
1	B	220	ASP	2.5
1	C	29	SER	2.5
1	A	218	ILE	2.5
1	A	209	MET	2.5
1	A	45	LYS	2.5
1	C	208	PRO	2.5
1	B	149	THR	2.5
1	C	30	ALA	2.5
1	A	43	GLU	2.4
1	D	114	ASN	2.4
1	C	87	LYS	2.4
1	D	197	ASN	2.4
1	A	86	LEU	2.4
1	D	189	PHE	2.4
1	D	1	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	152	ARG	2.4
1	D	75	LEU	2.4
1	C	88	ALA	2.4
1	B	46	VAL	2.4
1	C	122	LEU	2.4
1	C	162	LEU	2.4
1	A	110	ARG	2.3
1	A	118	GLY	2.3
1	C	63	HIS	2.3
1	C	113	GLY	2.3
1	D	202	TRP	2.3
1	C	49	ALA	2.3
1	D	46	VAL	2.3
1	D	48	LEU	2.3
1	B	135	LEU	2.3
1	C	90	MET	2.3
1	B	176	ILE	2.3
1	D	78	LEU	2.3
1	C	221	PHE	2.3
1	A	32	ILE	2.3
1	D	28	LEU	2.3
1	C	61	LEU	2.2
1	B	38	THR	2.2
1	D	221	PHE	2.2
1	C	108	GLY	2.2
1	D	122	LEU	2.2
1	A	133	ILE	2.2
1	C	139	PHE	2.2
1	D	185	PRO	2.2
1	A	139	PHE	2.2
1	B	26	LEU	2.2
1	A	213	VAL	2.2
1	C	107	TYR	2.2
1	A	92	ILE	2.2
1	A	134	GLU	2.2
1	A	223	LEU	2.2
1	A	76	GLY	2.2
1	A	159	SER	2.2
1	A	44	VAL	2.1
1	C	156	VAL	2.1
1	D	133	ILE	2.1
1	C	195	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	151	LYS	2.1
1	D	135	LEU	2.1
1	C	25	PHE	2.1
1	D	88	ALA	2.1
1	D	218	ILE	2.1
1	A	101	LEU	2.1
1	B	139	PHE	2.1
1	D	155	ASP	2.1
1	D	26	LEU	2.1
1	A	179	THR	2.1
1	B	92	ILE	2.1
1	B	14	LEU	2.1
1	B	122	LEU	2.1
1	D	150	ASP	2.1
1	B	75	LEU	2.1
1	C	96	MET	2.1
1	B	218	ILE	2.0
1	C	136	LEU	2.0
1	C	94	ALA	2.0
1	B	39	ASN	2.0
1	B	108	GLY	2.0
1	D	116	ASN	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.