



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:41 PM BST

PDB ID : 3WIP
Title : Crystal structure of acetylcholine bound to Ls-AChBP
Authors : Olsen, J.A.; Balle, T.; Gajhede, M.; Ahring, P.K.; Kastrup, J.S.
Deposited on : 2013-09-24
Resolution : 2.60 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

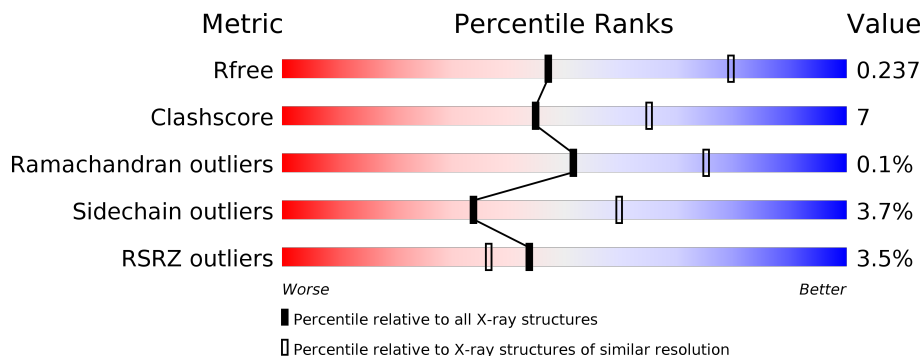
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	229	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">74% 14% 12%</p>
1	B	229	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">78% 12% 9%</p>
1	C	229	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">75% 13% 12%</p>
1	D	229	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">75% 13% 12%</p>
1	E	229	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">73% 14% 12%</p>
1	F	229	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">78% 12% 10%</p>

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Mol	Chain	Length	Quality of chain
1	G	229	
1	H	229	
1	I	229	
1	J	229	

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
3	1PE	A	303	-	-	X	-
3	1PE	A	304	-	-	X	-
3	1PE	B	304	-	-	X	-
3	1PE	E	303	-	-	X	-
3	1PE	G	303	-	-	X	-
3	1PE	H	302	-	-	X	-
4	SO4	J	302	-	-	-	X

2 Entry composition [i](#)

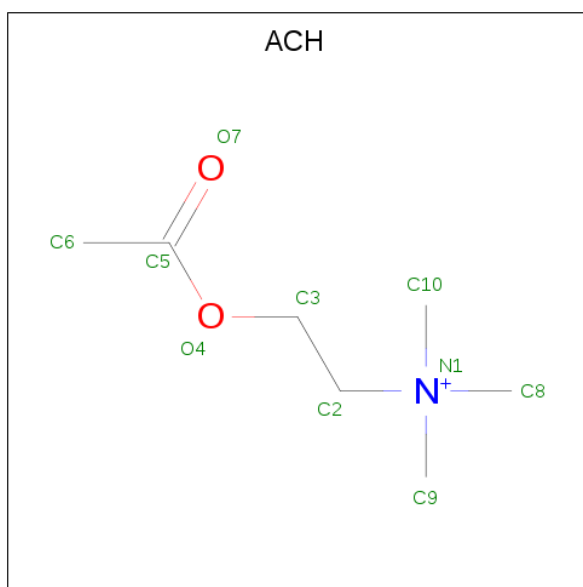
There are 7 unique types of molecules in this entry. The entry contains 17146 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylcholine-binding protein.

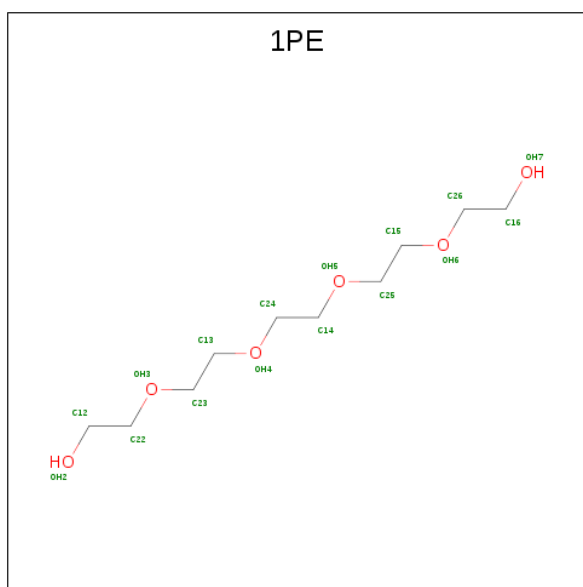
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	202	Total 1631	C 1022	N 282	O 321	S 6	0	3	0
1	B	208	Total 1683	C 1052	N 291	O 335	S 5	0	3	0
1	C	202	Total 1678	C 1048	N 294	O 331	S 5	0	8	0
1	D	202	Total 1653	C 1035	N 286	O 327	S 5	0	5	0
1	E	202	Total 1644	C 1036	N 280	O 321	S 7	0	5	0
1	F	206	Total 1648	C 1032	N 283	O 328	S 5	0	0	0
1	G	202	Total 1615	C 1012	N 276	O 322	S 5	0	0	0
1	H	198	Total 1587	C 998	N 272	O 312	S 5	0	1	0
1	I	200	Total 1611	C 1013	N 274	O 319	S 5	0	1	0
1	J	201	Total 1649	C 1039	N 283	O 321	S 6	0	5	0

- Molecule 2 is ACETYLCHOLINE (three-letter code: ACH) (formula: C₇H₁₆NO₂).



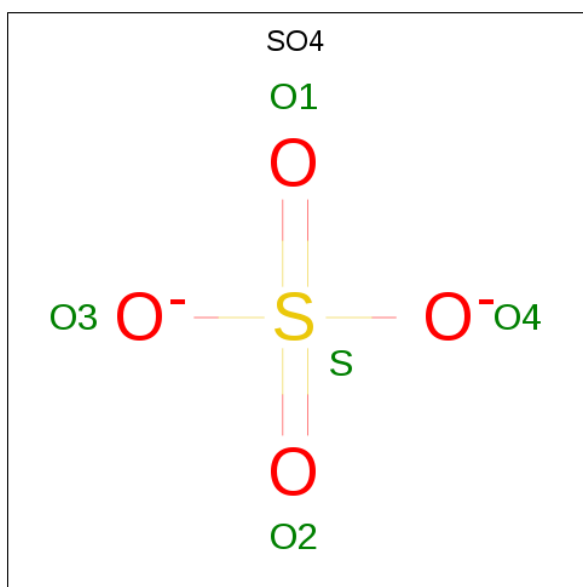
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 10	C 7	N 1	O 2	0	0
2	B	1	Total 10	C 7	N 1	O 2	0	0
2	C	1	Total 10	C 7	N 1	O 2	0	0
2	D	1	Total 10	C 7	N 1	O 2	0	0
2	E	1	Total 10	C 7	N 1	O 2	0	0
2	F	1	Total 10	C 7	N 1	O 2	0	0
2	G	1	Total 10	C 7	N 1	O 2	0	0
2	H	1	Total 10	C 7	N 1	O 2	0	0
2	I	1	Total 10	C 7	N 1	O 2	0	0
2	J	1	Total 10	C 7	N 1	O 2	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



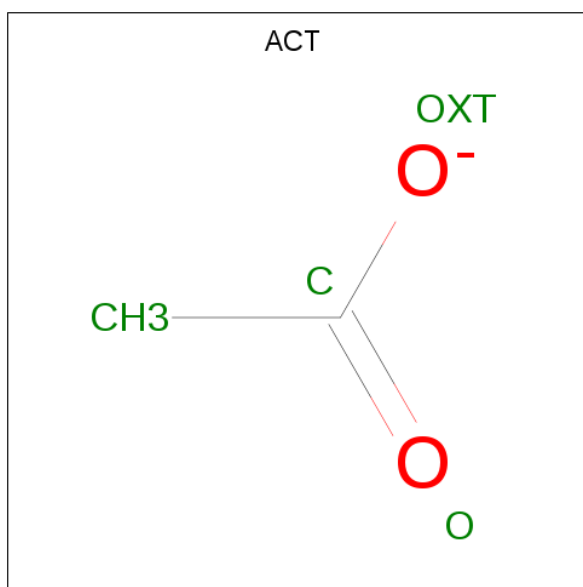
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 10 6	0	0
3	A	1	Total C O 16 10 6	0	0
3	A	1	Total C O 16 10 6	0	0
3	B	1	Total C O 16 10 6	0	0
3	B	1	Total C O 16 10 6	0	0
3	D	1	Total C O 16 10 6	0	0
3	D	1	Total C O 16 10 6	0	0
3	E	1	Total C O 16 10 6	0	0
3	G	1	Total C O 16 10 6	0	0
3	H	1	Total C O 11 7 4	0	0
3	I	1	Total C O 16 10 6	0	0
3	J	1	Total C O 16 10 6	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



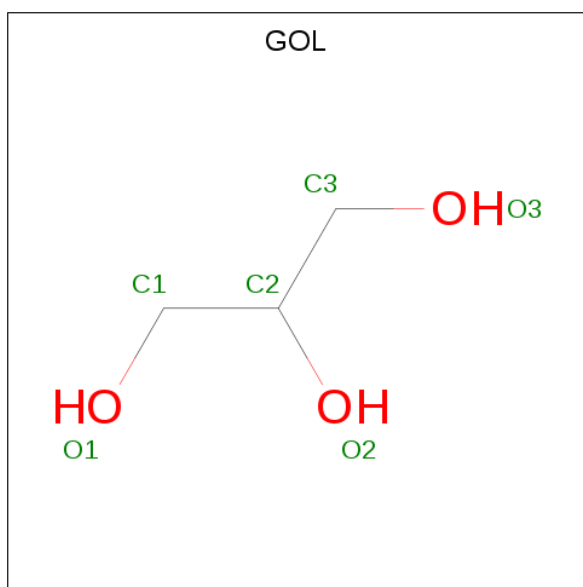
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			6	3	3		

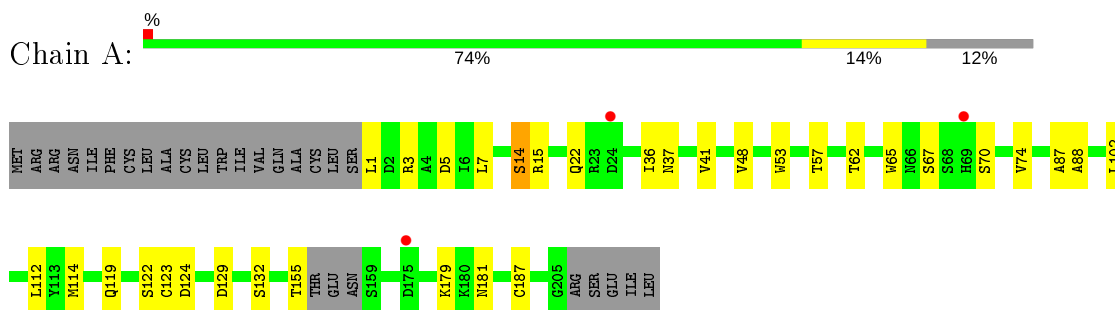
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	46	Total O 46 46	0	0
7	B	57	Total O 57 57	0	0
7	C	61	Total O 61 61	0	0
7	D	44	Total O 44 44	0	0
7	E	41	Total O 41 41	0	0
7	F	27	Total O 27 27	0	0
7	G	36	Total O 36 36	0	0
7	H	28	Total O 28 28	0	0
7	I	37	Total O 37 37	0	0
7	J	30	Total O 30 30	0	0

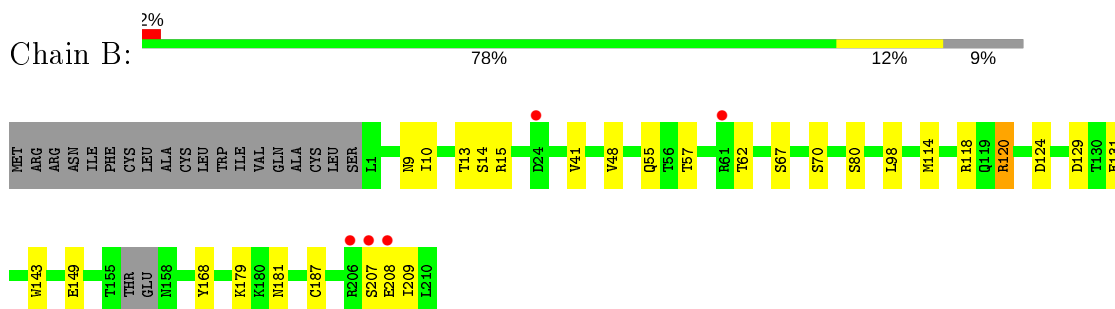
3 Residue-property plots [i](#)

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.

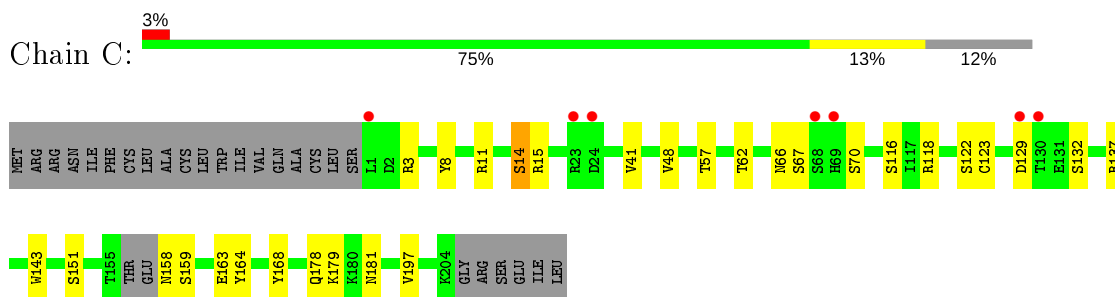
- Molecule 1: Acetylcholine-binding protein



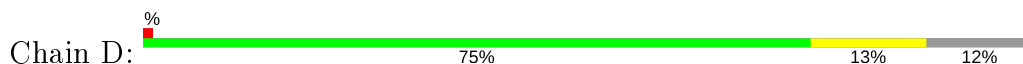
- Molecule 1: Acetylcholine-binding protein

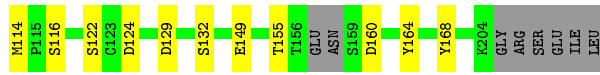
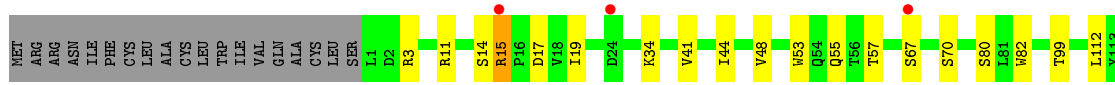


- Molecule 1: Acetylcholine-binding protein

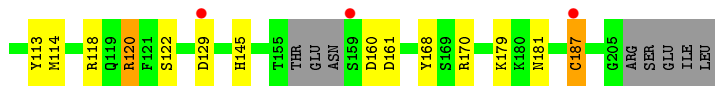
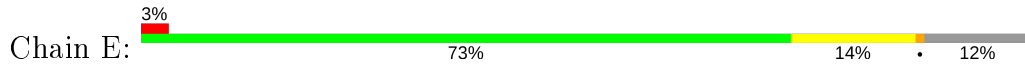


- Molecule 1: Acetylcholine-binding protein

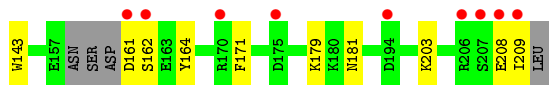
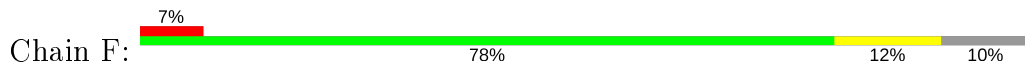




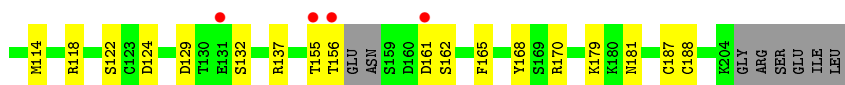
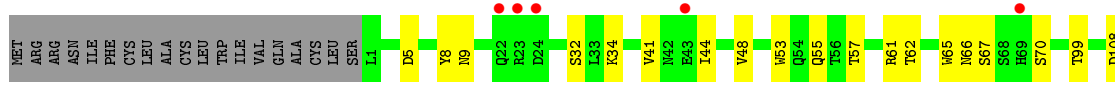
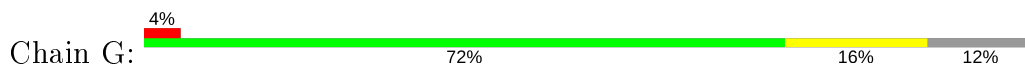
• Molecule 1: Acetylcholine-binding protein



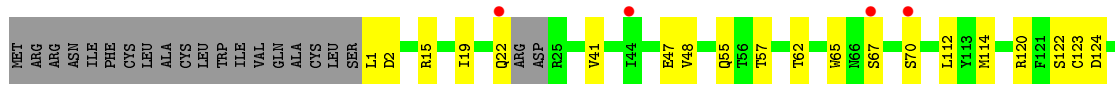
• Molecule 1: Acetylcholine-binding protein



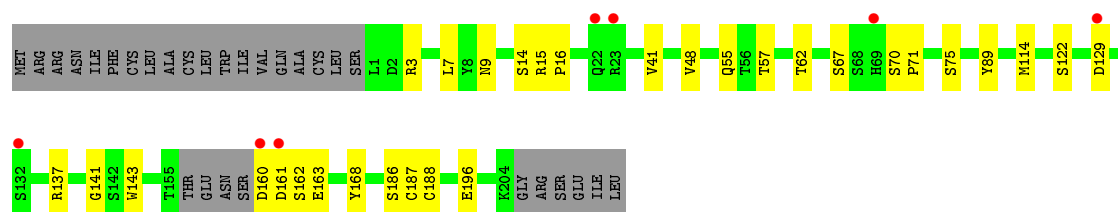
• Molecule 1: Acetylcholine-binding protein



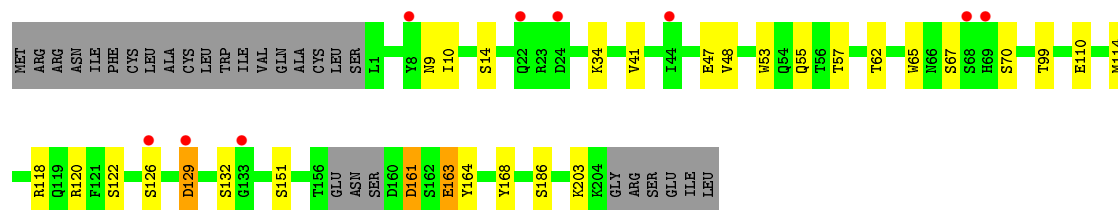
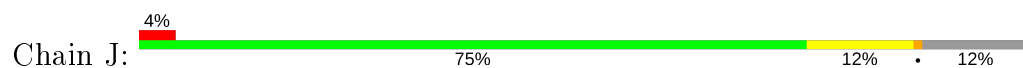
• Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	236.85Å 73.15Å 132.47Å 90.00° 101.45° 90.00°	Depositor
Resolution (Å)	46.17 – 2.60 47.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.17-2.60) 98.9 (47.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.179 , 0.239 0.180 , 0.237	Depositor DCC
R_{free} test set	3446 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtrriage
Anisotropy	0.232	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17146	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, GOL, ACH, SO4, 1PE

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	0.47	0/1675	0.61	0/2283
1	B	0.49	0/1721	0.62	2/2345 (0.1%)
1	C	0.49	0/1723	0.61	1/2348 (0.0%)
1	D	0.48	0/1694	0.63	0/2309
1	E	0.49	0/1696	0.60	2/2314 (0.1%)
1	F	0.45	0/1683	0.61	1/2294 (0.0%)
1	G	0.44	0/1650	0.56	0/2251
1	H	0.44	0/1624	0.60	0/2214
1	I	0.46	0/1650	0.59	0/2251
1	J	0.45	0/1698	0.57	0/2317
All	All	0.47	0/16814	0.60	6/22926 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	118	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	E	118	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	118	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	F	118	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	118	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	118	ARG	NE-CZ-NH2	-5.25	117.68	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1631	0	1592	34	0
1	B	1683	0	1637	19	0
1	C	1678	0	1634	19	0
1	D	1653	0	1618	22	0
1	E	1644	0	1609	28	0
1	F	1648	0	1600	16	0
1	G	1615	0	1565	24	0
1	H	1587	0	1547	25	0
1	I	1611	0	1562	24	0
1	J	1649	0	1615	20	0
2	A	10	0	16	0	0
2	B	10	0	16	0	0
2	C	10	0	16	0	0
2	D	10	0	16	1	0
2	E	10	0	16	0	0
2	F	10	0	16	0	0
2	G	10	0	16	1	0
2	H	10	0	16	1	0
2	I	10	0	16	0	0
2	J	10	0	16	0	0
3	A	48	0	66	19	0
3	B	32	0	44	10	0
3	D	32	0	44	8	0
3	E	16	0	22	15	0
3	G	16	0	22	9	0
3	H	11	0	13	10	0
3	I	16	0	22	4	0
3	J	16	0	22	6	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	1	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	J	5	0	0	0	0
5	B	4	0	3	0	0
5	G	8	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	6	0	8	2	0
7	A	46	0	0	3	0
7	B	57	0	0	1	0
7	C	61	0	0	4	0
7	D	44	0	0	1	0
7	E	41	0	0	0	0
7	F	27	0	0	0	0
7	G	36	0	0	2	0
7	H	28	0	0	2	0
7	I	37	0	0	2	0
7	J	30	0	0	2	0
All	All	17146	0	16411	217	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 (217) 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)
3:H:302:1PE:H161	1:I:75:SER:H	1.20	1.02
1:H:19:ILE:HG22	3:H:302:1PE:H261	1.50	0.93
1:H:145:HIS:HE1	3:H:302:1PE:H162	1.36	0.90
1:E:47:GLU:HB3	1:E:120:ARG:HH12	1.39	0.86
1:F:15:ARG:HH11	3:G:303:1PE:H232	1.42	0.85
1:I:9:ASN:HD22	3:I:302:1PE:H162	1.44	0.83
1:I:160:ASP:HB3	1:I:161:ASP:HA	1.62	0.81
1:A:88:ALA:H	3:A:304:1PE:H241	1.45	0.81
3:D:303:1PE:H162	1:E:101:GLN:H	1.46	0.80
1:D:82:TRP:HE1	3:D:303:1PE:H131	1.52	0.74
1:A:3[B]:ARG:NH1	3:E:303:1PE:OH7	2.21	0.74
1:D:19:ILE:HG22	3:D:303:1PE:H122	1.69	0.73
1:D:112:LEU:HD21	1:D:114:MET:HE3	1.71	0.72
1:C:66:ASN:ND2	7:C:458:HOH:O	2.22	0.71
3:A:302:1PE:H161	1:H:65:TRP:HB3	1.74	0.70
1:A:88:ALA:O	3:A:304:1PE:H222	1.92	0.69
1:C:143:TRP:HH2	3:D:304:1PE:H252	1.56	0.69
1:H:22:GLN:NE2	7:H:409:HOH:O	2.25	0.68
1:D:116:SER:OG	3:D:304:1PE:H262	1.95	0.67
1:B:13[A]:THR:O	1:B:13[A]:THR:OG1	2.11	0.67
1:F:171:PHE:CE2	1:F:203:LYS:HB2	2.31	0.66
1:E:82:TRP:HE1	3:E:303:1PE:H251	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:LEU:O	3:E:303:1PE:H122	1.96	0.65
1:D:15[B]:ARG:NH2	1:D:17:ASP:OD2	2.24	0.65
1:F:15:ARG:NH1	3:G:303:1PE:H232	2.11	0.65
1:D:55:GLN:HA	1:D:114:MET:HG2	1.79	0.64
1:D:3[B]:ARG:NH1	4:D:302:SO4:O2	2.29	0.64
1:H:145:HIS:CE1	3:H:302:1PE:H162	2.27	0.64
1:G:53:TRP:CE3	1:G:114:MET:HE2	2.32	0.64
1:D:34[A]:LYS:NZ	7:D:444:HOH:O	2.31	0.63
1:I:160:ASP:CB	1:I:161:ASP:HA	2.27	0.63
1:D:34[B]:LYS:NZ	1:D:160:ASP:O	2.31	0.63
1:A:65:TRP:HB3	3:A:302:1PE:H222	1.81	0.63
3:B:303:1PE:H162	1:C:116:SER:OG	1.99	0.62
1:C:143:TRP:CH2	3:D:304:1PE:H252	2.34	0.61
1:F:209:ILE:HG21	1:J:126:SER:HB3	1.81	0.61
1:G:8:TYR:CD2	3:G:303:1PE:H152	2.35	0.61
1:C:178[A]:GLN:HG2	1:C:197:VAL:HG22	1.82	0.60
1:E:14:SER:OG	1:E:80:SER:O	2.17	0.60
1:J:47:GLU:OE1	1:J:120[A]:ARG:NH1	2.33	0.60
1:D:149:GLU:OE2	1:E:3[A]:ARG:NH2	2.35	0.60
1:I:137:ARG:HD2	1:I:196:GLU:OE2	2.00	0.60
3:H:302:1PE:H161	1:I:75:SER:N	2.04	0.60
1:A:37:ASN:HB2	3:A:303:1PE:H122	1.84	0.59
1:A:53:TRP:HE1	1:A:114:MET:HB3	1.66	0.59
1:J:55:GLN:HG2	1:J:114[A]:MET:SD	2.42	0.59
1:D:164:TYR:HD1	3:D:304:1PE:H221	1.67	0.59
1:A:119:GLN:HE22	3:A:304:1PE:H131	1.68	0.59
1:I:9:ASN:HD22	3:I:302:1PE:C16	2.15	0.58
1:I:9:ASN:ND2	3:I:302:1PE:H162	2.16	0.58
1:A:14:SER:HA	7:A:444:HOH:O	2.04	0.58
3:A:303:1PE:H222	1:E:90:ASN:HA	1.86	0.58
1:E:19:ILE:H	3:E:303:1PE:H152	1.69	0.57
1:B:131:GLU:OE2	1:B:207:SER:HA	2.04	0.57
1:E:83:VAL:HB	3:E:303:1PE:H121	1.86	0.57
1:H:41:VAL:HG22	1:H:48:VAL:HG23	1.86	0.57
1:E:82:TRP:NE1	3:E:303:1PE:H251	2.20	0.57
1:F:41:VAL:HG22	1:F:48:VAL:HG23	1.87	0.57
1:I:55:GLN:HG2	1:I:114:MET:SD	2.44	0.57
1:A:88:ALA:N	3:A:304:1PE:H241	2.19	0.56
3:H:302:1PE:C16	1:I:75:SER:H	2.06	0.56
1:C:8:TYR:CD2	3:G:303:1PE:H221	2.40	0.56
1:I:14:SER:HA	7:I:435:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:HG13	3:A:303:1PE:H142	1.86	0.56
1:A:3[B]:ARG:NH1	3:E:303:1PE:HO7	2.04	0.56
1:B:149:GLU:OE2	1:C:3[A]:ARG:NH2	2.37	0.56
1:J:65:TRP:HB3	3:J:303:1PE:H162	1.87	0.56
1:E:160:ASP:OD1	1:E:161:ASP:N	2.38	0.56
1:F:53:TRP:HB3	1:F:114:MET:SD	2.46	0.55
1:B:143:TRP:HH2	3:B:303:1PE:H152	1.71	0.55
1:E:10:ILE:O	1:E:14:SER:HB3	2.06	0.55
1:A:1:LEU:HB2	1:A:70:SER:OG	2.07	0.55
1:A:41:VAL:HG22	1:A:48:VAL:HG23	1.87	0.55
2:G:301:ACH:H62	1:H:112:LEU:HD23	1.89	0.55
1:G:41:VAL:HG22	1:G:48:VAL:HG23	1.89	0.55
1:H:187:CYS:SG	1:H:188:CYS:N	2.80	0.54
1:D:124:ASP:HB2	1:E:168:TYR:CE1	2.42	0.54
1:F:208:GLU:N	1:F:208:GLU:OE1	2.28	0.54
1:D:41:VAL:HG22	1:D:48:VAL:HG23	1.90	0.54
1:B:41:VAL:HG22	1:B:48:VAL:HG23	1.90	0.54
1:A:87:ALA:HB1	3:A:304:1PE:H231	1.89	0.53
1:A:53:TRP:NE1	1:A:114:MET:HB3	2.23	0.53
1:E:47:GLU:HB3	1:E:120:ARG:NH1	2.18	0.53
1:G:32:SER:HB3	1:G:155:THR:HG22	1.91	0.53
1:J:65:TRP:HB3	3:J:303:1PE:C26	2.39	0.53
1:G:137:ARG:NH2	7:G:434:HOH:O	2.41	0.52
1:A:53:TRP:HE1	1:A:114:MET:CB	2.21	0.52
1:B:9:ASN:HB3	3:B:304:1PE:H132	1.92	0.52
1:C:41:VAL:HG22	1:C:48:VAL:HG23	1.91	0.52
1:J:161:ASP:N	1:J:161:ASP:OD1	2.42	0.52
1:F:14:SER:OG	1:F:80:SER:O	2.25	0.52
3:B:304:1PE:H161	1:G:65:TRP:CB	2.41	0.51
1:I:137:ARG:NH1	1:J:168:TYR:OH	2.42	0.51
1:J:9:ASN:HB3	3:J:303:1PE:H251	1.93	0.51
3:B:304:1PE:H161	1:G:65:TRP:HB2	1.92	0.51
1:E:41:VAL:HG22	1:E:48:VAL:HG23	1.93	0.51
1:J:41:VAL:HG22	1:J:48:VAL:HG23	1.93	0.51
3:A:303:1PE:H121	1:E:92:ILE:HG22	1.92	0.50
1:J:151:SER:HB3	7:J:415:HOH:O	2.12	0.50
1:E:82:TRP:HE1	3:E:303:1PE:H142	1.76	0.50
1:G:124:ASP:HB2	1:H:168:TYR:CE1	2.47	0.50
1:G:34:LYS:HD3	1:G:161:ASP:HA	1.93	0.49
1:I:67:SER:HA	1:I:70:SER:HB2	1.94	0.49
1:H:161:ASP:C	1:H:163:GLU:H	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13[B]:THR:HG21	3:B:304:1PE:H242	1.95	0.49
1:A:65:TRP:CB	3:A:302:1PE:H222	2.42	0.49
1:A:5:ASP:OD1	1:H:15[B]:ARG:NH2	2.46	0.49
1:B:14[B]:SER:OG	1:B:80:SER:O	2.29	0.49
1:G:8:TYR:CE2	3:G:303:1PE:H152	2.48	0.49
1:G:53:TRP:HE3	1:G:114:MET:HE2	1.76	0.49
1:D:67:SER:HA	1:D:70:SER:HB2	1.95	0.49
1:C:14[A]:SER:O	1:C:15[A]:ARG:HD2	2.13	0.48
1:E:145:HIS:HE1	3:E:303:1PE:H161	1.78	0.48
1:I:14:SER:O	1:I:15:ARG:HD2	2.13	0.48
1:H:19:ILE:CG2	3:H:302:1PE:H261	2.35	0.47
1:J:34:LYS:HB2	1:J:53[B]:TRP:HB3	1.96	0.47
1:A:7:LEU:HD11	3:E:303:1PE:H261	1.95	0.47
1:B:124:ASP:HB2	1:C:168:TYR:CE1	2.49	0.47
3:B:304:1PE:OH7	1:G:9:ASN:ND2	2.45	0.47
1:D:44:ILE:HG22	1:E:170:ARG:HD3	1.96	0.47
1:F:143:TRP:CZ2	1:G:99:THR:HG21	2.49	0.47
1:I:41:VAL:HG22	1:I:48:VAL:HG23	1.95	0.47
1:A:22:GLN:NE2	7:A:428:HOH:O	2.24	0.47
1:B:10:ILE:HG13	3:B:304:1PE:H222	1.96	0.47
1:D:15[B]:ARG:HH21	1:D:17:ASP:CG	2.13	0.47
1:G:67:SER:HA	1:G:70:SER:HB2	1.97	0.47
3:A:304:1PE:H132	1:B:98:LEU:O	2.15	0.47
1:B:15:ARG:CG	3:G:303:1PE:H151	2.45	0.47
1:H:67:SER:HA	1:H:70:SER:HB2	1.97	0.46
1:C:67:SER:HA	1:C:70:SER:HB2	1.98	0.46
3:B:304:1PE:H132	3:B:304:1PE:H221	1.48	0.46
1:A:102:LEU:HD21	3:E:303:1PE:H131	1.96	0.46
1:A:179:LYS:HE2	1:A:181:ASN:OD1	2.16	0.46
1:A:74:VAL:HB	3:E:303:1PE:H262	1.98	0.46
1:H:55:GLN:HG2	1:H:114:MET:SD	2.56	0.45
1:B:179:LYS:HE2	1:B:181:ASN:OD1	2.17	0.45
1:F:208:GLU:HB2	1:F:209:ILE:HA	1.97	0.45
1:J:65:TRP:HB3	3:J:303:1PE:C16	2.46	0.45
1:G:66:ASN:HD21	6:G:304:GOL:C2	2.29	0.45
1:H:124:ASP:HB2	1:I:168:TYR:CE1	2.51	0.45
1:J:67:SER:HA	1:J:70:SER:HB2	1.98	0.45
1:E:145:HIS:HE1	3:E:303:1PE:C16	2.30	0.45
1:I:160:ASP:CG	1:I:162:SER:H	2.19	0.45
3:I:302:1PE:H232	3:I:302:1PE:H241	1.42	0.45
1:A:123:CYS:HB2	7:A:427:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:HB2	1:B:168:TYR:CE1	2.51	0.45
1:H:55:GLN:HA	1:H:114:MET:HG3	1.99	0.45
1:F:164:TYR:OH	1:J:186:SER:HB2	2.17	0.45
1:G:66:ASN:ND2	6:G:304:GOL:O2	2.50	0.45
1:C:151:SER:HB3	7:C:425:HOH:O	2.16	0.45
1:J:129:ASP:OD1	1:J:203:LYS:HD3	2.17	0.44
1:F:15:ARG:CG	3:G:303:1PE:H222	2.47	0.44
1:E:67:SER:HA	1:E:70:SER:HB2	1.99	0.44
1:G:44:ILE:HG22	1:H:170:ARG:HD3	2.00	0.44
1:F:67:SER:HA	1:F:70:SER:HB2	2.00	0.44
1:H:145:HIS:CE1	3:H:302:1PE:H151	2.52	0.44
1:H:123:CYS:HB2	7:H:424:HOH:O	2.17	0.44
1:I:143:TRP:CZ2	1:J:99:THR:HG21	2.52	0.44
1:B:120[B]:ARG:NH2	7:B:413:HOH:O	2.51	0.44
1:H:202:ARG:HG3	1:H:203:LYS:O	2.18	0.43
1:D:11:ARG:O	1:D:14[A]:SER:HB2	2.17	0.43
1:E:179:LYS:HE2	1:E:181:ASN:OD1	2.18	0.43
1:C:143:TRP:CZ2	1:D:99:THR:HG21	2.54	0.43
1:J:110:GLU:OE2	7:J:429:HOH:O	2.21	0.43
1:A:112:LEU:HD11	1:A:114:MET:HE3	2.00	0.43
1:F:179:LYS:HE2	1:F:181:ASN:OD1	2.19	0.43
1:H:185:TYR:CD2	2:H:301:ACH:H82	2.54	0.43
3:H:302:1PE:H262	1:I:7:LEU:HD11	1.99	0.43
1:C:123:CYS:HB2	7:C:404:HOH:O	2.17	0.43
1:I:163:GLU:HG2	1:I:163:GLU:H	1.69	0.43
1:J:65:TRP:CB	3:J:303:1PE:H162	2.49	0.43
3:A:302:1PE:C16	1:H:65:TRP:HB3	2.44	0.42
1:A:3[A]:ARG:HD3	3:E:303:1PE:OH7	2.19	0.42
1:C:158:ASN:HB3	1:C:159:SER:H	1.62	0.42
1:A:67:SER:HA	1:A:70:SER:HB2	2.01	0.42
1:E:113:TYR:C	1:E:114[B]:MET:HG2	2.39	0.42
1:C:11:ARG:O	1:C:14[A]:SER:HB2	2.19	0.42
1:C:179:LYS:HE2	1:C:181:ASN:OD1	2.19	0.42
2:D:301:ACH:H83	1:E:53[B]:TRP:CH2	2.54	0.42
1:B:67:SER:HA	1:B:70:SER:HB2	2.01	0.42
1:A:7:LEU:HD11	3:E:303:1PE:C26	2.50	0.42
3:A:303:1PE:H121	1:E:92:ILE:CG2	2.49	0.42
1:G:170:ARG:NH2	5:G:305:ACT:H2	2.35	0.42
1:G:55:GLN:HG2	1:G:114:MET:HG3	2.02	0.42
1:H:55:GLN:HG2	1:H:114:MET:HG3	2.01	0.42
1:H:19:ILE:HB	3:H:302:1PE:H152	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLN:HE22	3:A:304:1PE:H242	1.84	0.42
1:B:15:ARG:HG2	3:G:303:1PE:H151	2.02	0.41
1:A:112:LEU:HD11	1:A:114:MET:CE	2.50	0.41
7:C:406:HOH:O	3:D:304:1PE:H261	2.19	0.41
1:E:55:GLN:HG2	1:E:114[A]:MET:HG3	2.01	0.41
1:I:14:SER:HB3	1:I:16:PRO:HD3	2.02	0.41
1:J:10:ILE:O	1:J:14:SER:HB2	2.19	0.41
1:C:137:ARG:NH1	1:D:168:TYR:OH	2.52	0.41
1:A:37:ASN:HD22	3:A:303:1PE:C12	2.34	0.41
1:I:188:CYS:HB3	7:I:418:HOH:O	2.21	0.41
1:J:163:GLU:HG2	1:J:164:TYR:CZ	2.55	0.41
1:B:55:GLN:HG2	1:B:114:MET:SD	2.61	0.41
1:D:53:TRP:NE1	1:D:114:MET:HB3	2.36	0.41
1:C:163:GLU:HG2	1:C:164:TYR:CE2	2.56	0.41
1:I:89[A]:TYR:OH	1:I:141:GLY:HA3	2.21	0.41
1:G:165:PHE:O	7:G:430:HOH:O	2.22	0.41
1:G:5:ASP:OD1	3:G:303:1PE:H251	2.21	0.41
1:D:34[A]:LYS:HB2	1:D:53:TRP:HB3	2.03	0.41
3:A:303:1PE:H232	1:E:89:TYR:O	2.21	0.41
1:D:14[B]:SER:OG	1:D:80:SER:O	2.27	0.41
1:G:179:LYS:HE2	1:G:181:ASN:OD1	2.21	0.41
1:A:88:ALA:O	3:A:304:1PE:H232	2.21	0.40
1:I:3:ARG:HG3	1:I:71:PRO:HG2	2.03	0.40
1:A:14:SER:O	1:A:15:ARG:HD2	2.21	0.40
1:F:137:ARG:NH1	1:G:168:TYR:OH	2.52	0.40
3:J:303:1PE:H232	3:J:303:1PE:H241	1.31	0.40
1:G:61:ARG:NH1	1:G:108:ASP:O	2.55	0.40
1:B:9:ASN:HB3	3:B:304:1PE:H221	2.03	0.40
1:F:55:GLN:HG2	1:F:114:MET:CG	2.52	0.40
1:H:47:GLU:OE1	1:H:120:ARG:NH1	2.55	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	201/229 (88%)	200 (100%)	1 (0%)	0	100	100
1	B	207/229 (90%)	205 (99%)	2 (1%)	0	100	100
1	C	206/229 (90%)	201 (98%)	5 (2%)	0	100	100
1	D	203/229 (89%)	201 (99%)	0	2 (1%)	15	32
1	E	203/229 (89%)	201 (99%)	2 (1%)	0	100	100
1	F	202/229 (88%)	198 (98%)	4 (2%)	0	100	100
1	G	198/229 (86%)	197 (100%)	1 (0%)	0	100	100
1	H	193/229 (84%)	190 (98%)	2 (1%)	1 (0%)	29	52
1	I	197/229 (86%)	195 (99%)	2 (1%)	0	100	100
1	J	202/229 (88%)	199 (98%)	3 (2%)	0	100	100
All	All	2012/2290 (88%)	1987 (99%)	22 (1%)	3 (0%)	51	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	162	SER
1	D	15[A]	ARG
1	D	15[B]	ARG

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	191/213 (90%)	183 (96%)	8 (4%)	30	55
1	B	197/213 (92%)	189 (96%)	8 (4%)	30	56
1	C	197/213 (92%)	190 (96%)	7 (4%)	35	61
1	D	194/213 (91%)	189 (97%)	5 (3%)	46	72
1	E	193/213 (91%)	188 (97%)	5 (3%)	46	72
1	F	192/213 (90%)	185 (96%)	7 (4%)	35	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	189/213 (89%)	179 (95%)	10 (5%)	22	45
1	H	185/213 (87%)	178 (96%)	7 (4%)	33	59
1	I	188/213 (88%)	182 (97%)	6 (3%)	39	65
1	J	193/213 (91%)	185 (96%)	8 (4%)	30	56
All	All	1919/2130 (90%)	1848 (96%)	71 (4%)	34	60

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	57	THR
1	A	62	THR
1	A	122	SER
1	A	129	ASP
1	A	132	SER
1	A	155	THR
1	A	187	CYS
1	B	57	THR
1	B	62	THR
1	B	120[A]	ARG
1	B	120[B]	ARG
1	B	129	ASP
1	B	187	CYS
1	B	208	GLU
1	B	209	ILE
1	C	14[A]	SER
1	C	14[B]	SER
1	C	57	THR
1	C	62	THR
1	C	122	SER
1	C	129	ASP
1	C	132	SER
1	D	57	THR
1	D	122	SER
1	D	129	ASP
1	D	132	SER
1	D	155	THR
1	E	57	THR
1	E	120	ARG
1	E	122	SER
1	E	129	ASP

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Mol	Chain	Res	Type
1	E	187	CYS
1	F	57	THR
1	F	62	THR
1	F	122	SER
1	F	129	ASP
1	F	132	SER
1	F	161	ASP
1	F	162	SER
1	G	57	THR
1	G	62	THR
1	G	118	ARG
1	G	122	SER
1	G	129	ASP
1	G	132	SER
1	G	156	THR
1	G	162	SER
1	G	187	CYS
1	G	188	CYS
1	H	1	LEU
1	H	2	ASP
1	H	57	THR
1	H	62	THR
1	H	122	SER
1	H	129	ASP
1	H	188	CYS
1	I	57	THR
1	I	62	THR
1	I	122	SER
1	I	129	ASP
1	I	186	SER
1	I	187	CYS
1	J	57	THR
1	J	62	THR
1	J	118	ARG
1	J	122	SER
1	J	129	ASP
1	J	132	SER
1	J	161	ASP
1	J	163	GLU

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

Mol	Chain	Res	Type
1	A	9	ASN
1	G	9	ASN
1	I	9	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](#)

33 ligands are modelled in this entry.

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
3	1PE	D	303	-	15,15,15	0.92	0	14,14,14	1.54	1 (7%)
2	ACH	A	301	-	9,9,9	1.17	0	12,12,12	1.64	4 (33%)
4	SO4	F	302	-	4,4,4	0.17	0	6,6,6	0.14	0
3	1PE	E	303	-	15,15,15	0.92	0	14,14,14	1.24	3 (21%)
2	ACH	H	301	-	9,9,9	1.16	0	12,12,12	1.50	2 (16%)
4	SO4	D	302	-	4,4,4	0.67	0	6,6,6	0.84	0
4	SO4	J	302	-	4,4,4	0.17	0	6,6,6	0.18	0
2	ACH	B	301	-	9,9,9	1.19	0	12,12,12	1.64	4 (33%)
3	1PE	G	303	-	15,15,15	0.70	0	14,14,14	1.54	2 (14%)
3	1PE	A	303	-	15,15,15	0.93	0	14,14,14	1.14	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	302	-	4,4,4	0.29	0	6,6,6	0.19	0
3	1PE	B	304	-	15,15,15	0.74	0	14,14,14	1.19	1 (7%)
2	ACH	G	301	-	9,9,9	1.20	0	12,12,12	1.43	2 (16%)
3	1PE	H	302	-	10,10,15	0.77	0	9,9,14	0.82	0
3	1PE	B	303	-	15,15,15	0.87	0	14,14,14	0.95	0
4	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.25	0
4	SO4	G	302	-	4,4,4	0.13	0	6,6,6	0.13	0
4	SO4	E	302	-	4,4,4	0.17	0	6,6,6	0.25	0
2	ACH	F	301	-	9,9,9	1.14	0	12,12,12	1.56	3 (25%)
3	1PE	A	304	-	15,15,15	1.30	0	14,14,14	2.14	7 (50%)
3	1PE	J	303	-	15,15,15	0.76	0	14,14,14	2.06	4 (28%)
5	ACT	G	305	-	1,3,3	1.96	0	0,3,3	0.00	-
2	ACH	E	301	-	9,9,9	1.25	0	12,12,12	1.46	2 (16%)
5	ACT	G	306	-	1,3,3	1.90	0	0,3,3	0.00	-
2	ACH	C	301	-	9,9,9	1.29	0	12,12,12	1.47	2 (16%)
6	GOL	G	304	-	5,5,5	0.29	0	5,5,5	0.21	0
3	1PE	A	302	-	15,15,15	0.85	0	14,14,14	1.76	3 (21%)
2	ACH	D	301	-	9,9,9	1.14	0	12,12,12	1.49	1 (8%)
5	ACT	B	305	-	1,3,3	1.75	0	0,3,3	0.00	-
3	1PE	D	304	-	15,15,15	0.76	0	14,14,14	1.97	4 (28%)
3	1PE	I	302	-	15,15,15	0.85	0	14,14,14	1.94	6 (42%)
2	ACH	J	301	-	9,9,9	1.20	0	12,12,12	1.39	3 (25%)
2	ACH	I	301	-	9,9,9	1.34	0	12,12,12	1.51	3 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	D	303	-	-	2/13/13/13	-
2	ACH	A	301	-	-	3/7/7/7	-
2	ACH	H	301	-	-	3/7/7/7	-
3	1PE	E	303	-	-	4/13/13/13	-
2	ACH	B	301	-	-	4/7/7/7	-
3	1PE	G	303	-	-	4/13/13/13	-
3	1PE	A	303	-	-	7/13/13/13	-
3	1PE	B	304	-	-	2/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACH	G	301	-	-	4/7/7/7	-
3	1PE	H	302	-	-	4/8/8/13	-
3	1PE	B	303	-	-	6/13/13/13	-
6	GOL	G	304	-	-	2/4/4/4	-
2	ACH	F	301	-	-	3/7/7/7	-
3	1PE	A	304	-	-	4/13/13/13	-
3	1PE	J	303	-	-	6/13/13/13	-
2	ACH	E	301	-	-	3/7/7/7	-
2	ACH	C	301	-	-	3/7/7/7	-
3	1PE	A	302	-	-	3/13/13/13	-
2	ACH	D	301	-	-	3/7/7/7	-
3	1PE	D	304	-	-	4/13/13/13	-
3	1PE	I	302	-	-	4/13/13/13	-
2	ACH	J	301	-	-	4/7/7/7	-
2	ACH	I	301	-	-	3/7/7/7	-

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	303	1PE	OH5-C14-C24	5.20	133.82	110.39
3	J	303	1PE	OH5-C14-C24	4.29	129.76	110.39
3	A	302	1PE	OH3-C22-C12	4.11	128.13	110.07
3	I	302	1PE	OH6-C15-C25	4.05	128.67	110.39
3	D	304	1PE	C25-OH5-C14	-3.98	96.05	113.29
3	J	303	1PE	OH3-C23-C13	3.93	128.10	110.39
3	A	304	1PE	OH4-C24-C14	3.87	127.82	110.39
3	G	303	1PE	OH4-C24-C14	3.61	126.67	110.39
3	A	302	1PE	OH5-C14-C24	3.61	126.66	110.39
3	D	304	1PE	OH5-C14-C24	3.49	126.15	110.39
3	I	302	1PE	OH3-C22-C12	-3.49	94.75	110.07
3	A	304	1PE	OH5-C14-C24	3.48	126.09	110.39
3	G	303	1PE	C24-OH4-C13	-3.24	99.23	113.29
3	A	304	1PE	OH5-C25-C15	3.17	124.70	110.39
2	B	301	ACH	O4-C3-C2	2.76	118.78	109.14
3	J	303	1PE	OH4-C13-C23	-2.74	98.04	110.39
3	A	304	1PE	OH4-C13-C23	2.67	122.41	110.39
3	E	303	1PE	C23-OH3-C22	-2.66	101.74	113.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	304	1PE	OH3-C22-C12	2.64	121.64	110.07
3	J	303	1PE	OH6-C26-C16	2.61	121.53	110.07
3	D	304	1PE	C23-OH3-C22	-2.59	102.08	113.29
2	D	301	ACH	O4-C3-C2	2.58	118.13	109.14
2	A	301	ACH	C9-N1-C8	-2.57	102.36	108.97
2	A	301	ACH	O4-C3-C2	2.56	118.07	109.14
3	A	304	1PE	C25-OH5-C14	2.54	124.29	113.29
3	I	302	1PE	OH4-C13-C23	-2.53	98.97	110.39
2	H	301	ACH	O4-C3-C2	2.48	117.79	109.14
3	A	302	1PE	OH6-C15-C25	-2.48	99.23	110.39
2	F	301	ACH	C10-N1-C9	-2.46	102.64	108.97
2	B	301	ACH	C9-N1-C8	-2.45	102.67	108.97
3	B	304	1PE	C23-OH3-C22	-2.45	102.66	113.29
2	H	301	ACH	C9-N1-C8	-2.44	102.71	108.97
3	E	303	1PE	OH4-C13-C23	-2.42	99.47	110.39
2	G	301	ACH	O4-C3-C2	2.42	117.56	109.14
3	E	303	1PE	C24-OH4-C13	-2.39	102.94	113.29
2	E	301	ACH	O4-C3-C2	2.35	117.34	109.14
3	A	304	1PE	OH6-C15-C25	2.33	120.90	110.39
2	C	301	ACH	O4-C3-C2	2.27	117.07	109.14
2	B	301	ACH	C10-N1-C9	-2.27	103.13	108.97
2	C	301	ACH	C10-N1-C9	-2.26	103.16	108.97
2	F	301	ACH	O4-C3-C2	2.23	116.92	109.14
2	I	301	ACH	C10-N1-C9	-2.21	103.30	108.97
3	I	302	1PE	OH5-C25-C15	2.19	120.26	110.39
3	I	302	1PE	C24-OH4-C13	-2.17	103.88	113.29
3	I	302	1PE	OH3-C23-C13	2.13	119.98	110.39
3	A	304	1PE	OH6-C26-C16	2.10	119.29	110.07
2	I	301	ACH	O4-C3-C2	2.09	116.44	109.14
2	J	301	ACH	O4-C3-C2	2.09	116.43	109.14
2	I	301	ACH	O4-C5-C6	2.08	121.44	112.38
2	G	301	ACH	O4-C5-C6	2.08	121.44	112.38
2	A	301	ACH	C10-N1-C9	-2.08	103.64	108.97
2	J	301	ACH	C10-N1-C9	-2.07	103.65	108.97
2	A	301	ACH	C10-N1-C8	2.05	114.24	108.97
3	A	303	1PE	OH4-C24-C14	2.03	119.57	110.39
2	F	301	ACH	O4-C5-C6	2.03	121.25	112.38
3	A	303	1PE	C23-OH3-C22	-2.03	104.50	113.29
2	E	301	ACH	O4-C5-C6	2.02	121.20	112.38
2	B	301	ACH	O4-C5-C6	2.02	121.20	112.38
2	J	301	ACH	O4-C5-C6	2.01	121.13	112.38

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	304	GOL	C1-C2-C3-O3
3	D	304	1PE	C15-C25-OH5-C14
3	A	302	1PE	C12-C22-OH3-C23
3	J	303	1PE	C24-C14-OH5-C25
6	G	304	GOL	O2-C2-C3-O3
3	J	303	1PE	C25-C15-OH6-C26
3	G	303	1PE	C23-C13-OH4-C24
3	I	302	1PE	C13-C23-OH3-C22
3	A	303	1PE	C24-C14-OH5-C25
3	A	303	1PE	C14-C24-OH4-C13
3	H	302	1PE	C14-C24-OH4-C13
3	G	303	1PE	C25-C15-OH6-C26
3	J	303	1PE	C23-C13-OH4-C24
3	J	303	1PE	C12-C22-OH3-C23
3	H	302	1PE	C16-C26-OH6-C15
3	A	302	1PE	C16-C26-OH6-C15
2	D	301	ACH	C3-C2-N1-C10
2	I	301	ACH	C3-C2-N1-C10
3	A	302	1PE	C24-C14-OH5-C25
3	I	302	1PE	C15-C25-OH5-C14
3	A	303	1PE	C23-C13-OH4-C24
3	A	304	1PE	C16-C26-OH6-C15
2	A	301	ACH	C3-C2-N1-C10
2	H	301	ACH	C3-C2-N1-C9
2	H	301	ACH	C3-C2-N1-C10
2	G	301	ACH	C3-C2-N1-C10
2	B	301	ACH	C3-C2-N1-C10
2	F	301	ACH	C3-C2-N1-C10
2	C	301	ACH	C3-C2-N1-C10
2	D	301	ACH	C3-C2-N1-C9
3	B	303	1PE	C23-C13-OH4-C24
2	A	301	ACH	C3-C2-N1-C9
2	B	301	ACH	C3-C2-N1-C9
2	G	301	ACH	C3-C2-N1-C9
2	F	301	ACH	C3-C2-N1-C9
2	C	301	ACH	C3-C2-N1-C9
2	J	301	ACH	C3-C2-N1-C10
2	I	301	ACH	C3-C2-N1-C9
3	B	303	1PE	C24-C14-OH5-C25
3	E	303	1PE	C24-C14-OH5-C25
3	B	303	1PE	C25-C15-OH6-C26
2	J	301	ACH	C3-C2-N1-C9

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Mol	Chain	Res	Type	Atoms
2	B	301	ACH	N1-C2-C3-O4
2	F	301	ACH	N1-C2-C3-O4
2	E	301	ACH	C3-C2-N1-C10
3	A	303	1PE	C25-C15-OH6-C26
2	E	301	ACH	C3-C2-N1-C9
3	B	303	1PE	C13-C23-OH3-C22
3	E	303	1PE	C16-C26-OH6-C15
3	E	303	1PE	C23-C13-OH4-C24
3	B	303	1PE	OH5-C14-C24-OH4
3	A	303	1PE	OH6-C15-C25-OH5
3	B	304	1PE	OH5-C14-C24-OH4
3	A	303	1PE	OH4-C13-C23-OH3
3	H	302	1PE	OH6-C15-C25-OH5
2	J	301	ACH	N1-C2-C3-O4
2	E	301	ACH	C2-C3-O4-C5
3	B	303	1PE	OH6-C15-C25-OH5
2	I	301	ACH	C3-C2-N1-C8
3	E	303	1PE	OH5-C14-C24-OH4
3	G	303	1PE	OH6-C15-C25-OH5
3	H	302	1PE	OH5-C14-C24-OH4
3	A	304	1PE	OH4-C13-C23-OH3
3	J	303	1PE	OH4-C13-C23-OH3
3	D	303	1PE	OH4-C13-C23-OH3
3	D	303	1PE	OH6-C15-C25-OH5
2	B	301	ACH	C2-C3-O4-C5
3	G	303	1PE	OH4-C13-C23-OH3
3	B	304	1PE	OH4-C13-C23-OH3
3	J	303	1PE	OH6-C15-C25-OH5
3	A	304	1PE	C15-C25-OH5-C14
3	A	304	1PE	C24-C14-OH5-C25
3	D	304	1PE	OH6-C15-C25-OH5
3	I	302	1PE	OH4-C13-C23-OH3
3	D	304	1PE	OH5-C14-C24-OH4
3	I	302	1PE	C25-C15-OH6-C26
2	A	301	ACH	N1-C2-C3-O4
2	G	301	ACH	N1-C2-C3-O4
2	C	301	ACH	N1-C2-C3-O4
2	G	301	ACH	C3-C2-N1-C8
2	D	301	ACH	C3-C2-N1-C8
3	A	303	1PE	OH5-C14-C24-OH4
3	D	304	1PE	OH4-C13-C23-OH3
2	J	301	ACH	C2-C3-O4-C5

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Mol	Chain	Res	Type	Atoms
2	H	301	ACH	C3-C2-N1-C8

There are no ring outliers.

18 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	303	1PE	3	0
3	E	303	1PE	15	0
2	H	301	ACH	1	0
4	D	302	SO4	1	0
3	G	303	1PE	9	0
3	A	303	1PE	7	0
3	B	304	1PE	8	0
2	G	301	ACH	1	0
3	H	302	1PE	10	0
3	B	303	1PE	2	0
3	A	304	1PE	8	0
3	J	303	1PE	6	0
5	G	305	ACT	1	0
6	G	304	GOL	2	0
3	A	302	1PE	4	0
2	D	301	ACH	1	0
3	D	304	1PE	5	0
3	I	302	1PE	4	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	202/229 (88%)	0.01	3 (1%) 73 70	14, 28, 50, 80	0
1	B	208/229 (90%)	0.10	5 (2%) 59 53	14, 28, 59, 78	0
1	C	202/229 (88%)	-0.01	7 (3%) 44 36	12, 25, 49, 82	0
1	D	202/229 (88%)	0.01	3 (1%) 73 70	12, 26, 53, 73	0
1	E	202/229 (88%)	0.04	7 (3%) 44 36	13, 26, 52, 67	0
1	F	206/229 (89%)	0.24	15 (7%) 15 11	16, 35, 62, 85	0
1	G	202/229 (88%)	0.18	9 (4%) 33 26	17, 34, 62, 89	0
1	H	198/229 (86%)	0.18	6 (3%) 50 43	18, 34, 59, 74	0
1	I	200/229 (87%)	0.12	7 (3%) 44 36	14, 30, 59, 86	0
1	J	201/229 (87%)	0.20	9 (4%) 33 26	13, 32, 60, 76	0
All	All	2023/2290 (88%)	0.11	71 (3%) 44 36	12, 30, 59, 89	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	161	ASP	5.1
1	D	24	ASP	4.7
1	G	23	ARG	4.2
1	B	207	SER	4.1
1	C	24	ASP	4.1
1	F	208	GLU	3.8
1	I	161	ASP	3.7
1	F	131	GLU	3.6
1	A	24	ASP	3.5
1	D	67	SER	3.5
1	H	22	GLN	3.4
1	G	24	ASP	3.4
1	H	70	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	24	ASP	3.3
1	F	162	SER	3.2
1	E	129	ASP	3.2
1	B	208	GLU	3.1
1	G	69	HIS	3.1
1	I	69	HIS	3.0
1	J	69	HIS	2.9
1	I	22	GLN	2.9
1	G	156	THR	2.9
1	H	129	ASP	2.9
1	J	44	ILE	2.9
1	B	24	ASP	2.9
1	J	129	ASP	2.8
1	A	69	HIS	2.8
1	C	23	ARG	2.8
1	F	132	SER	2.7
1	F	209	ILE	2.7
1	I	129	ASP	2.7
1	C	129	ASP	2.7
1	E	159	SER	2.7
1	G	22	GLN	2.6
1	G	131	GLU	2.6
1	H	128	VAL	2.6
1	F	23	ARG	2.6
1	C	130	THR	2.6
1	J	22	GLN	2.6
1	J	126	SER	2.6
1	F	161	ASP	2.6
1	E	44	ILE	2.5
1	F	44	ILE	2.5
1	H	67	SER	2.5
1	A	175	ASP	2.5
1	J	68	SER	2.5
1	C	69[A]	HIS	2.5
1	G	43	GLU	2.4
1	C	1	LEU	2.4
1	E	69	HIS	2.4
1	G	155	THR	2.4
1	E	187	CYS	2.4
1	I	132	SER	2.3
1	J	8	TYR	2.3
1	B	61	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	24	ASP	2.3
1	F	175	ASP	2.3
1	F	207	SER	2.2
1	H	44	ILE	2.2
1	D	15[A]	ARG	2.2
1	F	194	ASP	2.1
1	B	206	ARG	2.1
1	F	128	VAL	2.1
1	J	133	GLY	2.1
1	I	160	ASP	2.1
1	C	68[A]	SER	2.1
1	E	2	ASP	2.1
1	I	23	ARG	2.0
1	F	130	THR	2.0
1	F	170	ARG	2.0
1	F	206	ARG	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, 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(Å ²)	Q<0.9
4	SO4	J	302	5/5	0.68	0.52	56,88,107,109	0
6	GOL	G	304	6/6	0.69	0.24	49,66,72,72	0
4	SO4	B	302	5/5	0.82	0.55	42,69,85,100	0
4	SO4	E	302	5/5	0.82	0.27	38,64,72,92	0
3	1PE	D	303	16/16	0.82	0.31	18,40,55,69	0
3	1PE	E	303	16/16	0.83	0.39	19,39,58,64	0
5	ACT	G	306	4/4	0.83	0.19	25,43,57,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	G	302	5/5	0.83	0.41	65,67,96,96	0
3	1PE	A	303	16/16	0.84	0.32	25,40,50,54	0
3	1PE	I	302	16/16	0.84	0.26	32,44,58,59	0
4	SO4	D	302	5/5	0.85	0.48	48,55,84,100	0
3	1PE	A	302	16/16	0.85	0.28	33,45,61,68	0
3	1PE	H	302	11/16	0.85	0.33	18,35,41,42	0
2	ACH	J	301	10/10	0.85	0.24	15,25,43,44	0
5	ACT	G	305	4/4	0.87	0.19	30,57,58,65	0
2	ACH	B	301	10/10	0.87	0.28	9,25,33,35	0
3	1PE	J	303	16/16	0.87	0.27	27,44,53,60	0
3	1PE	D	304	16/16	0.88	0.30	17,42,51,54	0
2	ACH	F	301	10/10	0.88	0.27	18,26,38,47	0
3	1PE	G	303	16/16	0.88	0.37	42,52,59,61	0
4	SO4	F	302	5/5	0.89	0.43	64,67,71,75	0
5	ACT	B	305	4/4	0.89	0.15	33,34,35,38	0
2	ACH	H	301	10/10	0.89	0.24	15,25,33,39	0
2	ACH	A	301	10/10	0.89	0.25	12,25,33,36	0
3	1PE	B	303	16/16	0.89	0.19	24,42,53,53	0
3	1PE	B	304	16/16	0.90	0.28	27,38,49,51	0
2	ACH	D	301	10/10	0.90	0.23	7,18,29,30	0
2	ACH	E	301	10/10	0.91	0.23	11,23,36,38	0
2	ACH	G	301	10/10	0.91	0.21	11,29,34,41	0
3	1PE	A	304	16/16	0.91	0.22	27,40,50,56	0
2	ACH	I	301	10/10	0.91	0.22	8,20,30,32	0
4	SO4	C	302	5/5	0.94	0.31	53,55,63,90	0
2	ACH	C	301	10/10	0.94	0.22	9,24,31,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.