



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2021 – 10:04 AM EST

PDB ID : 7N43
Title : Alpha-conotoxin OmIA with unusual pharmacological properties at alpha7 nicotinic receptors
Authors : Ho, T.N.T.; Abraham, N.; Lewis, R.J.
Deposited on : 2021-06-03
Resolution : 2.47 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	:	2.23.2
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)	:	2.23.2

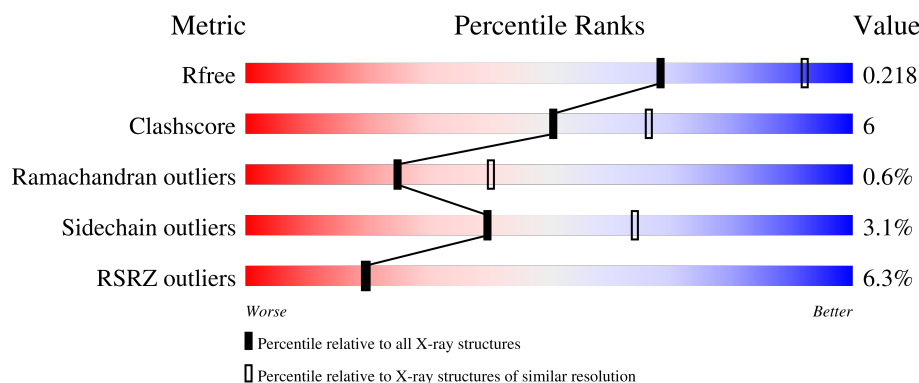
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 $\leq 5\%$. 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	210	<div> <div>0%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>
1	B	210	<div> <div>5%</div> <div>86%</div> <div>10%</div> <div>..</div> </div>
1	C	210	<div> <div>11%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	D	210	<div> <div>4%</div> <div>83%</div> <div>12%</div> <div>..</div> </div>
1	E	210	<div> <div>3%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	18	<div><div></div><div>11%</div><div>78%</div><div>17%</div><div>6%</div></div>
2	G	18	<div><div></div><div>6%</div><div>89%</div><div>6%</div><div>6%</div></div>
2	H	18	<div><div></div><div>72%</div><div>61%</div><div>33%</div><div>6%</div></div>
2	I	18	<div><div></div><div>6%</div><div>78%</div><div>17%</div><div>6%</div></div>
2	J	18	<div><div></div><div>11%</div><div>83%</div><div>11%</div><div>6%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8868 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
1	A	202	Total	C	N	O	S	0	0	0
			1614	1012	276	321	5			
1	B	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			
1	C	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			
1	D	202	Total	C	N	O	S	0	0	0
			1615	1012	277	321	5			
1	E	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			

- Molecule 2 is a protein called Alpha-conotoxin OmIA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	18	Total	C	N	O	S	0	0	1
			117	67	25	21	4			
2	G	18	Total	C	N	O	S	0	0	1
			117	67	25	21	4			
2	H	18	Total	C	N	O	S	0	0	1
			117	67	25	21	4			
2	I	18	Total	C	N	O	S	0	0	1
			117	67	25	21	4			
2	J	18	Total	C	N	O	S	0	0	1
			117	67	25	21	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	18	NH2	-	amidation	UNP P0C1R7
G	18	NH2	-	amidation	UNP P0C1R7
H	18	NH2	-	amidation	UNP P0C1R7
I	18	NH2	-	amidation	UNP P0C1R7
J	18	NH2	-	amidation	UNP P0C1R7

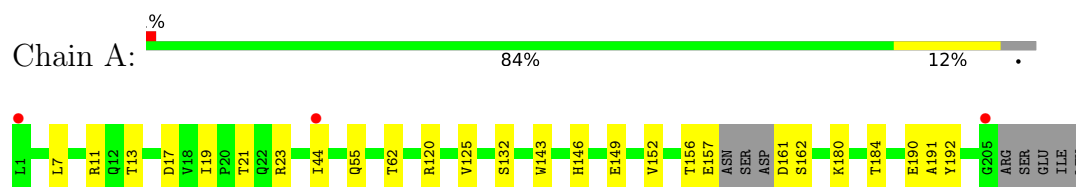
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total 37	O 37	0	0
3	B	25	Total 25	O 25	0	0
3	C	18	Total 18	O 18	0	0
3	D	26	Total 26	O 26	0	0
3	E	33	Total 33	O 33	0	0
3	F	3	Total 3	O 3	0	0
3	G	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0
3	I	1	Total 1	O 1	0	0
3	J	1	Total 1	O 1	0	0

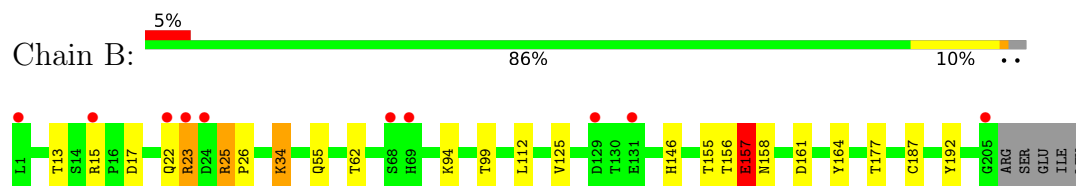
3 Residue-property plots [i](#)

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.

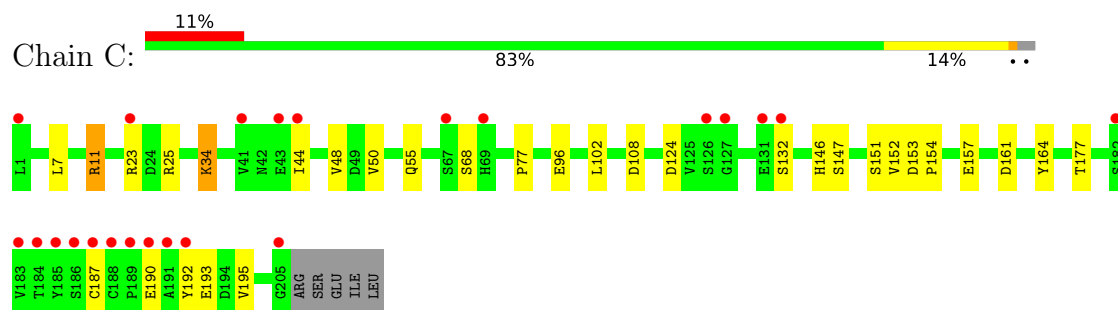
- Molecule 1: Acetylcholine-binding protein



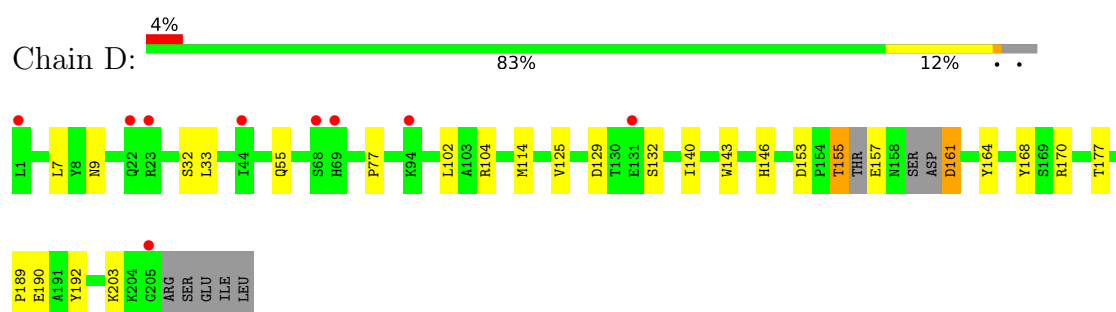
- Molecule 1: Acetylcholine-binding protein



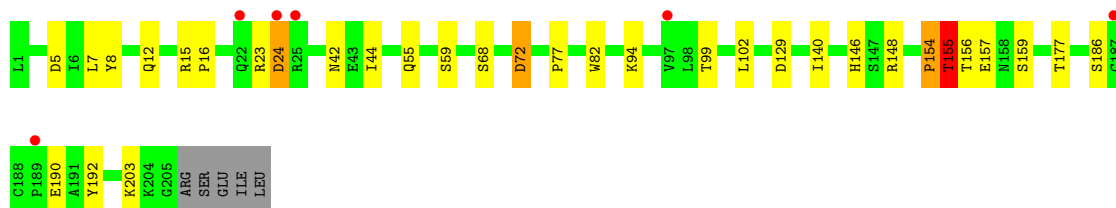
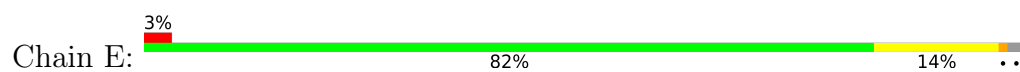
- Molecule 1: Acetylcholine-binding protein



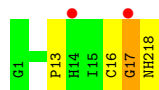
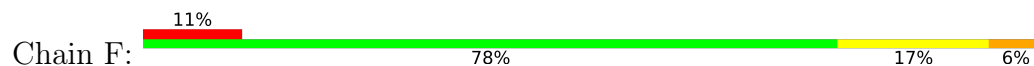
- Molecule 1: Acetylcholine-binding protein



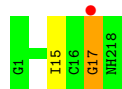
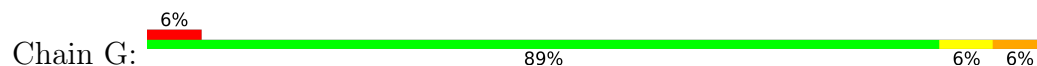
- Molecule 1: Acetylcholine-binding protein



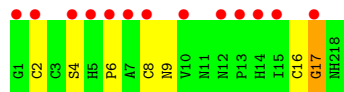
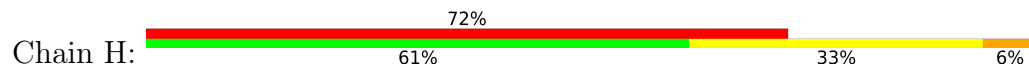
- Molecule 2: Alpha-conotoxin OmIA



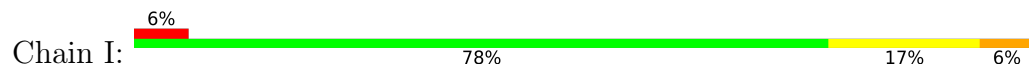
- Molecule 2: Alpha-conotoxin OmIA



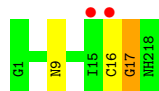
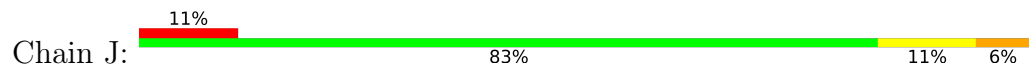
- Molecule 2: Alpha-conotoxin OmIA



- Molecule 2: Alpha-conotoxin OmIA



- Molecule 2: Alpha-conotoxin OmIA



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	169.36Å 169.36Å 124.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.19 – 2.47 49.19 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.19-2.47) 99.6 (49.19-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.187 , 0.212 0.196 , 0.218	Depositor DCC
R_{free} test set	2000 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8868	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

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	0.70	0/1649	0.93	4/2249 (0.2%)
1	B	0.64	0/1672	0.83	1/2282 (0.0%)
1	C	0.71	0/1672	0.89	2/2282 (0.1%)
1	D	0.70	0/1649	0.88	2/2247 (0.1%)
1	E	0.69	1/1672 (0.1%)	0.90	3/2282 (0.1%)
2	F	0.58	0/119	0.67	0/162
2	G	0.54	0/119	0.64	0/162
2	H	0.56	0/119	0.66	0/162
2	I	0.65	0/119	0.77	0/162
2	J	0.51	0/119	0.62	0/162
All	All	0.68	1/8909 (0.0%)	0.87	12/12152 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	155	THR	N-CA	5.38	1.57	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ASP	CB-CG-OD1	8.67	126.10	118.30
1	D	104	ARG	NE-CZ-NH2	-6.32	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	153	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	A	17	ASP	CB-CG-OD2	5.93	123.64	118.30
1	C	153	ASP	CB-CG-OD1	5.77	123.50	118.30
1	C	108	ASP	CB-CG-OD2	-5.72	113.16	118.30
1	B	161	ASP	CB-CG-OD2	5.53	123.28	118.30
1	E	5	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	149	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	E	72	ASP	CB-CA-C	-5.09	100.23	110.40
1	A	7	LEU	CB-CG-CD2	5.07	119.62	111.00
1	E	154	PRO	CB-CA-C	-5.06	99.36	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	SER	Peptide

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	1614	0	1565	13	0
1	B	1636	0	1581	20	0
1	C	1636	0	1581	18	0
1	D	1615	0	1563	17	0
1	E	1636	0	1581	25	0
2	F	117	0	100	5	0
2	G	117	0	100	3	0
2	H	117	0	100	7	0
2	I	117	0	100	8	0
2	J	117	0	100	4	0
3	A	37	0	0	0	0
3	B	25	0	0	0	0
3	C	18	0	0	0	0
3	D	26	0	0	1	0
3	E	33	0	0	4	0
3	F	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	2	0
3	J	1	0	0	0	0
All	All	8868	0	8371	97	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 6.

All (97) 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:44:ILE:O	1:D:170:ARG:HD3	1.61	0.99
1:E:155:THR:CG2	1:E:156:THR:H	1.84	0.90
1:E:155:THR:HG22	1:E:156:THR:H	1.40	0.83
1:D:161:ASP:OD1	3:D:301:HOH:O	2.03	0.76
2:I:16:CYS:O	2:I:17:GLY:O	2.03	0.74
1:E:155:THR:HG21	3:E:302:HOH:O	1.88	0.73
1:D:55:GLN:NE2	2:H:9:ASN:OD1	2.21	0.73
1:C:154:PRO:HG3	1:C:195:VAL:HG22	1.71	0.71
1:B:25:ARG:HG2	1:B:26:PRO:HD2	1.74	0.70
1:D:164:TYR:CE1	2:H:4:SER:HA	2.27	0.69
1:B:112:LEU:HD21	2:F:13:PRO:HB3	1.76	0.68
1:E:155:THR:CG2	1:E:156:THR:N	2.52	0.68
1:B:25:ARG:NH1	1:B:26:PRO:O	2.26	0.68
1:A:55:GLN:OE1	2:J:17:GLY:HA3	1.94	0.68
3:E:302:HOH:O	2:I:17:GLY:HA2	1.94	0.67
2:J:16:CYS:O	2:J:17:GLY:O	2.16	0.64
2:I:16:CYS:O	2:I:17:GLY:C	2.34	0.64
1:A:184:THR:HG22	1:A:191:ALA:HB2	1.80	0.62
1:E:55:GLN:OE1	2:I:17:GLY:HA3	2.00	0.62
1:B:156:THR:O	1:B:157:GLU:HB3	2.00	0.60
2:J:16:CYS:O	2:J:17:GLY:C	2.39	0.60
2:F:16:CYS:O	2:F:17:GLY:C	2.40	0.59
2:H:16:CYS:O	2:H:17:GLY:O	2.20	0.59
2:H:16:CYS:O	2:H:17:GLY:C	2.39	0.58
1:E:23:ARG:HG2	1:E:23:ARG:O	2.03	0.58
1:E:42:ASN:OD1	1:E:44:ILE:HG12	2.03	0.58
1:B:55:GLN:OE1	2:F:17:GLY:HA3	2.04	0.57
1:E:42:ASN:OD1	1:E:44:ILE:CG1	2.53	0.57
1:E:148:ARG:HH21	1:E:190:GLU:HB3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:GLN:HE22	2:G:17:GLY:CA	2.18	0.56
3:E:302:HOH:O	2:I:17:GLY:CA	2.50	0.56
1:A:143:TRP:CZ2	1:B:99:THR:HG21	2.41	0.56
1:A:13:THR:HG21	1:A:62:THR:O	2.05	0.55
1:E:155:THR:HG23	1:E:156:THR:H	1.72	0.55
1:A:152:VAL:O	1:A:180:LYS:HE2	2.07	0.54
1:D:33:LEU:HD11	1:D:140:ILE:HD11	1.90	0.54
1:C:55:GLN:HE22	2:G:17:GLY:HA3	1.72	0.54
2:F:16:CYS:O	2:F:17:GLY:O	2.25	0.54
1:B:23:ARG:HG2	1:B:23:ARG:O	2.08	0.52
1:A:146:HIS:CE1	1:A:190:GLU:HG3	2.45	0.52
1:C:25:ARG:NE	1:C:25:ARG:HA	2.25	0.52
1:B:22:GLN:O	1:B:23:ARG:HD3	2.10	0.52
1:B:155:THR:HG21	2:F:18:NH2:N	2.25	0.52
1:D:114:MET:CE	2:H:6:PRO:HA	2.40	0.52
1:C:48:VAL:HG22	1:C:50:VAL:HG13	1.92	0.51
1:E:55:GLN:NE2	2:I:9:ASN:OD1	2.41	0.51
1:E:155:THR:HG22	1:E:156:THR:N	2.19	0.51
1:A:19:ILE:HD12	1:A:21:THR:HG23	1.94	0.50
1:C:146:HIS:HB3	1:C:192:TYR:CE1	2.47	0.50
1:E:129:ASP:OD1	1:E:203:LYS:HE2	2.13	0.49
1:A:156:THR:O	1:A:157:GLU:HG3	2.13	0.49
1:B:157:GLU:O	1:B:177:THR:HA	2.13	0.49
2:I:15:ILE:CD1	3:I:101:HOH:O	2.61	0.49
1:C:192:TYR:CZ	2:H:8:CYS:HA	2.48	0.48
1:C:157:GLU:O	1:C:177:THR:HA	2.13	0.48
1:D:32:SER:HB2	1:D:155:THR:HB	1.96	0.47
1:B:13:THR:HG21	1:B:62:THR:O	2.15	0.47
1:B:187:CYS:HB2	2:G:15:ILE:HG12	1.97	0.46
1:E:155:THR:HG23	1:E:156:THR:N	2.28	0.46
1:A:55:GLN:NE2	2:J:9:ASN:OD1	2.44	0.46
1:D:190:GLU:OE1	1:D:190:GLU:N	2.35	0.46
1:C:190:GLU:OE1	1:C:190:GLU:N	2.35	0.45
1:B:22:GLN:O	1:B:23:ARG:CD	2.65	0.45
1:D:129:ASP:OD1	1:D:203:LYS:HE3	2.16	0.45
1:B:94:LYS:HE2	1:C:96:GLU:HG2	1.97	0.45
1:B:146:HIS:HB3	1:B:192:TYR:CE1	2.52	0.44
1:E:154:PRO:O	1:E:155:THR:HB	2.18	0.44
1:C:147:SER:HB3	1:C:193:GLU:HG3	1.99	0.44
1:C:124:ASP:HB2	1:D:168:TYR:CE1	2.53	0.44
1:C:152:VAL:CG1	1:C:195:VAL:HG23	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:HIS:HB3	1:A:192:TYR:CE1	2.53	0.43
1:E:24:ASP:O	1:E:24:ASP:CG	2.55	0.43
1:E:146:HIS:HB3	1:E:192:TYR:CE1	2.53	0.43
1:A:143:TRP:CH2	1:B:99:THR:HG21	2.54	0.43
1:C:187:CYS:SG	2:H:2:CYS:HB2	2.59	0.43
1:D:146:HIS:HB3	1:D:192:TYR:CE1	2.53	0.42
1:D:157:GLU:O	1:D:177:THR:HA	2.19	0.42
1:D:143:TRP:CH2	1:E:99:THR:HG21	2.54	0.42
1:E:72:ASP:HB3	3:E:326:HOH:O	2.19	0.42
1:D:189:PRO:HD2	1:D:190:GLU:OE1	2.20	0.42
1:B:158:ASN:ND2	1:B:177:THR:HG22	2.35	0.42
1:B:17:ASP:OD2	1:C:11:ARG:NH2	2.51	0.41
1:E:42:ASN:OD1	1:E:44:ILE:HG13	2.18	0.41
1:A:44:ILE:HD12	1:A:44:ILE:N	2.35	0.41
1:E:8:TYR:CE1	1:E:12:GLN:HG3	2.56	0.41
1:D:77:PRO:HA	1:D:102:LEU:HD23	2.02	0.41
1:D:125:VAL:O	1:D:125:VAL:HG12	2.20	0.41
1:E:77:PRO:HA	1:E:102:LEU:HD23	2.03	0.41
1:A:125:VAL:HG12	1:A:125:VAL:O	2.21	0.41
1:B:125:VAL:O	1:B:125:VAL:HG12	2.19	0.41
1:C:77:PRO:HA	1:C:102:LEU:HD23	2.02	0.41
1:C:34:LYS:HG2	1:C:164:TYR:CE2	2.56	0.41
2:I:15:ILE:HD13	3:I:101:HOH:O	2.21	0.41
1:D:143:TRP:CZ2	1:E:99:THR:HG21	2.57	0.40
1:E:16:PRO:HA	1:E:82:TRP:HA	2.03	0.40
1:E:157:GLU:O	1:E:177:THR:HA	2.20	0.40
1:B:34:LYS:HG2	1:B:164:TYR:CZ	2.56	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	198/210 (94%)	197 (100%)	1 (0%)	0	100	100
1	B	203/210 (97%)	201 (99%)	1 (0%)	1 (0%)	29	46
1	C	203/210 (97%)	203 (100%)	0	0	100	100
1	D	196/210 (93%)	195 (100%)	1 (0%)	0	100	100
1	E	203/210 (97%)	202 (100%)	0	1 (0%)	29	46
2	F	16/18 (89%)	14 (88%)	1 (6%)	1 (6%)	1	1
2	G	16/18 (89%)	14 (88%)	1 (6%)	1 (6%)	1	1
2	H	16/18 (89%)	14 (88%)	1 (6%)	1 (6%)	1	1
2	I	16/18 (89%)	14 (88%)	1 (6%)	1 (6%)	1	1
2	J	16/18 (89%)	14 (88%)	1 (6%)	1 (6%)	1	1
All	All	1083/1140 (95%)	1068 (99%)	8 (1%)	7 (1%)	25	40

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	17	GLY
2	I	17	GLY
2	J	17	GLY
1	B	157	GLU
2	F	17	GLY
1	E	155	THR
2	G	17	GLY

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	188/196 (96%)	184 (98%)	4 (2%)	53	76
1	B	191/196 (97%)	186 (97%)	5 (3%)	46	70
1	C	191/196 (97%)	183 (96%)	8 (4%)	30	51
1	D	188/196 (96%)	183 (97%)	5 (3%)	44	69
1	E	191/196 (97%)	181 (95%)	10 (5%)	23	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	14/14 (100%)	14 (100%)	0	100	100
2	G	14/14 (100%)	14 (100%)	0	100	100
2	H	14/14 (100%)	14 (100%)	0	100	100
2	I	14/14 (100%)	14 (100%)	0	100	100
2	J	14/14 (100%)	14 (100%)	0	100	100
All	All	1019/1050 (97%)	987 (97%)	32 (3%)	40	64

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	23	ARG
1	A	120	ARG
1	A	132	SER
1	B	15	ARG
1	B	23	ARG
1	B	25	ARG
1	B	34	LYS
1	B	157	GLU
1	C	7	LEU
1	C	11	ARG
1	C	23	ARG
1	C	34	LYS
1	C	68	SER
1	C	132	SER
1	C	151	SER
1	C	161	ASP
1	D	7	LEU
1	D	9	ASN
1	D	132	SER
1	D	155	THR
1	D	161	ASP
1	E	7	LEU
1	E	15	ARG
1	E	24	ASP
1	E	59	SER
1	E	68	SER
1	E	94	LYS
1	E	140	ILE
1	E	155	THR

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Mol	Chain	Res	Type
1	E	159	SER
1	E	186	SER

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

Mol	Chain	Res	Type
1	B	158	ASN
1	C	55	GLN
2	H	5	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	202/210 (96%)	0.25	3 (1%) 73 75	37, 55, 91, 119	0
1	B	205/210 (97%)	0.30	10 (4%) 29 31	39, 59, 89, 149	0
1	C	205/210 (97%)	0.49	23 (11%) 5 4	39, 58, 99, 137	0
1	D	202/210 (96%)	0.31	9 (4%) 33 35	35, 57, 95, 120	0
1	E	205/210 (97%)	0.19	6 (2%) 51 54	33, 51, 84, 118	0
2	F	17/18 (94%)	0.35	2 (11%) 4 4	43, 56, 94, 98	0
2	G	17/18 (94%)	0.13	1 (5%) 22 22	50, 61, 95, 98	0
2	H	17/18 (94%)	3.19	13 (76%) 0 0	71, 90, 106, 115	0
2	I	17/18 (94%)	0.18	1 (5%) 22 22	35, 40, 60, 61	0
2	J	17/18 (94%)	0.65	2 (11%) 4 4	47, 63, 93, 98	0
All	All	1104/1140 (96%)	0.35	70 (6%) 20 20	33, 56, 96, 149	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	184	THR	6.5
2	H	8	CYS	6.4
1	C	187	CYS	5.9
2	H	17	GLY	5.8
1	B	23	ARG	5.3
2	H	14	HIS	4.9
1	D	205	GLY	4.8
2	H	15	ILE	4.2
1	C	23	ARG	4.0
1	B	24	ASP	4.0
2	H	2	CYS	3.6
1	C	185	TYR	3.6
2	G	17	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	205	GLY	3.6
1	C	189	PRO	3.5
2	J	15	ILE	3.5
1	C	205	GLY	3.5
1	E	189	PRO	3.4
2	F	17	GLY	3.4
2	H	13	PRO	3.4
1	C	186	SER	3.4
1	B	69	HIS	3.3
1	C	182	SER	3.1
1	D	23	ARG	3.1
1	C	132	SER	3.1
1	A	44	ILE	3.0
1	B	205	GLY	3.0
1	D	22	GLN	3.0
2	H	5	HIS	3.0
2	H	1	GLY	3.0
2	H	4	SER	3.0
2	H	12	ASN	3.0
1	B	22	GLN	3.0
1	C	44	ILE	2.9
1	A	1	LEU	2.9
1	C	191	ALA	2.9
2	H	7	ALA	2.9
1	C	69	HIS	2.9
1	C	183	VAL	2.8
2	H	10	VAL	2.8
1	B	1	LEU	2.8
1	C	190	GLU	2.8
1	C	1	LEU	2.7
1	D	131	GLU	2.7
1	C	188	CYS	2.7
1	D	69	HIS	2.6
1	B	68	SER	2.5
1	C	43	GLU	2.5
1	C	126	SER	2.5
1	C	131	GLU	2.5
1	E	22	GLN	2.4
1	D	44	ILE	2.4
2	F	14	HIS	2.4
1	C	67	SER	2.4
1	E	24	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	6	PRO	2.3
1	B	129	ASP	2.3
1	C	127	GLY	2.3
1	B	15	ARG	2.3
2	I	17	GLY	2.2
2	J	16	CYS	2.2
1	B	131	GLU	2.2
1	E	97	VAL	2.1
1	D	68	SER	2.1
1	E	25	ARG	2.1
1	C	41	VAL	2.0
1	D	94	LYS	2.0
1	E	187	CYS	2.0
1	D	1	LEU	2.0
1	C	192	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.