Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2022 – 12:15 PM JST

PDB ID	:	6IVP
Title	:	Crystal structure of a membrane protein P262A
Authors	:	Kittredge, A.; Fukuda, F.; Zhang, Y.; Yang, T.
Deposited on	:	2018-12-04
Resolution	:	3.80 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:

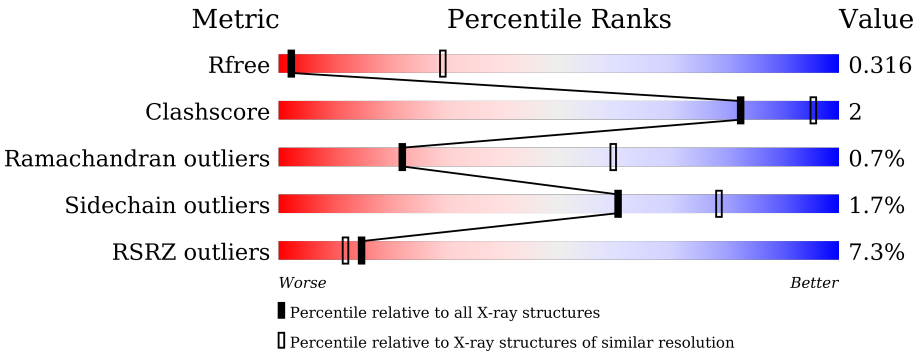
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	297	6% 86% 6% 8%
1	B	297	6% 80% 10% 9%
1	C	297	6% 82% 8% • 9%
1	D	297	12% 83% 7% 10%
1	E	297	4% 82% 8% 9%

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
2	ZN	C	305	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10751 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 bestrophin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2175	1408	368	390	9			
1	B	269	Total	C	N	O	S	0	0	0
			2143	1387	364	383	9			
1	C	269	Total	C	N	O	S	0	0	0
			2138	1383	364	382	9			
1	D	268	Total	C	N	O	S	0	0	0
			2127	1375	361	382	9			
1	E	269	Total	C	N	O	S	0	0	0
			2143	1387	364	383	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP W9BH30
A	-1	ASN	-	expression tag	UNP W9BH30
A	0	ALA	-	expression tag	UNP W9BH30
A	262	ALA	PRO	engineered mutation	UNP W9BH30
B	-2	SER	-	expression tag	UNP W9BH30
B	-1	ASN	-	expression tag	UNP W9BH30
B	0	ALA	-	expression tag	UNP W9BH30
B	262	ALA	PRO	engineered mutation	UNP W9BH30
C	-2	SER	-	expression tag	UNP W9BH30
C	-1	ASN	-	expression tag	UNP W9BH30
C	0	ALA	-	expression tag	UNP W9BH30
C	262	ALA	PRO	engineered mutation	UNP W9BH30
D	-2	SER	-	expression tag	UNP W9BH30
D	-1	ASN	-	expression tag	UNP W9BH30
D	0	ALA	-	expression tag	UNP W9BH30
D	262	ALA	PRO	engineered mutation	UNP W9BH30
E	-2	SER	-	expression tag	UNP W9BH30
E	-1	ASN	-	expression tag	UNP W9BH30
E	0	ALA	-	expression tag	UNP W9BH30

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Chain	Residue	Modelled	Actual	Comment	Reference
E	262	ALA	PRO	engineered mutation	UNP W9BH30

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Zn 3 3	0	0
2	B	3	Total Zn 3 3	0	0
2	C	4	Total Zn 4 4	0	0
2	D	3	Total Zn 3 3	0	0
2	E	1	Total Zn 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0
3	B	2	Total Cl 2 2	0	0
3	C	2	Total Cl 2 2	0	0
3	D	3	Total Cl 3 3	0	0
3	E	1	Total Cl 1 1	0	0

- Molecule 4 is water.

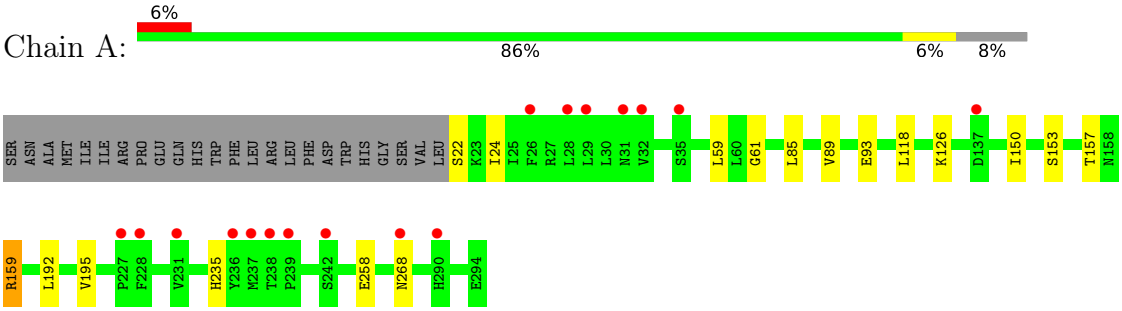
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O 1 1	0	0

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.

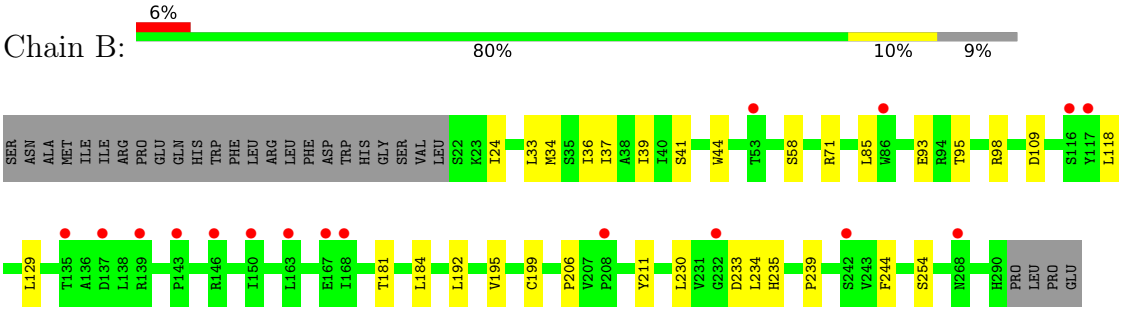
• Molecule 1: bestrophin

Chain A:



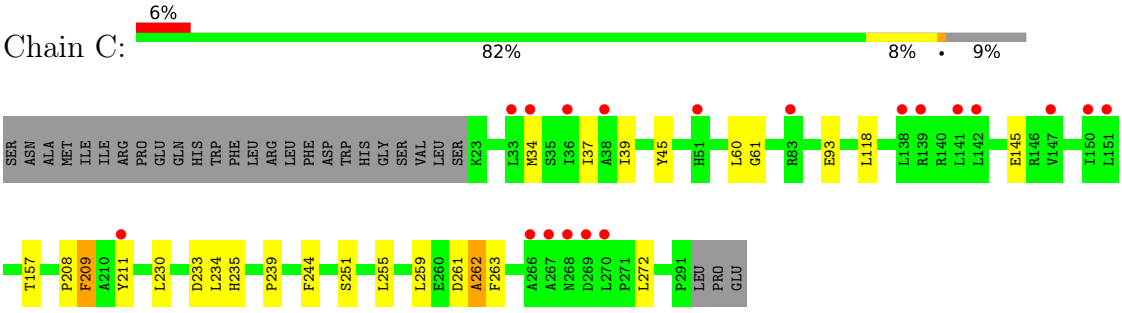
• Molecule 1: bestrophin

Chain B:



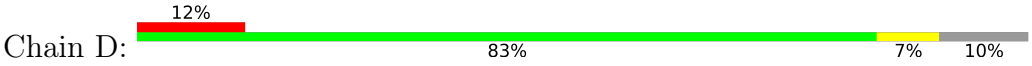
• Molecule 1: bestrophin

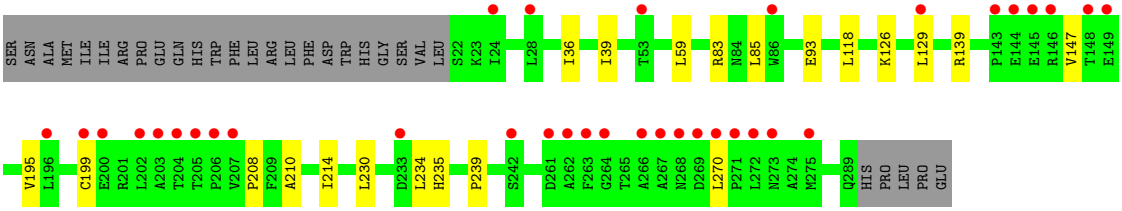
Chain C:



• Molecule 1: bestrophin

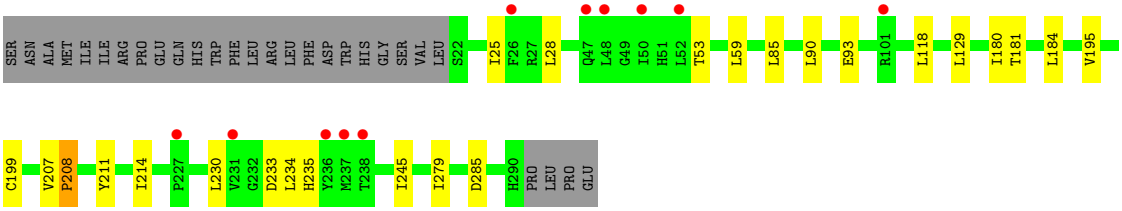
Chain D:





- Molecule 1: bestrophin

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	114.48Å 162.41Å 161.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.80 48.94 – 3.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.01-3.80) 97.6 (48.94-3.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.266 , 0.315 0.266 , 0.316	Depositor DCC
R_{free} test set	1526 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	149.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 71.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	10751	wwPDB-VP
Average B, all atoms (Å^2)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: CL, ZN

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	0.40	0/2223	0.58	0/3025
1	B	0.40	0/2189	0.58	0/2978
1	C	0.40	0/2184	0.60	0/2973
1	D	0.40	0/2171	0.59	0/2954
1	E	0.40	0/2189	0.58	0/2978
All	All	0.40	0/10956	0.59	0/14908

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	2175	0	2217	10	0
1	B	2143	0	2186	14	0
1	C	2138	0	2181	13	0
1	D	2127	0	2172	12	0
1	E	2143	0	2186	13	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3	0	0	0	0
2	E	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
3	E	1	0	0	0	0
4	C	1	0	0	0	0
All	All	10751	0	10942	54	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 2.

All (54) 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:261:ASP:HA	1:C:262:ALA:HB2	1.37	1.03
1:C:261:ASP:HA	1:C:262:ALA:CB	2.16	0.67
1:E:207:VAL:HG23	1:E:208:PRO:HD3	1.79	0.65
1:E:90:LEU:HA	1:E:279:ILE:HD13	1.84	0.58
1:D:139:ARG:HG3	1:D:147:VAL:HG11	1.87	0.56
1:B:129:LEU:HD21	1:B:199:CYS:HB3	1.89	0.54
1:A:22:SER:HB3	1:A:24:ILE:HG22	1.91	0.53
1:E:129:LEU:HD21	1:E:199:CYS:HB3	1.90	0.52
1:D:230:LEU:HB3	1:D:234:LEU:HD12	1.90	0.52
1:C:39:ILE:HD11	1:C:239:PRO:HD3	1.93	0.51
1:E:230:LEU:HB3	1:E:234:LEU:HD12	1.93	0.51
1:E:211:TYR:HA	1:E:214:ILE:HB	1.93	0.50
1:A:89:VAL:HG22	1:A:195:VAL:HG11	1.93	0.50
1:C:230:LEU:HB3	1:C:234:LEU:HD12	1.93	0.50
1:D:93:GLU:HG2	1:D:118:LEU:HD22	1.93	0.50
1:A:153:SER:HB2	1:A:159:ARG:HD2	1.93	0.50
1:B:85:LEU:HB3	1:B:195:VAL:HG13	1.94	0.50
1:A:93:GLU:HG2	1:A:118:LEU:HD22	1.94	0.49
1:B:39:ILE:HD11	1:B:239:PRO:HD3	1.95	0.49
1:D:85:LEU:HD22	1:D:195:VAL:HA	1.95	0.48
1:B:230:LEU:HB3	1:B:234:LEU:HD12	1.94	0.48
1:B:34:MET:HA	1:B:37:ILE:HD12	1.96	0.48
1:C:61:GLY:HA3	1:D:59:LEU:HD11	1.96	0.48
1:D:83:ARG:HG2	1:D:270:LEU:HD21	1.95	0.48
1:B:85:LEU:HD22	1:B:195:VAL:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:SER:HB3	1:D:214:ILE:HG12	1.96	0.47
1:B:93:GLU:HG2	1:B:118:LEU:HD22	1.96	0.47
1:C:93:GLU:HG2	1:C:118:LEU:HD22	1.97	0.47
1:E:93:GLU:HG2	1:E:118:LEU:HD22	1.96	0.47
1:B:95:THR:HG22	1:B:98:ARG:HE	1.79	0.46
1:D:39:ILE:HD11	1:D:239:PRO:HD3	1.99	0.45
1:D:36:ILE:HA	1:D:39:ILE:HD12	1.98	0.45
1:C:34:MET:HA	1:C:37:ILE:HD12	1.98	0.45
1:C:263:PHE:HB3	1:C:272:LEU:HD11	1.99	0.45
1:C:60:LEU:HB2	1:E:245:ILE:HG12	1.99	0.44
1:B:33:LEU:HA	1:B:36:ILE:HD12	1.99	0.44
1:C:60:LEU:HD13	1:E:245:ILE:HA	2.00	0.44
1:E:85:LEU:HD22	1:E:195:VAL:HA	1.99	0.44
1:C:259:LEU:HD21	1:D:208:PRO:HG2	2.01	0.43
1:A:258:GLU:HB3	1:A:268:ASN:HB2	2.00	0.43
1:E:25:ILE:HA	1:E:28:LEU:HD12	2.00	0.43
1:B:24:ILE:HD11	1:B:254:SER:HB3	2.01	0.42
1:A:150:ILE:HA	1:A:159:ARG:HG2	2.02	0.42
1:B:181:THR:HA	1:B:184:LEU:HD12	2.01	0.42
1:B:93:GLU:HG3	1:B:192:LEU:HD21	2.00	0.42
1:E:181:THR:HA	1:E:184:LEU:HD12	2.02	0.42
1:A:93:GLU:HG3	1:A:192:LEU:HD21	2.02	0.42
1:A:61:GLY:HA3	1:E:59:LEU:HD11	2.01	0.42
1:A:85:LEU:HD22	1:A:195:VAL:HA	2.02	0.41
1:E:85:LEU:HB3	1:E:195:VAL:HG13	2.03	0.41
1:D:129:LEU:HD21	1:D:199:CYS:HB3	2.01	0.41
1:A:59:LEU:HD13	1:B:58:SER:HA	2.03	0.40
1:B:41:SER:HA	1:B:44:TRP:HD1	1.87	0.40
1:C:255:LEU:HD13	1:D:210:ALA:HB3	2.03	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	271/297 (91%)	266 (98%)	4 (2%)	1 (0%)	34	70
1	B	267/297 (90%)	262 (98%)	3 (1%)	2 (1%)	22	60
1	C	267/297 (90%)	259 (97%)	4 (2%)	4 (2%)	10	46
1	D	266/297 (90%)	263 (99%)	2 (1%)	1 (0%)	34	70
1	E	267/297 (90%)	259 (97%)	6 (2%)	2 (1%)	22	60
All	All	1338/1485 (90%)	1309 (98%)	19 (1%)	10 (1%)	22	60

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	209	PHE
1	C	262	ALA
1	A	235	HIS
1	C	235	HIS
1	B	235	HIS
1	D	235	HIS
1	E	235	HIS
1	B	206	PRO
1	C	208	PRO
1	E	208	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	237/259 (92%)	234 (99%)	3 (1%)	69	82
1	B	233/259 (90%)	228 (98%)	5 (2%)	53	74
1	C	232/259 (90%)	225 (97%)	7 (3%)	41	66
1	D	231/259 (89%)	230 (100%)	1 (0%)	91	95
1	E	233/259 (90%)	229 (98%)	4 (2%)	60	78
All	All	1166/1295 (90%)	1146 (98%)	20 (2%)	60	78

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	LYS
1	A	157	THR
1	A	159	ARG
1	B	71	ARG
1	B	109	ASP
1	B	211	TYR
1	B	233	ASP
1	B	244	PHE
1	C	45	TYR
1	C	145	GLU
1	C	157	THR
1	C	209	PHE
1	C	211	TYR
1	C	233	ASP
1	C	244	PHE
1	D	126	LYS
1	E	53	THR
1	E	180	ILE
1	E	233	ASP
1	E	285	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	B	99	GLN
1	B	102	ASN
1	B	290	HIS
1	C	102	ASN
1	C	166	ASN
1	D	102	ASN
1	D	282	ASN
1	E	102	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 24 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	273/297 (91%)	0.23	17 (6%)	20 16	104, 149, 206, 261	0
1	B	269/297 (90%)	0.38	17 (6%)	20 15	108, 163, 210, 227	0
1	C	269/297 (90%)	0.40	19 (7%)	16 12	116, 163, 212, 229	0
1	D	268/297 (90%)	0.56	35 (13%)	3 4	110, 168, 216, 236	0
1	E	269/297 (90%)	0.15	11 (4%)	37 31	104, 145, 213, 231	0
All	All	1348/1485 (90%)	0.34	99 (7%)	15 12	104, 158, 213, 261	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	268	ASN	8.0
1	D	205	THR	7.1
1	D	268	ASN	6.9
1	D	204	THR	6.6
1	E	48	LEU	4.5
1	D	270	LEU	4.2
1	D	145	GLU	4.1
1	C	267	ALA	4.0
1	D	199	CYS	4.0
1	A	31	ASN	4.0
1	A	242	SER	3.8
1	D	86	TRP	3.8
1	A	231	VAL	3.7
1	D	272	LEU	3.7
1	D	200	GLU	3.6
1	A	237	MET	3.6
1	D	206	PRO	3.6
1	E	50	ILE	3.5
1	D	233	ASP	3.4
1	D	242	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	150	ILE	3.4
1	A	236	TYR	3.3
1	B	53	THR	3.1
1	A	227	PRO	3.1
1	D	269	ASP	3.1
1	D	146	ARG	3.1
1	B	116	SER	3.1
1	C	34	MET	3.0
1	D	148	THR	3.0
1	C	139	ARG	3.0
1	C	138	LEU	3.0
1	D	262	ALA	3.0
1	B	137	ASP	3.0
1	D	263	PHE	3.0
1	B	150	ILE	2.9
1	D	143	PRO	2.9
1	E	47	GLN	2.9
1	A	238	THR	2.8
1	A	228	PHE	2.8
1	C	142	LEU	2.8
1	D	28	LEU	2.8
1	B	117	TYR	2.8
1	A	35	SER	2.8
1	D	264	GLY	2.8
1	E	52	LEU	2.8
1	E	231	VAL	2.7
1	D	207	VAL	2.7
1	D	129	LEU	2.7
1	B	135	THR	2.6
1	C	141	LEU	2.6
1	E	237	MET	2.6
1	C	147	VAL	2.6
1	B	167	GLU	2.6
1	A	29	LEU	2.5
1	B	242	SER	2.5
1	D	203	ALA	2.5
1	C	38	ALA	2.5
1	E	236	TYR	2.4
1	D	196	LEU	2.4
1	C	266	ALA	2.4
1	B	163	LEU	2.4
1	E	26	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	232	GLY	2.4
1	E	101	ARG	2.3
1	C	33	LEU	2.3
1	C	270	LEU	2.3
1	B	139	ARG	2.3
1	B	146	ARG	2.3
1	E	227	PRO	2.2
1	D	24	ILE	2.2
1	C	269	ASP	2.2
1	A	28	LEU	2.2
1	A	239	PRO	2.2
1	C	51	HIS	2.2
1	A	268	ASN	2.2
1	B	143	PRO	2.2
1	C	211	TYR	2.2
1	A	137	ASP	2.2
1	A	32	VAL	2.2
1	C	36	ILE	2.2
1	B	268	ASN	2.2
1	E	238	THR	2.1
1	D	275	MET	2.1
1	C	83	ARG	2.1
1	D	202	LEU	2.1
1	B	86	TRP	2.1
1	A	290	HIS	2.1
1	D	273	ASN	2.1
1	B	208	PRO	2.1
1	D	271	PRO	2.1
1	D	144	GLU	2.1
1	D	266	ALA	2.1
1	A	26	PHE	2.1
1	B	168	ILE	2.1
1	D	53	THR	2.0
1	D	261	ASP	2.0
1	C	151	LEU	2.0
1	D	267	ALA	2.0
1	D	149	GLU	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 (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, 95^{th} 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(Å^2)	Q<0.9
2	ZN	D	302	1/1	0.64	0.12	169,169,169,169	0
2	ZN	D	303	1/1	0.68	0.13	230,230,230,230	0
2	ZN	C	305	1/1	0.69	0.49	260,260,260,260	0
3	CL	B	303	1/1	0.76	0.28	182,182,182,182	0
2	ZN	A	301	1/1	0.89	0.43	117,117,117,117	0
2	ZN	C	302	1/1	0.91	0.10	148,148,148,148	0
2	ZN	B	302	1/1	0.92	0.10	146,146,146,146	0
2	ZN	B	301	1/1	0.93	0.08	198,198,198,198	0
2	ZN	C	301	1/1	0.94	0.24	124,124,124,124	0
2	ZN	B	305	1/1	0.95	0.26	132,132,132,132	0
3	CL	D	305	1/1	0.95	0.12	150,150,150,150	0
3	CL	C	304	1/1	0.96	0.13	162,162,162,162	0
2	ZN	C	306	1/1	0.96	0.42	112,112,112,112	0
3	CL	B	304	1/1	0.97	0.12	151,151,151,151	0
2	ZN	A	302	1/1	0.97	0.34	120,120,120,120	0
2	ZN	A	303	1/1	0.97	0.10	132,132,132,132	0
3	CL	D	306	1/1	0.97	0.13	191,191,191,191	0
3	CL	A	304	1/1	0.98	0.09	141,141,141,141	0
2	ZN	E	301	1/1	0.98	0.06	120,120,120,120	0
2	ZN	D	301	1/1	0.99	0.08	167,167,167,167	0
3	CL	D	304	1/1	0.99	0.17	108,108,108,108	0
3	CL	A	305	1/1	0.99	0.22	103,103,103,103	0
3	CL	C	303	1/1	0.99	0.19	115,115,115,115	0
3	CL	E	302	1/1	0.99	0.10	116,116,116,116	0

6.5 Other polymers (i)

There are no such residues in this entry.