Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 10:15 am BST

PDB ID	:	8OEE
Title	:	Crystal structure of human AQP2 T126M mutant
Authors	:	Horsefield, S.; Hagstroemer, C.J.
Deposited on	:	2023-03-10
Resolution	:	3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

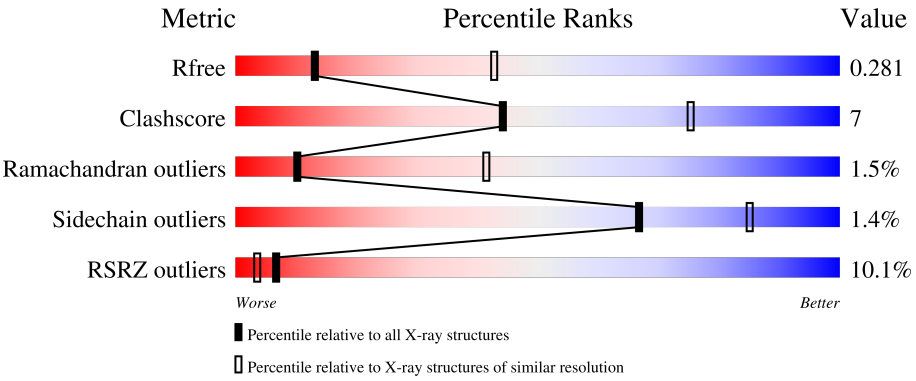
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	241	8% 80% 17%
1	B	241	6% 82% 15%
1	C	241	9% 80% 17%
1	D	241	16% 84% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6945 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1762	1151	296	308	7			
1	B	233	Total	C	N	O	S	0	0	0
			1716	1123	287	299	7			
1	C	236	Total	C	N	O	S	0	0	0
			1737	1136	290	304	7			
1	D	232	Total	C	N	O	S	0	0	0
			1713	1117	288	301	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P41181
A	2	SER	-	expression tag	UNP P41181
A	126	MET	THR	engineered mutation	UNP P41181
B	1	GLY	-	expression tag	UNP P41181
B	2	SER	-	expression tag	UNP P41181
B	126	MET	THR	engineered mutation	UNP P41181
C	1	GLY	-	expression tag	UNP P41181
C	2	SER	-	expression tag	UNP P41181
C	126	MET	THR	engineered mutation	UNP P41181
D	1	GLY	-	expression tag	UNP P41181
D	2	SER	-	expression tag	UNP P41181
D	126	MET	THR	engineered mutation	UNP P41181

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Cd	2	0
			2	2		

- Molecule 3 is water.

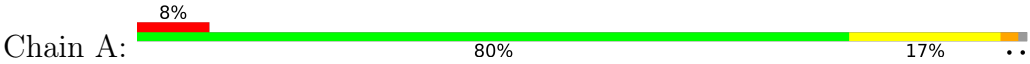
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	4	Total O 4 4	0	0
3	C	2	Total O 2 2	0	0
3	D	2	Total O 2 2	0	0

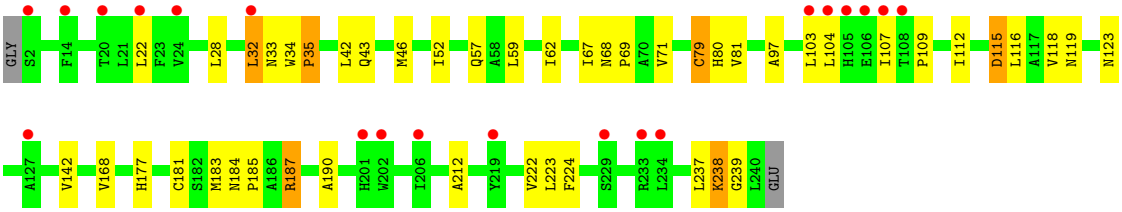
3 Residue-property plots (i)

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-2

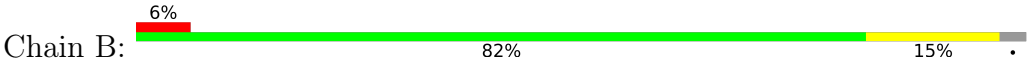
Chain A:

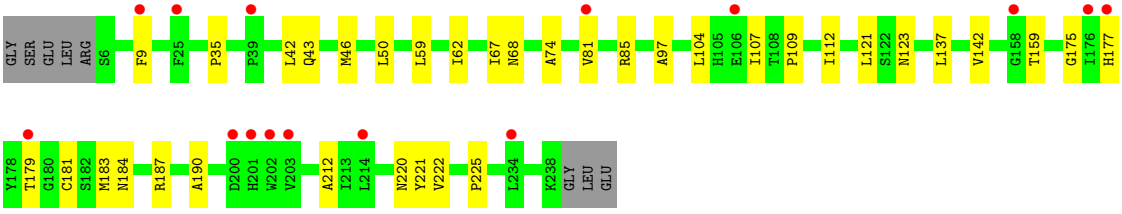




• Molecule 1: Aquaporin-2

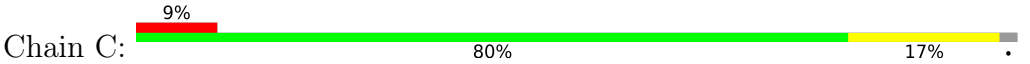
Chain B:

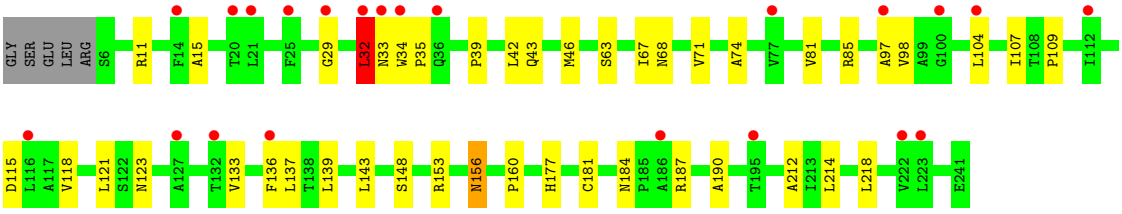




• Molecule 1: Aquaporin-2

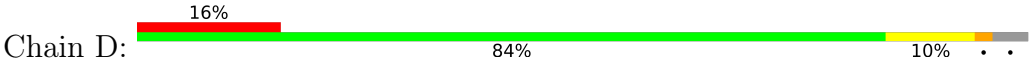
Chain C:

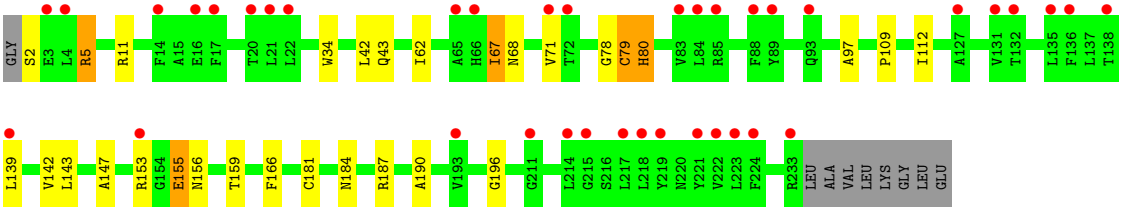




• Molecule 1: Aquaporin-2

Chain D:




GLY S2 E3 L4 R5 R11 F14 A15 E16 F17 T20 L21 L22 W34 L42 Q43 I62 A65 H66 I67 N68 V71 T72 G78 C79 H80 V83 L84 R85 F88 Y89 Q93 A97 P109 I112 A127 V131 T132 L135 F136 L137 T138
L139 V142 L143 A147 R153 G154 E155 N156 T159 F166 C181 N184 R187 A190 V193 G196 G211 L214 G215 S216 L217 L218 Y219 N220 Y221 V222 L223 P224 R233 LEU ALA VAL LEU LYS GLY LEU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α, β, γ	118.94Å 118.94Å 89.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.75 – 3.15 71.75 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.75-3.15) 88.7 (71.75-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.54 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.250 , 0.284 0.248 , 0.281	Depositor DCC
R_{free} test set	1090 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	80.6	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 101.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	6945	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

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

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	0.27	0/1803	0.49	1/2463 (0.0%)
1	B	0.25	0/1757	0.46	0/2402
1	C	0.25	0/1778	0.48	1/2430 (0.0%)
1	D	0.25	0/1754	0.46	0/2397
All	All	0.25	0/7092	0.47	2/9692 (0.0%)

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	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	32	LEU	CA-CB-CG	7.62	132.84	115.30
1	A	32	LEU	CA-CB-CG	5.39	127.69	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	5	ARG	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	1762	0	1806	33	0
1	B	1716	0	1759	24	0
1	C	1737	0	1777	31	0
1	D	1713	0	1743	23	0
2	D	2	0	0	0	0
3	A	7	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
All	All	6945	0	7085	92	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 7.

All (92) 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:155:GLU:HG2	1:D:156:ASN:H	1.32	0.91
1:A:238:LYS:HG2	1:A:239:GLY:H	1.45	0.81
1:D:34:TRP:HA	1:D:112:ILE:HD11	1.65	0.76
1:A:109:PRO:HG2	1:A:112:ILE:HD12	1.69	0.72
1:B:42:LEU:HB2	1:C:43:GLN:HG3	1.72	0.70
1:B:67:ILE:O	1:B:184:ASN:ND2	2.26	0.69
1:B:81:VAL:HG23	1:B:85:ARG:HD2	1.74	0.68
1:D:67:ILE:O	1:D:184:ASN:ND2	2.28	0.66
1:D:2:SER:HB3	1:D:5:ARG:HG3	1.78	0.66
1:B:43:GLN:HG3	1:D:42:LEU:HB2	1.78	0.65
1:C:74:ALA:HB2	1:C:212:ALA:HB1	1.79	0.64
1:A:104:LEU:HD12	1:A:107:ILE:HD11	1.81	0.63
1:B:68:ASN:ND2	1:B:183:MET:O	2.32	0.63
1:A:42:LEU:HB2	1:D:43:GLN:HG3	1.79	0.62
1:A:67:ILE:O	1:A:184:ASN:ND2	2.26	0.62
1:A:32:LEU:HD22	1:A:116:LEU:HA	1.82	0.61
1:A:68:ASN:ND2	1:A:183:MET:O	2.33	0.60
1:D:155:GLU:HG2	1:D:156:ASN:N	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ALA:HB1	1:D:190:ALA:HB2	1.84	0.60
1:A:69:PRO:HD2	1:A:185:PRO:HD2	1.84	0.60
1:A:35:PRO:HD3	1:A:112:ILE:HG12	1.84	0.58
1:B:59:LEU:HA	1:B:62:ILE:HD12	1.86	0.58
1:B:104:LEU:HD12	1:B:107:ILE:HD11	1.86	0.57
1:A:238:LYS:HG2	1:A:239:GLY:N	2.19	0.56
1:A:97:ALA:HB1	1:A:190:ALA:HB2	1.88	0.55
1:C:104:LEU:HD12	1:C:107:ILE:HD11	1.88	0.55
1:B:137:LEU:HD21	1:B:175:GLY:HA3	1.88	0.55
1:B:50:LEU:HD22	1:D:166:PHE:HB3	1.89	0.55
1:D:68:ASN:HB3	1:D:71:VAL:HG22	1.88	0.55
1:C:67:ILE:O	1:C:184:ASN:ND2	2.39	0.54
1:C:15:ALA:HB3	1:C:63:SER:HB3	1.90	0.54
1:C:123:ASN:ND2	1:C:177:HIS:O	2.41	0.53
1:B:123:ASN:O	1:C:109:PRO:HG3	2.08	0.53
1:D:139:LEU:O	1:D:143:LEU:HD13	2.09	0.53
1:A:177:HIS:HB3	1:D:34:TRP:CE3	2.44	0.53
1:A:119:ASN:OD1	1:A:187:ARG:NH1	2.42	0.52
1:C:32:LEU:HD12	1:C:33:ASN:H	1.75	0.52
1:A:52:ILE:HG13	1:A:168:VAL:HG21	1.91	0.51
1:C:34:TRP:HB3	1:C:39:PRO:HD3	1.93	0.51
1:B:221:TYR:HA	1:B:225:PRO:HB3	1.93	0.51
1:A:57:GLN:O	1:C:153:ARG:NH1	2.44	0.50
1:A:223:LEU:HB3	1:D:62:ILE:HD13	1.93	0.49
1:B:177:HIS:CG	1:C:33:ASN:HB3	2.47	0.49
1:B:9:PHE:HE1	1:B:85:ARG:HG3	1.77	0.49
1:C:81:VAL:HG13	1:C:85:ARG:HD2	1.94	0.49
1:C:148:SER:HB3	1:C:160:PRO:HD2	1.93	0.49
1:B:67:ILE:O	1:B:67:ILE:HG22	2.13	0.48
1:C:29:GLY:O	1:C:33:ASN:ND2	2.46	0.48
1:C:98:VAL:HG12	1:C:190:ALA:HA	1.94	0.48
1:A:43:GLN:HG3	1:C:42:LEU:HB2	1.95	0.48
1:C:67:ILE:O	1:C:67:ILE:HG22	2.14	0.47
1:C:68:ASN:HB3	1:C:71:VAL:HB	1.94	0.47
1:A:68:ASN:HB3	1:A:71:VAL:HB	1.96	0.47
1:A:222:VAL:O	1:D:11:ARG:HD3	2.15	0.47
1:B:121:LEU:HD12	1:B:179:THR:HG22	1.97	0.47
1:A:115:ASP:HB2	1:A:118:VAL:HG22	1.98	0.46
1:B:220:ASN:O	1:B:225:PRO:HA	2.15	0.46
1:A:142:VAL:HG21	1:A:212:ALA:HA	1.96	0.46
1:A:67:ILE:O	1:A:67:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ALA:O	1:D:153:ARG:NH1	2.47	0.46
1:B:46:MET:HG2	1:D:42:LEU:HD11	1.98	0.46
1:C:115:ASP:HB2	1:C:118:VAL:HG22	1.98	0.46
1:C:97:ALA:HB1	1:C:190:ALA:HB2	1.98	0.45
1:C:133:VAL:O	1:C:137:LEU:HG	2.17	0.45
1:D:67:ILE:O	1:D:67:ILE:HG22	2.16	0.45
1:B:159:THR:HG22	1:D:159:THR:HG21	1.98	0.45
1:A:33:ASN:C	1:A:35:PRO:HD2	2.37	0.45
1:B:142:VAL:HG21	1:B:212:ALA:HA	1.98	0.45
1:D:34:TRP:CE3	1:D:112:ILE:HD13	2.53	0.44
1:B:109:PRO:HG2	1:B:112:ILE:HD13	2.00	0.44
1:C:143:LEU:HD23	1:C:143:LEU:HA	1.87	0.44
1:D:71:VAL:HG12	1:D:142:VAL:HG12	1.99	0.44
1:B:74:ALA:HB2	1:B:212:ALA:HB1	1.99	0.44
1:B:42:LEU:HD11	1:C:46:MET:HG2	2.00	0.44
1:A:28:LEU:HB3	1:A:32:LEU:HD23	2.00	0.43
1:A:34:TRP:N	1:A:35:PRO:HD2	2.33	0.43
1:C:214:LEU:O	1:C:218:LEU:HB2	2.18	0.43
1:A:59:LEU:HA	1:A:62:ILE:HD12	2.00	0.43
1:B:97:ALA:HB1	1:B:190:ALA:HB2	2.00	0.43
1:C:32:LEU:HD12	1:C:33:ASN:N	2.33	0.43
1:D:78:GLY:O	1:D:80:HIS:N	2.52	0.43
1:A:79:CYS:O	1:A:81:VAL:N	2.52	0.43
1:A:103:LEU:HD11	1:C:136:PHE:CZ	2.54	0.42
1:A:237:LEU:HG	1:A:238:LYS:O	2.19	0.42
1:A:123:ASN:O	1:D:109:PRO:HG3	2.20	0.42
1:A:22:LEU:HD21	1:C:139:LEU:HD23	2.03	0.41
1:C:156:ASN:N	1:C:156:ASN:OD1	2.53	0.41
1:D:155:GLU:N	1:D:155:GLU:OE1	2.54	0.40
1:A:34:TRP:O	1:A:35:PRO:C	2.60	0.40
1:A:46:MET:HG2	1:C:42:LEU:HD11	2.03	0.40
1:C:121:LEU:HA	1:C:121:LEU:HD23	1.82	0.40
1:B:222:VAL:O	1:C:11:ARG:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	237/241 (98%)	221 (93%)	13 (6%)	3 (1%)	12	44
1	B	231/241 (96%)	216 (94%)	13 (6%)	2 (1%)	17	53
1	C	234/241 (97%)	221 (94%)	10 (4%)	3 (1%)	12	44
1	D	230/241 (95%)	216 (94%)	8 (4%)	6 (3%)	5	28
All	All	932/964 (97%)	874 (94%)	44 (5%)	14 (2%)	10	41

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	D	155	GLU
1	C	35	PRO
1	D	79	CYS
1	D	196	GLY
1	A	35	PRO
1	A	181	CYS
1	B	181	CYS
1	C	32	LEU
1	C	181	CYS
1	D	181	CYS
1	D	80	HIS
1	D	67	ILE
1	B	35	PRO

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	182/183 (100%)	177 (97%)	5 (3%)	44	73
1	B	177/183 (97%)	176 (99%)	1 (1%)	86	94
1	C	179/183 (98%)	177 (99%)	2 (1%)	73	88
1	D	177/183 (97%)	175 (99%)	2 (1%)	73	88
All	All	715/732 (98%)	705 (99%)	10 (1%)	67	85

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

Mol	Chain	Res	Type
1	A	79	CYS
1	A	115	ASP
1	A	187	ARG
1	A	224	PHE
1	A	238	LYS
1	B	187	ARG
1	C	156	ASN
1	C	187	ARG
1	D	79	CYS
1	D	187	ARG

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

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - 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, 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	239/241 (99%)	0.54	20 (8%) 11 5	62, 110, 179, 241	0
1	B	233/241 (96%)	0.59	15 (6%) 19 10	70, 125, 221, 435	1 (0%)
1	C	236/241 (97%)	0.64	22 (9%) 8 5	68, 111, 169, 216	0
1	D	232/241 (96%)	0.87	38 (16%) 1 1	64, 124, 192, 328	1 (0%)
All	All	940/964 (97%)	0.66	95 (10%) 7 3	62, 118, 185, 435	2 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	VAL	8.1
1	D	222	VAL	6.4
1	A	107	ILE	6.2
1	C	112	ILE	5.8
1	D	139	LEU	4.9
1	D	223	LEU	4.6
1	B	202	TRP	4.5
1	A	108	THR	4.5
1	D	135	LEU	4.4
1	D	84	LEU	4.2
1	A	106	GLU	4.2
1	B	158	GLY	4.1
1	D	219	TYR	4.1
1	B	203	VAL	3.8
1	D	65	ALA	3.7
1	D	131	VAL	3.7
1	A	229	SER	3.7
1	C	21	LEU	3.7
1	C	34	TRP	3.6
1	D	83	VAL	3.6
1	D	71	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	39	PRO	3.6
1	C	100	GLY	3.6
1	C	116	LEU	3.5
1	D	4	LEU	3.2
1	D	21	LEU	3.2
1	A	105	HIS	3.2
1	C	33	ASN	3.2
1	D	138	THR	3.1
1	D	211	GLY	3.1
1	B	9	PHE	3.0
1	A	201	HIS	3.0
1	C	127	ALA	3.0
1	D	20	THR	2.9
1	D	214	LEU	2.9
1	B	234	LEU	2.9
1	D	72	THR	2.8
1	C	25	PHE	2.8
1	B	201	HIS	2.8
1	B	177	HIS	2.8
1	D	88	PHE	2.8
1	B	200	ASP	2.7
1	D	217	LEU	2.7
1	A	104	LEU	2.7
1	A	127	ALA	2.6
1	A	103	LEU	2.6
1	D	218	LEU	2.6
1	D	89	TYR	2.6
1	C	32	LEU	2.6
1	D	3	GLU	2.6
1	D	233	ARG	2.6
1	A	22	LEU	2.5
1	D	132	THR	2.5
1	B	106	GLU	2.5
1	C	20	THR	2.5
1	D	153	ARG	2.5
1	D	22	LEU	2.4
1	C	132	THR	2.4
1	A	233	ARG	2.4
1	D	93	GLN	2.4
1	C	222	VAL	2.4
1	D	193	VAL	2.4
1	B	25	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	104	LEU	2.4
1	C	136	PHE	2.4
1	A	20	THR	2.4
1	A	202	TRP	2.3
1	C	97	ALA	2.3
1	A	234	LEU	2.3
1	D	221	TYR	2.3
1	A	32	LEU	2.3
1	D	16	GLU	2.3
1	C	29	GLY	2.3
1	D	136	PHE	2.3
1	D	17	PHE	2.3
1	D	215	GLY	2.3
1	A	2	SER	2.3
1	D	224	PHE	2.3
1	C	223	LEU	2.2
1	A	206	ILE	2.2
1	B	214	LEU	2.2
1	A	219	TYR	2.2
1	A	14	PHE	2.2
1	D	66	HIS	2.2
1	C	77	VAL	2.1
1	C	36	GLN	2.1
1	C	14	PHE	2.1
1	D	85	ARG	2.1
1	A	24	VAL	2.1
1	B	179	THR	2.1
1	C	195	THR	2.1
1	D	14	PHE	2.1
1	C	186	ALA	2.1
1	D	127	ALA	2.1
1	B	176	ILE	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 monosaccharides in this entry.

6.4 Ligands

LIGAND-RSR INFOmissingINFO

6.5 Other polymers

There are no such residues in this entry.