



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2018 – 11:28 AM EST

PDB ID : 3U8L
Title : Crystal structure of the acetylcholine binding protein (AChBP) from *Lymnaea stagnalis* in complex with NS3570 (1-(5-phenylpyridin-3-yl)-1,4-diazepane)
Authors : Rohde, L.A.H.; Ahring, P.K.; Jensen, M.L.; Nielsen, E.O.; Peters, D.; Helgstrand, C.; Krintel, C.; Harpsoe, K.; Gajhede, M.; Kastrup, J.S.; Balle, T.
Deposited on : 2011-10-17
Resolution : 2.32 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

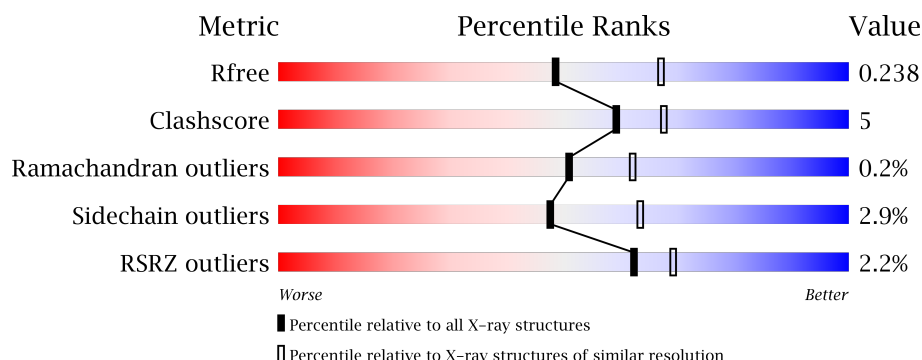
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	100719	4787 (2.34-2.30)
Clashscore	112137	5439 (2.34-2.30)
Ramachandran outliers	110173	5386 (2.34-2.30)
Sidechain outliers	110143	5385 (2.34-2.30)
RSRZ outliers	101464	4814 (2.34-2.30)

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. 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>2%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>••</div> </div> </div>
1	B	210	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>•</div> </div> </div>
1	C	210	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>•</div> </div> </div>
1	D	210	<div> <div>•%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
1	E	210	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	210	 3% 86% 10% •
1	G	210	 2% 83% 11% • 5%
1	H	210	 3% 85% 9% • 5%
1	I	210	 % 88% 9% •
1	J	210	 % 84% 10% • 5%

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	09Q	A	211	-	-	-	X
2	09Q	B	212	-	-	X	-
2	09Q	B	213	-	-	-	X

2 Entry composition

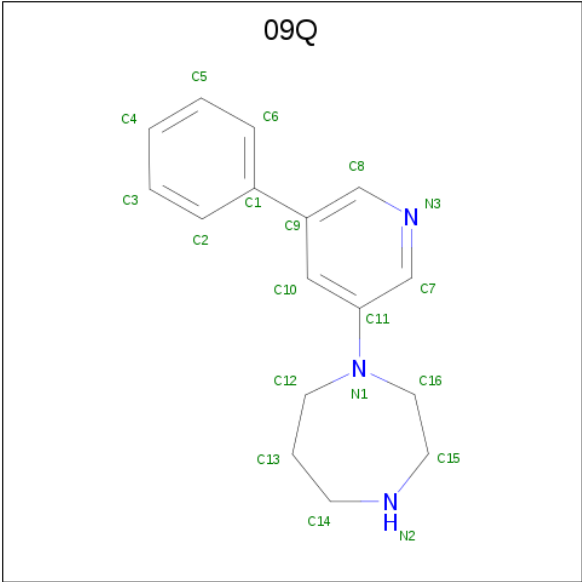
There are 4 unique types of molecules in this entry. The entry contains 17072 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1	0
			1618	1015	276	321	6			
1	B	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			
1	C	201	Total	C	N	O	S	0	2	0
			1619	1015	279	320	5			
1	D	199	Total	C	N	O	S	0	0	0
			1590	999	273	313	5			
1	E	206	Total	C	N	O	S	0	0	0
			1647	1029	284	329	5			
1	F	202	Total	C	N	O	S	0	1	0
			1618	1015	276	321	6			
1	G	200	Total	C	N	O	S	0	1	0
			1607	1009	274	318	6			
1	H	200	Total	C	N	O	S	0	2	0
			1609	1010	277	316	6			
1	I	204	Total	C	N	O	S	0	1	0
			1635	1023	282	325	5			
1	J	200	Total	C	N	O	S	0	1	0
			1613	1012	280	317	4			

- Molecule 2 is 1-(5-phenylpyridin-3-yl)-1,4-diazepane (three-letter code: 09Q) (formula: C₁₆H₁₉N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			19	16	3		
2	B	1	Total	C	N	0	0
			19	16	3		
2	B	1	Total	C	N	0	0
			19	16	3		
2	B	1	Total	C	N	0	0
			19	16	3		
2	C	1	Total	C	N	0	0
			19	16	3		
2	D	1	Total	C	N	0	0
			19	16	3		
2	E	1	Total	C	N	0	0
			19	16	3		
2	F	1	Total	C	N	0	0
			19	16	3		
2	G	1	Total	C	N	0	0
			19	16	3		
2	H	1	Total	C	N	0	0
			19	16	3		
2	H	1	Total	C	N	0	0
			19	16	3		
2	H	1	Total	C	N	0	0
			19	16	3		
2	I	1	Total	C	N	0	0
			19	16	3		
2	J	1	Total	C	N	0	0
			19	16	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	49	Total	O	0	0
			49	49		
4	C	65	Total	O	0	0
			65	65		
4	D	59	Total	O	0	0
			59	59		
4	E	67	Total	O	0	0
			67	67		
4	F	49	Total	O	0	0
			49	49		
4	G	58	Total	O	0	0
			58	58		
4	H	73	Total	O	0	0
			73	73		

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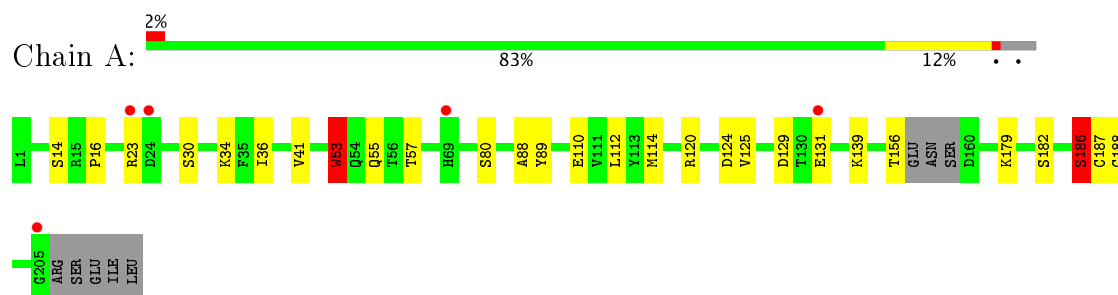
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	66	Total	O	0	0
			66	66		
4	J	54	Total	O	0	0
			54	54		

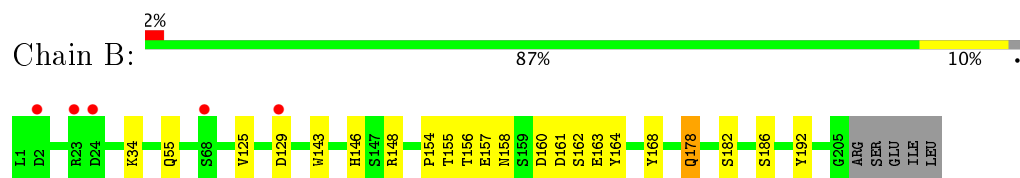
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

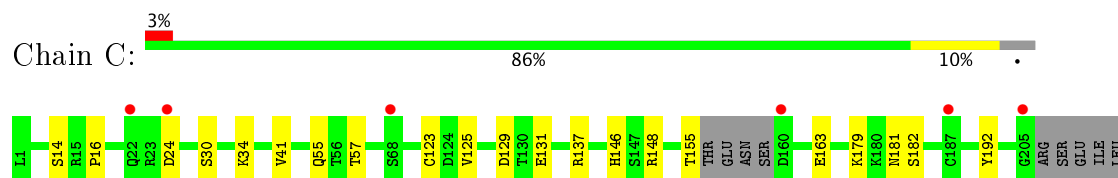
- Molecule 1: Acetylcholine-binding protein



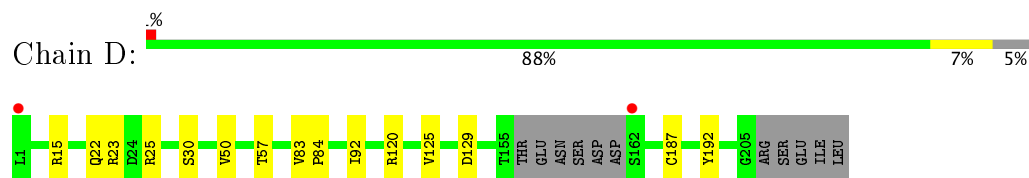
- Molecule 1: Acetylcholine-binding protein



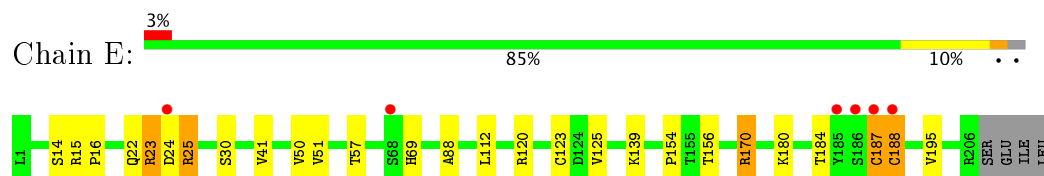
- Molecule 1: Acetylcholine-binding protein



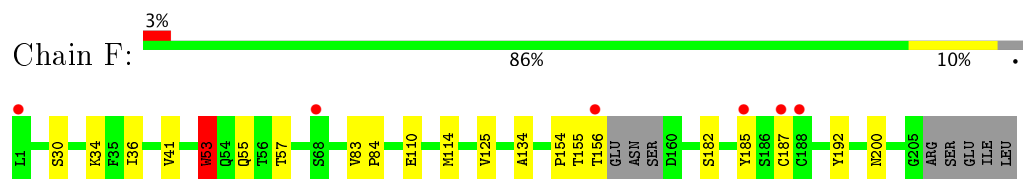
- Molecule 1: Acetylcholine-binding protein



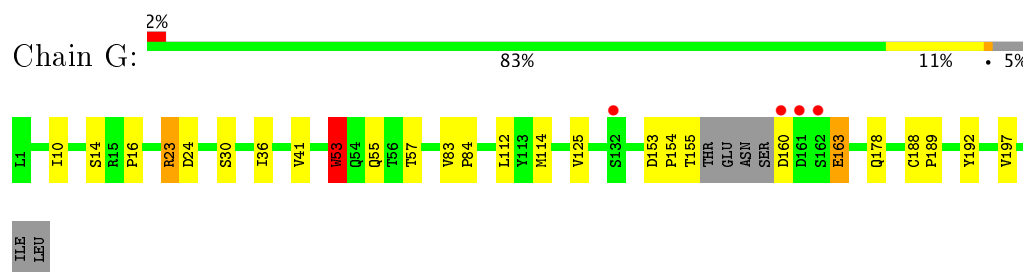
- Molecule 1: Acetylcholine-binding protein



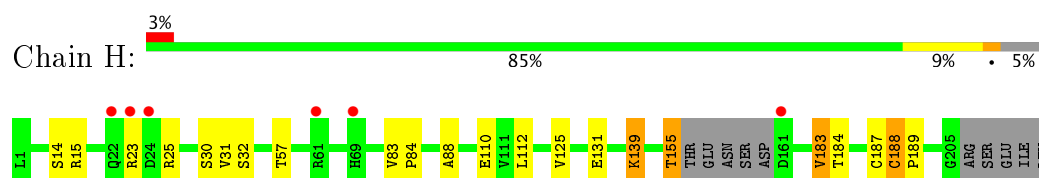
- Molecule 1: Acetylcholine-binding protein



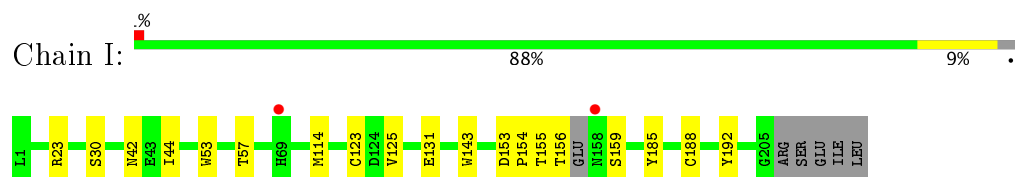
- Molecule 1: Acetylcholine-binding protein



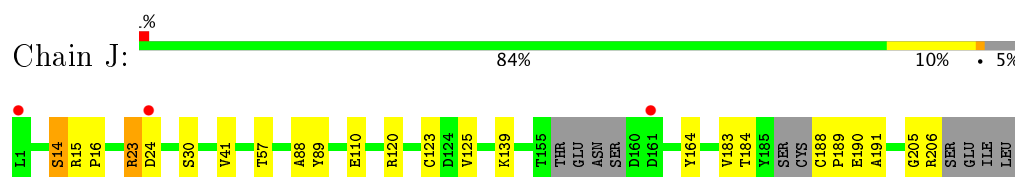
- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.96 Å 114.81 Å 127.06 Å 90.00° 91.08° 90.00°	Depositor
Resolution (Å)	42.35 – 2.32 44.08 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.35-2.32) 99.9 (44.08-2.32)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.32 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.191 , 0.244 0.183 , 0.238	Depositor DCC
R_{free} test set	4593 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17072	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: 09Q, SO4

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	0.39	0/1656	0.57	1/2259 (0.0%)
1	B	0.39	0/1672	0.54	0/2282
1	C	0.39	0/1660	0.53	0/2264
1	D	0.40	0/1625	0.54	0/2216
1	E	0.40	0/1683	0.56	0/2296
1	F	0.38	0/1656	0.55	1/2259 (0.0%)
1	G	0.39	0/1645	0.57	1/2244 (0.0%)
1	H	0.40	0/1650	0.55	0/2251
1	I	0.40	0/1673	0.54	0/2281
1	J	0.38	0/1650	0.52	0/2247
All	All	0.39	0/16570	0.55	3/22599 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	53	TRP	CA-CB-CG	6.46	125.98	113.70
1	G	53	TRP	CA-CB-CG	5.78	124.69	113.70
1	A	53	TRP	CA-CB-CG	5.74	124.61	113.70

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	1618	0	1574	23	0
1	B	1636	0	1583	24	0
1	C	1619	0	1575	14	0
1	D	1590	0	1548	6	0
1	E	1647	0	1594	21	0
1	F	1618	0	1572	17	0
1	G	1607	0	1562	19	0
1	H	1609	0	1570	12	0
1	I	1635	0	1589	20	0
1	J	1613	0	1573	24	0
2	A	19	0	19	1	0
2	B	57	0	57	12	0
2	C	19	0	19	1	0
2	D	19	0	19	2	0
2	E	19	0	19	1	0
2	F	19	0	19	3	0
2	G	19	0	19	2	0
2	H	57	0	57	6	0
2	I	19	0	19	4	0
2	J	19	0	19	1	0
3	B	10	0	0	0	0
3	G	5	0	0	0	0
4	A	59	0	0	3	0
4	B	49	0	0	0	0
4	C	65	0	0	4	0
4	D	59	0	0	0	0
4	E	67	0	0	4	0
4	F	49	0	0	1	0
4	G	58	0	0	1	0
4	H	73	0	0	0	0
4	I	66	0	0	2	0
4	J	54	0	0	1	0
All	All	17072	0	16006	175	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 5.

All (175) 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:B:154:PRO:HB3	1:B:178:GLN:HE21	1.29	0.98
1:A:89:TYR:HD2	2:B:212:09Q:H4	1.38	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:120[B]:ARG:CG	1:J:120[B]:ARG:HH11	1.87	0.87
1:A:186:SER:HB2	1:B:160:ASP:HB2	1.56	0.85
1:G:55:GLN:HA	1:G:114[B]:MET:HG3	1.59	0.83
1:H:188[B]:CYS:SG	1:H:189:PRO:HD2	2.19	0.83
1:A:131:GLU:CD	1:A:131:GLU:H	1.83	0.82
1:A:120:ARG:HD2	4:A:230:HOH:O	1.82	0.80
1:B:154:PRO:HB3	1:B:178:GLN:NE2	1.98	0.79
2:A:211:09Q:H4	4:A:827:HOH:O	1.83	0.78
1:C:14:SER:HA	4:C:818:HOH:O	1.84	0.76
1:F:55:GLN:HA	1:F:114[B]:MET:HG2	1.71	0.72
1:J:14:SER:HB3	1:J:16:PRO:HD3	1.70	0.72
1:J:15:ARG:N	1:J:16:PRO:HD3	2.05	0.72
1:J:120[B]:ARG:HH11	1:J:120[B]:ARG:HG2	1.54	0.71
1:B:164:TYR:O	2:B:212:09Q:H2	1.93	0.69
1:E:22:GLN:O	1:E:25:ARG:HG2	1.92	0.69
1:A:89:TYR:CD2	2:B:212:09Q:H4	2.27	0.66
1:G:154:PRO:O	1:G:155:THR:HG23	1.95	0.66
1:G:36:ILE:HG13	1:G:53:TRP:CZ3	2.31	0.65
1:G:23:ARG:N	1:G:23:ARG:HD3	2.11	0.65
1:A:89:TYR:HD2	2:B:212:09Q:C5	2.08	0.65
1:F:57:THR:HG22	4:F:663:HOH:O	1.97	0.64
2:H:211:09Q:H10	2:H:213:09Q:H3	1.79	0.64
1:G:160:ASP:HB3	1:G:163:GLU:HG3	1.81	0.63
1:E:23:ARG:N	1:E:23:ARG:HD3	2.13	0.62
1:A:55:GLN:HA	1:A:114[B]:MET:CG	2.30	0.62
1:I:155:THR:HG22	1:I:156:THR:N	2.15	0.62
1:C:192:TYR:OH	2:C:211:09Q:H1	2.00	0.61
1:A:55:GLN:HA	1:A:114[B]:MET:HG3	1.83	0.60
1:G:10:ILE:O	1:G:14:SER:HB2	2.01	0.60
1:E:123:CYS:HB2	4:E:499:HOH:O	2.01	0.59
1:G:14:SER:HB3	4:G:823:HOH:O	2.00	0.59
1:F:36:ILE:HD11	1:F:53:TRP:CE3	2.38	0.59
1:J:120[B]:ARG:HG3	1:J:120[B]:ARG:HH11	1.64	0.59
1:B:157:GLU:HG2	1:B:161:ASP:OD2	2.02	0.59
1:C:146:HIS:HD2	1:C:148:ARG:H	1.51	0.59
1:E:154:PRO:HB3	1:E:195:VAL:HG22	1.84	0.58
1:G:23:ARG:H	1:G:23:ARG:HD3	1.69	0.58
1:H:30:SER:HB2	1:H:57:THR:HB	1.86	0.57
1:F:36:ILE:HG13	1:F:53:TRP:CE3	2.41	0.56
1:G:36:ILE:HG13	1:G:53:TRP:CE3	2.40	0.56
1:G:14:SER:O	1:G:16:PRO:HD3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:HIS:HD2	1:I:23:ARG:HH21	1.53	0.56
1:A:36:ILE:HD11	1:A:53:TRP:CE3	2.40	0.56
1:H:183:VAL:HG13	2:H:212:09Q:H15	1.86	0.55
1:B:186:SER:HB2	1:C:163:GLU:OE1	2.07	0.55
1:B:163:GLU:HG3	2:B:212:09Q:H18	1.89	0.54
1:B:157:GLU:HG3	2:B:213:09Q:H9	1.90	0.53
1:I:42:ASN:OD1	1:I:44:ILE:HB	2.09	0.53
1:E:170:ARG:HA	1:E:170:ARG:NE	2.23	0.53
1:I:53:TRP:NE1	1:I:114:MET:HB3	2.24	0.53
1:A:34:LYS:HB2	1:A:53:TRP:HB2	1.90	0.52
1:F:125:VAL:HG12	1:F:125:VAL:O	2.10	0.52
1:B:125:VAL:O	1:B:125:VAL:HG12	2.09	0.52
1:D:125:VAL:O	1:D:125:VAL:HG12	2.09	0.52
1:J:15:ARG:N	1:J:16:PRO:CD	2.72	0.52
1:A:125:VAL:O	1:A:125:VAL:HG12	2.09	0.52
1:A:112:LEU:HD13	2:E:211:09Q:H4	1.90	0.52
1:H:14:SER:O	1:H:15[B]:ARG:HG2	2.09	0.52
1:C:14:SER:C	1:C:16:PRO:HD3	2.30	0.51
1:G:125:VAL:HG12	1:G:125:VAL:O	2.08	0.51
1:I:125:VAL:HG12	1:I:125:VAL:O	2.10	0.51
1:J:125:VAL:O	1:J:125:VAL:HG12	2.09	0.51
1:E:14:SER:O	1:E:16:PRO:HD3	2.10	0.51
1:E:154:PRO:HG3	1:E:180:LYS:HB2	1.92	0.51
2:H:211:09Q:H10	2:H:213:09Q:C4	2.41	0.51
1:I:188:CYS:HB3	4:I:794:HOH:O	2.11	0.51
1:E:125:VAL:HG12	1:E:125:VAL:O	2.11	0.50
1:B:160:ASP:OD1	2:B:212:09Q:H16	2.12	0.50
1:C:125:VAL:HG12	1:C:125:VAL:O	2.11	0.50
1:H:83:VAL:HG13	1:H:84:PRO:HD2	1.93	0.50
1:E:187:CYS:SG	1:E:188:CYS:N	2.85	0.49
1:J:190:GLU:OE1	1:J:190:GLU:HA	2.12	0.49
1:E:120:ARG:HD3	4:E:357:HOH:O	2.12	0.49
1:F:36:ILE:HG13	1:F:53:TRP:CZ3	2.48	0.49
1:B:192:TYR:OH	2:B:211:09Q:H1	2.12	0.49
1:H:125:VAL:O	1:H:125:VAL:HG12	2.13	0.49
1:F:185:TYR:CE2	2:F:211:09Q:H14	2.47	0.49
1:F:36:ILE:CD1	1:F:53:TRP:CE3	2.96	0.49
1:E:88:ALA:HA	1:E:139:LYS:O	2.12	0.48
1:I:192:TYR:OH	2:I:211:09Q:H1	2.12	0.48
1:C:55:GLN:NE2	1:C:155:THR:HG21	2.28	0.48
1:D:92:ILE:HD11	1:D:120:ARG:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLU:CG	1:B:163:GLU:O	2.62	0.48
2:G:211:09Q:H4	1:H:112:LEU:HD22	1.94	0.48
1:C:30:SER:HB2	1:C:57:THR:HB	1.94	0.48
1:H:32:SER:HB2	1:H:155:THR:HB	1.96	0.48
1:A:55:GLN:HA	1:A:114[B]:MET:HG2	1.96	0.48
1:J:205:GLY:O	1:J:206:ARG:C	2.52	0.48
1:C:137:ARG:HD2	4:C:863:HOH:O	2.14	0.47
1:D:83:VAL:HG13	1:D:84:PRO:HD2	1.97	0.47
1:J:30:SER:HB2	1:J:57:THR:HB	1.96	0.47
1:J:183:VAL:HG12	1:J:184:THR:N	2.29	0.47
1:B:162:SER:HA	2:B:213:09Q:C1	2.45	0.47
1:J:183:VAL:CG1	1:J:184:THR:N	2.78	0.47
1:J:14:SER:CB	1:J:16:PRO:HD3	2.41	0.47
1:C:123:CYS:HB2	4:C:864:HOH:O	2.15	0.46
1:J:89:TYR:OH	2:J:211:09Q:N2	2.48	0.46
1:E:23:ARG:HE	1:E:25:ARG:HH12	1.64	0.46
1:I:123:CYS:HB2	4:I:791:HOH:O	2.14	0.46
1:I:143:TRP:CE3	2:I:211:09Q:H16	2.51	0.46
1:A:188:CYS:HB3	4:A:503:HOH:O	2.16	0.46
1:A:187:CYS:HB3	1:B:158:ASN:OD1	2.15	0.46
1:G:41:VAL:HG13	1:G:125:VAL:HG11	1.98	0.46
1:I:23:ARG:HD3	1:I:23:ARG:N	2.32	0.45
1:B:157:GLU:HG2	1:B:158:ASN:H	1.82	0.45
1:J:120[B]:ARG:NH1	1:J:120[B]:ARG:CG	2.59	0.45
1:J:23:ARG:HG2	1:J:23:ARG:HH11	1.82	0.45
1:D:92:ILE:CG1	1:D:120:ARG:HG2	2.47	0.45
1:C:41:VAL:HG13	1:C:125:VAL:HG11	1.98	0.45
1:A:124:ASP:HB2	1:B:168:TYR:CZ	2.51	0.45
1:B:160:ASP:CG	2:B:212:09Q:H19	2.20	0.44
1:A:131:GLU:CD	1:A:131:GLU:N	2.63	0.44
1:F:36:ILE:CG1	1:F:53:TRP:CE3	3.01	0.44
1:F:34:LYS:HB2	1:F:53:TRP:HB2	2.00	0.44
1:I:30:SER:HB2	1:I:57:THR:HB	1.98	0.44
1:B:157:GLU:HG2	1:B:158:ASN:N	2.32	0.44
2:D:211:09Q:H4	1:E:112:LEU:HD13	1.98	0.44
1:J:123:CYS:HB2	4:J:446:HOH:O	2.16	0.44
1:B:146:HIS:CE1	1:B:148:ARG:HB2	2.53	0.44
1:H:187:CYS:SG	2:H:213:09Q:C1	3.06	0.44
1:I:155:THR:HG22	1:I:156:THR:H	1.83	0.44
1:J:89:TYR:CG	1:J:139:LYS:HE2	2.53	0.44
1:E:23:ARG:HB3	1:E:24:ASP:H	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:THR:HG23	4:E:349:HOH:O	2.17	0.43
1:I:143:TRP:CZ3	2:I:211:09Q:H16	2.52	0.43
1:J:183:VAL:O	1:J:191:ALA:HA	2.18	0.43
1:E:41:VAL:HG13	1:E:125:VAL:HG11	2.00	0.43
1:G:83:VAL:HG13	1:G:84:PRO:HD2	2.00	0.43
1:C:34:LYS:HE2	1:C:55:GLN:OE1	2.17	0.43
1:H:183:VAL:HG11	2:H:212:09Q:H18	1.99	0.43
1:G:153:ASP:HA	1:G:154:PRO:HD3	1.82	0.43
1:G:192:TYR:OH	2:G:211:09Q:H1	2.18	0.43
1:I:155:THR:CG2	1:I:156:THR:N	2.81	0.43
1:J:41:VAL:HG13	1:J:125:VAL:HG11	2.00	0.43
1:F:83:VAL:HG13	1:F:84:PRO:HD2	2.01	0.43
1:J:188:CYS:HA	1:J:189:PRO:HD3	1.88	0.43
1:A:88:ALA:HA	1:A:139:LYS:O	2.18	0.43
1:G:178:GLN:HG2	1:G:197:VAL:HG22	2.00	0.43
1:I:53:TRP:HE1	1:I:114:MET:HB3	1.84	0.43
1:B:34:LYS:HE2	1:B:55:GLN:OE1	2.19	0.42
1:F:192:TYR:OH	2:F:211:09Q:H1	2.19	0.42
1:F:36:ILE:HD11	1:F:53:TRP:CD2	2.53	0.42
1:A:14:SER:O	1:A:16:PRO:HD3	2.19	0.42
1:F:134:ALA:O	1:F:200:ASN:HA	2.19	0.42
1:A:30:SER:HB2	1:A:57:THR:HB	2.01	0.42
1:H:183:VAL:CG1	2:H:212:09Q:H15	2.50	0.42
1:A:41:VAL:HG13	1:A:125:VAL:HG11	2.00	0.42
1:G:188:CYS:HA	1:G:189:PRO:HD3	1.83	0.42
1:I:185:TYR:HD1	1:J:164:TYR:HE1	1.67	0.42
1:I:153:ASP:HA	1:I:154:PRO:HD3	1.87	0.42
1:J:120[B]:ARG:NH1	1:J:120[B]:ARG:HG2	2.28	0.42
1:F:41:VAL:HG13	1:F:125:VAL:HG11	2.00	0.42
1:I:143:TRP:CE2	2:I:211:09Q:H17	2.55	0.42
1:J:88:ALA:HA	1:J:139:LYS:O	2.20	0.42
1:I:42:ASN:OD1	1:I:44:ILE:N	2.51	0.41
1:D:30:SER:HB2	1:D:57:THR:HB	2.02	0.41
1:E:30:SER:HB2	1:E:57:THR:HB	2.02	0.41
1:E:69:HIS:CD2	1:I:23:ARG:HH21	2.36	0.41
1:B:163:GLU:CD	1:B:163:GLU:O	2.58	0.41
1:H:88:ALA:HA	1:H:139:LYS:O	2.20	0.41
1:B:143:TRP:CE2	2:B:211:09Q:H17	2.55	0.41
1:F:30:SER:HB2	1:F:57:THR:HB	2.02	0.41
1:G:30:SER:HB2	1:G:57:THR:HB	2.02	0.41
1:E:50:VAL:HG12	1:E:51:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:LYS:HG3	4:C:222:HOH:O	2.20	0.41
1:C:181[A]:ASN:OD1	1:C:182:SER:N	2.50	0.41
1:A:14:SER:OG	1:A:80:SER:O	2.35	0.40
1:B:143:TRP:CZ3	2:B:211:09Q:H16	2.56	0.40
1:D:192:TYR:OH	2:D:211:09Q:H1	2.21	0.40
1:A:124:ASP:HB2	1:B:168:TYR:CE1	2.56	0.40
1:E:120:ARG:CD	4:E:357:HOH:O	2.69	0.40
1:F:55:GLN:HA	1:F:114[B]:MET:CG	2.46	0.40
2:F:211:09Q:H4	1:G:112:LEU:HD22	2.04	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	199/210 (95%)	196 (98%)	2 (1%)	1 (0%)	32	39
1	B	203/210 (97%)	201 (99%)	2 (1%)	0	100	100
1	C	199/210 (95%)	197 (99%)	2 (1%)	0	100	100
1	D	195/210 (93%)	192 (98%)	3 (2%)	0	100	100
1	E	204/210 (97%)	199 (98%)	5 (2%)	0	100	100
1	F	199/210 (95%)	195 (98%)	3 (2%)	1 (0%)	32	39
1	G	197/210 (94%)	196 (100%)	1 (0%)	0	100	100
1	H	198/210 (94%)	194 (98%)	4 (2%)	0	100	100
1	I	201/210 (96%)	199 (99%)	2 (1%)	0	100	100
1	J	195/210 (93%)	191 (98%)	3 (2%)	1 (0%)	32	39
All	All	1990/2100 (95%)	1960 (98%)	27 (1%)	3 (0%)	51	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	14	SER
1	A	186	SER
1	F	154	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/196 (96%)	181 (96%)	8 (4%)	34	47
1	B	191/196 (97%)	186 (97%)	5 (3%)	51	68
1	C	189/196 (96%)	186 (98%)	3 (2%)	68	82
1	D	185/196 (94%)	178 (96%)	7 (4%)	38	52
1	E	192/196 (98%)	185 (96%)	7 (4%)	40	54
1	F	189/196 (96%)	183 (97%)	6 (3%)	44	59
1	G	188/196 (96%)	184 (98%)	4 (2%)	59	75
1	H	188/196 (96%)	177 (94%)	11 (6%)	23	30
1	I	191/196 (97%)	189 (99%)	2 (1%)	80	90
1	J	187/196 (95%)	184 (98%)	3 (2%)	68	82
All	All	1889/1960 (96%)	1833 (97%)	56 (3%)	48	62

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	53	TRP
1	A	110	GLU
1	A	129	ASP
1	A	156	THR
1	A	179	LYS
1	A	182	SER
1	A	186	SER
1	B	129	ASP
1	B	155	THR
1	B	156	THR

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Mol	Chain	Res	Type
1	B	178	GLN
1	B	182	SER
1	C	24	ASP
1	C	129	ASP
1	C	131	GLU
1	D	15	ARG
1	D	22	GLN
1	D	23	ARG
1	D	25	ARG
1	D	50	VAL
1	D	129	ASP
1	D	187	CYS
1	E	15	ARG
1	E	23	ARG
1	E	25	ARG
1	E	156	THR
1	E	170	ARG
1	E	187	CYS
1	E	188	CYS
1	F	53	TRP
1	F	110	GLU
1	F	155	THR
1	F	156	THR
1	F	182	SER
1	F	187	CYS
1	G	23	ARG
1	G	24	ASP
1	G	53	TRP
1	G	163	GLU
1	H	23	ARG
1	H	25	ARG
1	H	31	VAL
1	H	110	GLU
1	H	131	GLU
1	H	139	LYS
1	H	155	THR
1	H	183	VAL
1	H	184	THR
1	H	188[A]	CYS
1	H	188[B]	CYS
1	I	131	GLU
1	I	159	SER

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Mol	Chain	Res	Type
1	J	23	ARG
1	J	24	ASP
1	J	110	GLU

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

Mol	Chain	Res	Type
1	A	178	GLN
1	B	22	GLN
1	B	178	GLN
1	B	200	ASN
1	C	146	HIS
1	E	69	HIS
1	I	12	GLN
1	I	158	ASN
1	J	178	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

17 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
2	09Q	A	211	-	19,21,21	1.14	1 (5%)	21,27,27	1.61	4 (19%)
2	09Q	B	211	-	19,21,21	1.11	0	21,27,27	1.20	2 (9%)
2	09Q	B	212	-	19,21,21	1.18	1 (5%)	21,27,27	0.98	1 (4%)
2	09Q	B	213	-	19,21,21	1.15	0	21,27,27	1.24	2 (9%)
3	SO4	B	214	-	4,4,4	0.17	0	6,6,6	0.10	0
3	SO4	B	215	-	4,4,4	0.19	0	6,6,6	0.08	0
2	09Q	C	211	-	19,21,21	1.26	1 (5%)	21,27,27	1.13	1 (4%)
2	09Q	D	211	-	19,21,21	1.18	1 (5%)	21,27,27	1.08	1 (4%)
2	09Q	E	211	-	19,21,21	1.19	1 (5%)	21,27,27	0.94	1 (4%)
2	09Q	F	211	-	19,21,21	1.16	0	21,27,27	1.05	1 (4%)
2	09Q	G	211	-	19,21,21	1.23	1 (5%)	21,27,27	1.39	2 (9%)
3	SO4	G	212	-	4,4,4	0.14	0	6,6,6	0.12	0
2	09Q	H	211	-	19,21,21	1.17	0	21,27,27	0.88	1 (4%)
2	09Q	H	212	-	19,21,21	1.25	1 (5%)	21,27,27	1.22	3 (14%)
2	09Q	H	213	-	19,21,21	1.27	0	21,27,27	1.11	1 (4%)
2	09Q	I	211	-	19,21,21	1.24	1 (5%)	21,27,27	1.50	2 (9%)
2	09Q	J	211	-	19,21,21	1.16	0	21,27,27	1.15	1 (4%)

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
2	09Q	A	211	-	-	0/8/17/17	0/2/3/3
2	09Q	B	211	-	-	0/8/17/17	0/2/3/3
2	09Q	B	212	-	-	0/8/17/17	0/2/3/3
2	09Q	B	213	-	-	0/8/17/17	0/2/3/3
3	SO4	B	214	-	-	0/0/0/0	0/0/0/0
3	SO4	B	215	-	-	0/0/0/0	0/0/0/0
2	09Q	C	211	-	-	0/8/17/17	0/2/3/3
2	09Q	D	211	-	-	0/8/17/17	0/2/3/3
2	09Q	E	211	-	-	0/8/17/17	0/2/3/3
2	09Q	F	211	-	-	0/8/17/17	0/2/3/3
2	09Q	G	211	-	-	0/8/17/17	0/2/3/3
3	SO4	G	212	-	-	0/0/0/0	0/0/0/0
2	09Q	H	211	-	-	0/8/17/17	0/2/3/3
2	09Q	H	212	-	-	0/8/17/17	0/2/3/3
2	09Q	H	213	-	-	0/8/17/17	0/2/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	09Q	I	211	-	-	0/8/17/17	0/2/3/3
2	09Q	J	211	-	-	0/8/17/17	0/2/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	211	09Q	C7-C11	2.01	1.42	1.38
2	G	211	09Q	C7-C11	2.05	1.42	1.38
2	H	212	09Q	C7-C11	2.06	1.42	1.38
2	D	211	09Q	C7-C11	2.15	1.42	1.38
2	A	211	09Q	C7-C11	2.17	1.42	1.38
2	B	212	09Q	C7-C11	2.18	1.42	1.38
2	C	211	09Q	C7-C11	2.19	1.42	1.38
2	I	211	09Q	C7-C11	2.33	1.43	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	211	09Q	C10-C11-C7	-5.64	114.25	119.36
2	A	211	09Q	C10-C11-C7	-4.65	115.15	119.36
2	G	211	09Q	C10-C11-C7	-4.50	115.29	119.36
2	J	211	09Q	C10-C11-C7	-4.48	115.30	119.36
2	C	211	09Q	C10-C11-C7	-4.34	115.43	119.36
2	D	211	09Q	C10-C11-C7	-4.28	115.49	119.36
2	B	213	09Q	C10-C11-C7	-3.99	115.75	119.36
2	F	211	09Q	C10-C11-C7	-3.83	115.89	119.36
2	H	212	09Q	C10-C11-C7	-3.75	115.97	119.36
2	H	213	09Q	C10-C11-C7	-3.74	115.97	119.36
2	E	211	09Q	C10-C11-C7	-3.63	116.07	119.36
2	B	212	09Q	C10-C11-C7	-3.60	116.10	119.36
2	B	211	09Q	C10-C11-C7	-3.51	116.18	119.36
2	H	211	09Q	C10-C11-C7	-3.26	116.41	119.36
2	A	211	09Q	C10-C9-C1	-2.33	116.93	120.88
2	A	211	09Q	C8-C9-C1	2.13	125.54	121.81
2	H	212	09Q	C15-C16-N1	2.13	117.36	113.16
2	I	211	09Q	C11-C7-N3	2.13	125.56	122.97
2	B	211	09Q	C16-C15-N2	2.46	116.33	112.87
2	G	211	09Q	C16-C15-N2	2.59	116.51	112.87
2	H	212	09Q	C16-C15-N2	2.90	116.96	112.87
2	B	213	09Q	C16-C15-N2	2.91	116.97	112.87
2	A	211	09Q	C7-C11-N1	3.49	125.44	120.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	211	09Q	1	0
2	B	211	09Q	3	0
2	B	212	09Q	7	0
2	B	213	09Q	2	0
2	C	211	09Q	1	0
2	D	211	09Q	2	0
2	E	211	09Q	1	0
2	F	211	09Q	3	0
2	G	211	09Q	2	0
2	H	211	09Q	2	0
2	H	212	09Q	3	0
2	H	213	09Q	3	0
2	I	211	09Q	4	0
2	J	211	09Q	1	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 ⓘ

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%)	-0.12	5 (2%)	58	65	14, 26, 59, 78	0
1	B	205/210 (97%)	-0.05	5 (2%)	59	66	12, 26, 58, 85	0
1	C	201/210 (95%)	-0.13	6 (2%)	51	58	12, 24, 55, 84	0
1	D	199/210 (94%)	-0.18	2 (1%)	82	86	12, 24, 50, 74	0
1	E	206/210 (98%)	-0.08	6 (2%)	52	59	12, 23, 61, 93	0
1	F	202/210 (96%)	-0.02	6 (2%)	51	58	13, 26, 63, 86	0
1	G	200/210 (95%)	-0.09	4 (2%)	65	72	12, 25, 61, 85	0
1	H	200/210 (95%)	-0.16	6 (3%)	51	58	12, 24, 54, 81	0
1	I	204/210 (97%)	-0.16	2 (0%)	82	86	12, 24, 58, 84	0
1	J	200/210 (95%)	-0.08	3 (1%)	74	79	13, 24, 60, 92	0
All	All	2019/2100 (96%)	-0.11	45 (2%)	62	69	12, 25, 61, 93	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	187	CYS	5.1
1	F	187	CYS	5.0
1	E	188	CYS	4.8
1	J	24	ASP	4.2
1	A	23	ARG	4.1
1	B	68	SER	3.6
1	G	162	SER	3.6
1	A	24	ASP	3.5
1	G	161	ASP	3.3
1	A	205	GLY	3.3
1	E	186	SER	3.1
1	H	61	ARG	3.0
1	C	22	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	161	ASP	2.8
1	D	162	SER	2.8
1	B	24	ASP	2.7
1	H	69	HIS	2.7
1	I	69	HIS	2.7
1	D	1	LEU	2.6
1	E	68	SER	2.6
1	J	1	LEU	2.6
1	E	185	TYR	2.5
1	A	131	GLU	2.5
1	G	132	SER	2.4
1	I	158	ASN	2.4
1	H	22	GLN	2.4
1	C	24	ASP	2.3
1	C	187	CYS	2.3
1	F	156	THR	2.2
1	B	129	ASP	2.2
1	H	23	ARG	2.2
1	E	24	ASP	2.2
1	A	69	HIS	2.2
1	B	23	ARG	2.1
1	B	2	ASP	2.1
1	C	68	SER	2.1
1	J	161	ASP	2.1
1	F	188	CYS	2.1
1	G	160	ASP	2.1
1	H	24	ASP	2.1
1	F	185	TYR	2.1
1	C	205	GLY	2.1
1	C	160	ASP	2.0
1	F	1	LEU	2.0
1	F	68	SER	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 carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	09Q	A	211	19/19	0.91	0.22	3.74	29,38,76,76	0
2	09Q	B	213	19/19	0.83	0.23	2.04	39,47,65,71	0
2	09Q	H	211	19/19	0.96	0.14	1.59	13,23,28,31	0
2	09Q	H	212	19/19	0.93	0.15	1.52	20,34,48,53	0
2	09Q	H	213	19/19	0.93	0.17	1.02	16,44,66,67	0
2	09Q	D	211	19/19	0.97	0.14	0.61	11,21,40,44	0
2	09Q	B	212	19/19	0.90	0.17	0.43	33,53,73,75	0
2	09Q	B	211	19/19	0.96	0.14	0.38	20,29,35,40	0
2	09Q	G	211	19/19	0.95	0.13	0.34	9,24,39,40	0
2	09Q	C	211	19/19	0.95	0.14	0.27	17,26,47,50	0
3	SO4	G	212	5/5	0.74	0.18	0.24	119,127,137,139	0
2	09Q	J	211	19/19	0.96	0.14	0.04	17,33,42,45	0
2	09Q	F	211	19/19	0.96	0.16	-0.07	16,26,47,47	0
2	09Q	I	211	19/19	0.96	0.12	-0.11	16,27,47,48	0
3	SO4	B	214	5/5	0.97	0.15	-0.30	36,86,102,106	0
2	09Q	E	211	19/19	0.98	0.13	-0.49	14,23,33,37	0
3	SO4	B	215	5/5	0.97	0.12	-0.89	62,65,83,88	0

6.5 Other polymers ⓘ

There are no such residues in this entry.