wwPDB X-ray Structure Validation Summary Report (i)

Oct 21, 2024 – 07:56 AM EDT

PDB ID	:	2B5F
Title	:	Crystal structure of the spinach aquaporin SoPIP2;1 in an open conformation to 3.9 resolution
Authors	:	Tornroth-Horsefield, S.; Wang, Y.; Hedfalk, K.; Johanson, U.; Karlsson, M.; Tajkhorshid, E.; Neutze, R.; Kjellbom, P.
Deposited on	:	2005-09-28
Resolution	:	3.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

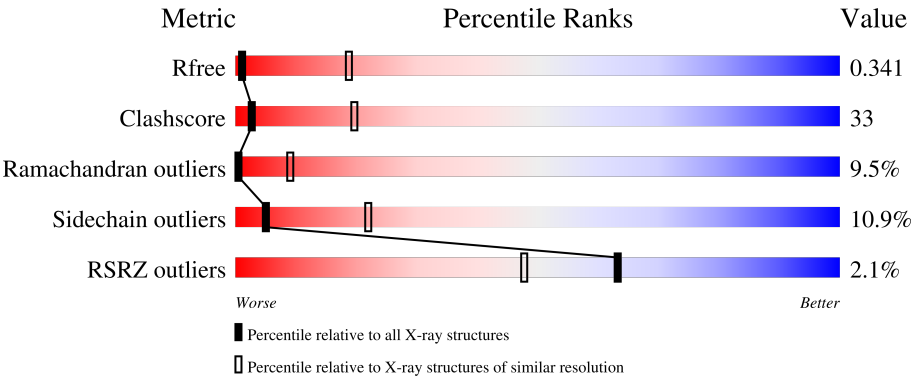
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1157 (4.10-3.70)
Clashscore	180529	1219 (4.10-3.70)
Ramachandran outliers	177936	1177 (4.10-3.70)
Sidechain outliers	177891	1169 (4.10-3.70)
RSRZ outliers	164620	1157 (4.10-3.70)

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	303	3% 39% 29% 9% • 22%
1	B	303	2% 39% 26% 8% • 26%
1	C	303	36% 28% 9% • 25%
1	D	303	% 40% 27% 8% • 24%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6854 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1767	1175	288	296	8			
1	B	224	Total	C	N	O	S	0	0	0
			1671	1116	267	280	8			
1	C	227	Total	C	N	O	S	0	0	0
			1696	1134	271	283	8			
1	D	230	Total	C	N	O	S	0	0	0
			1720	1150	276	286	8			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	LEU	-	expression tag	UNP Q41372
A	283	GLU	-	expression tag	UNP Q41372
A	284	GLN	-	expression tag	UNP Q41372
A	285	LYS	-	expression tag	UNP Q41372
A	286	LEU	-	expression tag	UNP Q41372
A	287	ILE	-	expression tag	UNP Q41372
A	288	SER	-	expression tag	UNP Q41372
A	289	GLU	-	expression tag	UNP Q41372
A	290	GLU	-	expression tag	UNP Q41372
A	291	ASP	-	expression tag	UNP Q41372
A	292	LEU	-	expression tag	UNP Q41372
A	293	ASN	-	expression tag	UNP Q41372
A	294	SER	-	expression tag	UNP Q41372
A	295	ALA	-	expression tag	UNP Q41372
A	296	VAL	-	expression tag	UNP Q41372
A	297	ASP	-	expression tag	UNP Q41372
A	298	HIS	-	expression tag	UNP Q41372
A	299	HIS	-	expression tag	UNP Q41372
A	300	HIS	-	expression tag	UNP Q41372
A	301	HIS	-	expression tag	UNP Q41372
A	302	HIS	-	expression tag	UNP Q41372

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Chain	Residue	Modelled	Actual	Comment	Reference
A	303	HIS	-	expression tag	UNP Q41372
B	282	LEU	-	expression tag	UNP Q41372
B	283	GLU	-	expression tag	UNP Q41372
B	284	GLN	-	expression tag	UNP Q41372
B	285	LYS	-	expression tag	UNP Q41372
B	286	LEU	-	expression tag	UNP Q41372
B	287	ILE	-	expression tag	UNP Q41372
B	288	SER	-	expression tag	UNP Q41372
B	289	GLU	-	expression tag	UNP Q41372
B	290	GLU	-	expression tag	UNP Q41372
B	291	ASP	-	expression tag	UNP Q41372
B	292	LEU	-	expression tag	UNP Q41372
B	293	ASN	-	expression tag	UNP Q41372
B	294	SER	-	expression tag	UNP Q41372
B	295	ALA	-	expression tag	UNP Q41372
B	296	VAL	-	expression tag	UNP Q41372
B	297	ASP	-	expression tag	UNP Q41372
B	298	HIS	-	expression tag	UNP Q41372
B	299	HIS	-	expression tag	UNP Q41372
B	300	HIS	-	expression tag	UNP Q41372
B	301	HIS	-	expression tag	UNP Q41372
B	302	HIS	-	expression tag	UNP Q41372
B	303	HIS	-	expression tag	UNP Q41372
C	282	LEU	-	expression tag	UNP Q41372
C	283	GLU	-	expression tag	UNP Q41372
C	284	GLN	-	expression tag	UNP Q41372
C	285	LYS	-	expression tag	UNP Q41372
C	286	LEU	-	expression tag	UNP Q41372
C	287	ILE	-	expression tag	UNP Q41372
C	288	SER	-	expression tag	UNP Q41372
C	289	GLU	-	expression tag	UNP Q41372
C	290	GLU	-	expression tag	UNP Q41372
C	291	ASP	-	expression tag	UNP Q41372
C	292	LEU	-	expression tag	UNP Q41372
C	293	ASN	-	expression tag	UNP Q41372
C	294	SER	-	expression tag	UNP Q41372
C	295	ALA	-	expression tag	UNP Q41372
C	296	VAL	-	expression tag	UNP Q41372
C	297	ASP	-	expression tag	UNP Q41372
C	298	HIS	-	expression tag	UNP Q41372
C	299	HIS	-	expression tag	UNP Q41372
C	300	HIS	-	expression tag	UNP Q41372

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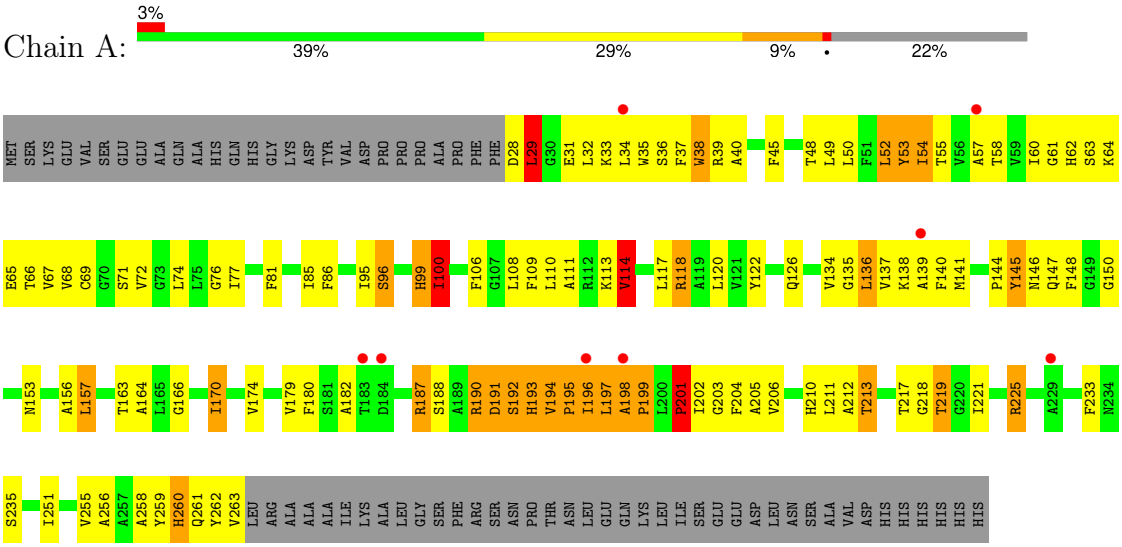
Chain	Residue	Modelled	Actual	Comment	Reference
C	301	HIS	-	expression tag	UNP Q41372
C	302	HIS	-	expression tag	UNP Q41372
C	303	HIS	-	expression tag	UNP Q41372
D	282	LEU	-	expression tag	UNP Q41372
D	283	GLU	-	expression tag	UNP Q41372
D	284	GLN	-	expression tag	UNP Q41372
D	285	LYS	-	expression tag	UNP Q41372
D	286	LEU	-	expression tag	UNP Q41372
D	287	ILE	-	expression tag	UNP Q41372
D	288	SER	-	expression tag	UNP Q41372
D	289	GLU	-	expression tag	UNP Q41372
D	290	GLU	-	expression tag	UNP Q41372
D	291	ASP	-	expression tag	UNP Q41372
D	292	LEU	-	expression tag	UNP Q41372
D	293	ASN	-	expression tag	UNP Q41372
D	294	SER	-	expression tag	UNP Q41372
D	295	ALA	-	expression tag	UNP Q41372
D	296	VAL	-	expression tag	UNP Q41372
D	297	ASP	-	expression tag	UNP Q41372
D	298	HIS	-	expression tag	UNP Q41372
D	299	HIS	-	expression tag	UNP Q41372
D	300	HIS	-	expression tag	UNP Q41372
D	301	HIS	-	expression tag	UNP Q41372
D	302	HIS	-	expression tag	UNP Q41372
D	303	HIS	-	expression tag	UNP Q41372

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.

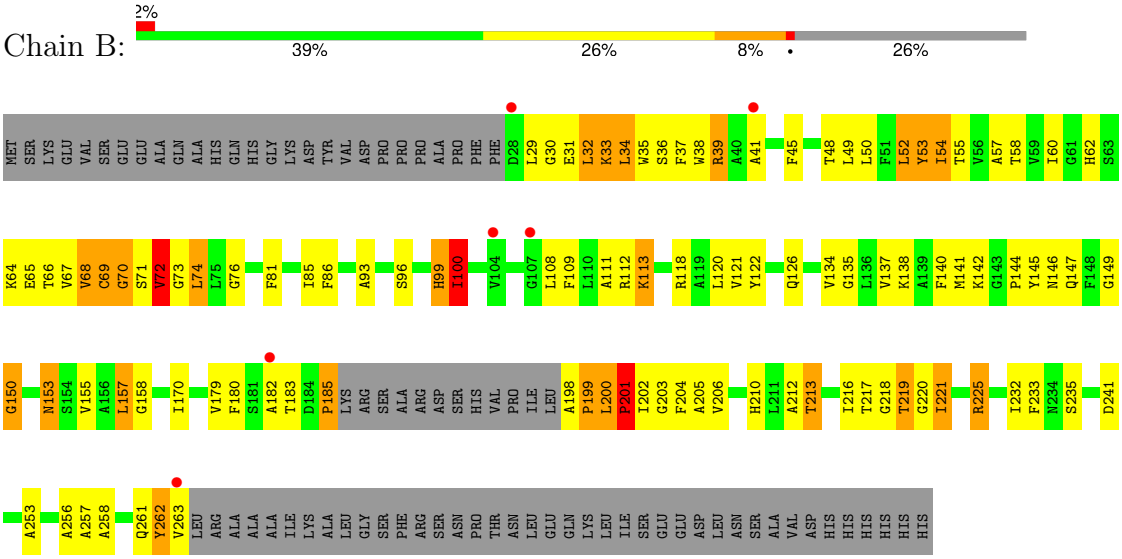
• Molecule 1: aquaporin

Chain A:



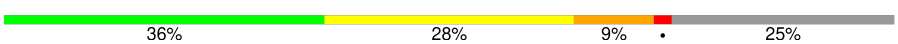
• Molecule 1: aquaporin

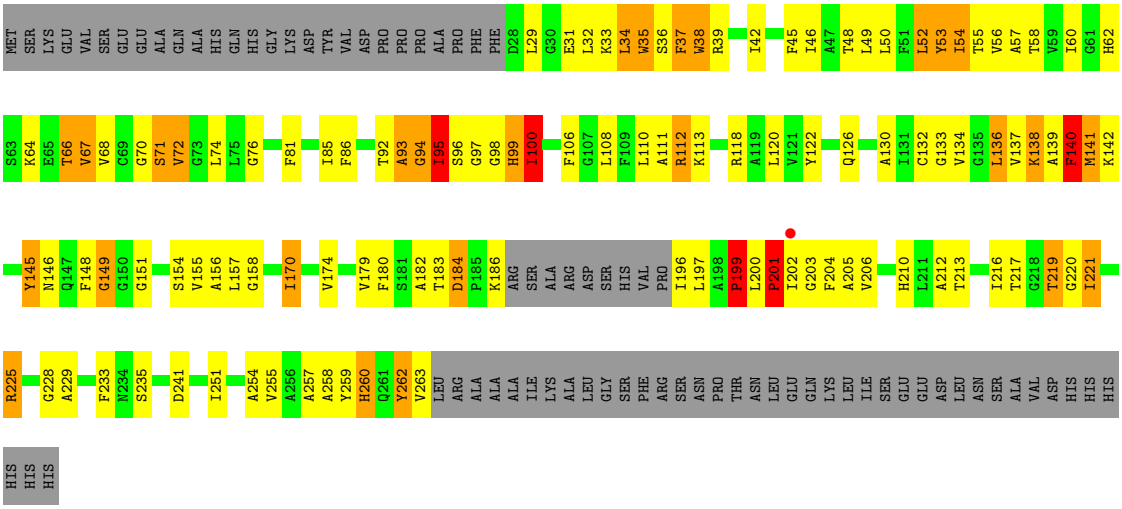
Chain B:



• Molecule 1: aquaporin

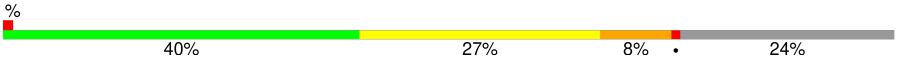
Chain C:

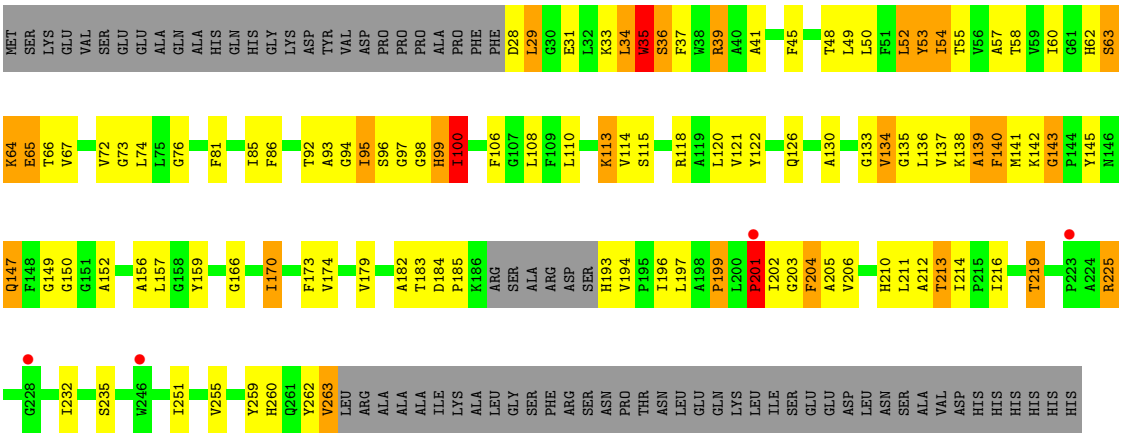




• Molecule 1: aquaporin

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	181.30Å 103.97Å 67.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 50.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.90) 89.6 (50.00-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 3.75Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.290 , 0.332 0.283 , 0.341	Depositor DCC
R_{free} test set	520 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	103.8	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , 63.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6854	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	1.11	4/1817 (0.2%)	0.97	6/2479 (0.2%)
1	B	1.12	4/1718 (0.2%)	1.03	7/2344 (0.3%)
1	C	1.12	4/1743 (0.2%)	1.01	6/2377 (0.3%)
1	D	1.12	5/1769 (0.3%)	1.00	7/2414 (0.3%)
All	All	1.12	17/7047 (0.2%)	1.00	26/9614 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	122	TYR	CE2-CZ	-12.34	1.22	1.38
1	C	122	TYR	CE2-CZ	-12.30	1.22	1.38
1	A	122	TYR	CE2-CZ	-12.30	1.22	1.38
1	B	122	TYR	CE2-CZ	-12.27	1.22	1.38
1	D	122	TYR	CG-CD1	-10.79	1.25	1.39

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	201	PRO	CA-N-CD	-15.52	89.77	111.50
1	D	201	PRO	CA-N-CD	-15.52	89.77	111.50
1	C	201	PRO	CA-N-CD	-15.48	89.82	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	201	PRO	CA-N-CD	-15.48	89.83	111.50
1	A	122	TYR	CB-CG-CD1	6.54	124.93	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	99	HIS	Sidechain
1	B	99	HIS	Sidechain
1	C	99	HIS	Sidechain
1	D	99	HIS	Sidechain

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	1767	0	1796	126	0
1	B	1671	0	1692	106	0
1	C	1696	0	1727	144	0
1	D	1720	0	1750	121	0
All	All	6854	0	6965	452	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 33.

The worst 5 of 452 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:39:ARG:HD3	1:D:263:VAL:HG13	1.42	1.01
1:C:66:THR:HG23	1:C:67:VAL:H	1.28	0.98
1:C:134:VAL:HG11	1:C:229:ALA:HA	1.48	0.95
1:C:202:ILE:O	1:C:203:GLY:C	2.02	0.95
1:A:202:ILE:O	1:A:203:GLY:C	2.02	0.95

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	234/303 (77%)	170 (73%)	42 (18%)	22 (9%)	0 9
1	B	220/303 (73%)	173 (79%)	29 (13%)	18 (8%)	1 11
1	C	223/303 (74%)	175 (78%)	21 (9%)	27 (12%)	0 5
1	D	226/303 (75%)	180 (80%)	27 (12%)	19 (8%)	0 10
All	All	903/1212 (74%)	698 (77%)	119 (13%)	86 (10%)	0 9

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	SER
1	A	96	SER
1	A	145	TYR
1	A	187	ARG
1	A	195	PRO

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	176/234 (75%)	157 (89%)	19 (11%)	5 22
1	B	165/234 (70%)	147 (89%)	18 (11%)	5 22
1	C	168/234 (72%)	151 (90%)	17 (10%)	6 24
1	D	171/234 (73%)	151 (88%)	20 (12%)	4 20
All	All	680/936 (73%)	606 (89%)	74 (11%)	5 22

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	52	LEU
1	D	260	HIS
1	D	66	THR
1	D	157	LEU
1	B	72	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	153	ASN
1	B	210	HIS
1	D	210	HIS
1	C	210	HIS
1	D	99	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)

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

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	236/303 (77%)	0.03	8 (3%)	48	37	17, 30, 43, 49	236 (100%)
1	B	224/303 (73%)	0.01	6 (2%)	56	42	21, 33, 45, 52	224 (100%)
1	C	227/303 (74%)	-0.01	1 (0%)	89	78	22, 34, 47, 52	227 (100%)
1	D	230/303 (75%)	0.02	4 (1%)	69	52	26, 38, 46, 53	230 (100%)
All	All	917/1212 (75%)	0.01	19 (2%)	63	48	17, 34, 46, 53	917 (100%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	THR	2.8
1	B	104	VAL	2.7
1	B	28	ASP	2.7
1	D	223	PRO	2.7
1	A	198	ALA	2.6

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 (i)

There are no such residues in this entry.