



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:39 PM GMT

PDB ID : 2WZY
Title : CRYSTAL STRUCTURE OF A-ACHBP IN COMPLEX WITH 13-DESMETHYL SPIROLIDE C
Authors : Bourne, Y.; Radic, Z.; Araoz, R.; Talley, T.T.; Benoit, E.; Servent, D.; Taylor, P.; Molgo, J.; Marchot, P.
Deposited on : 2009-12-03
Resolution : 2.51 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

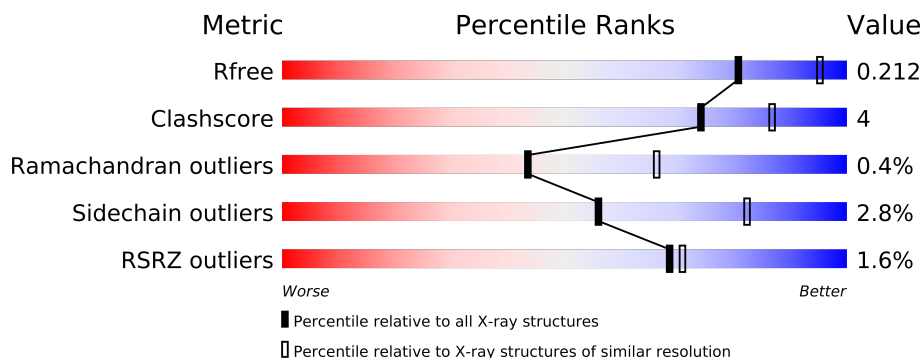
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.51 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	228	
1	B	228	
1	C	228	
1	D	228	
1	E	228	
1	F	228	
1	G	228	
1	H	228	
1	I	228	
1	J	228	

2 Entry composition

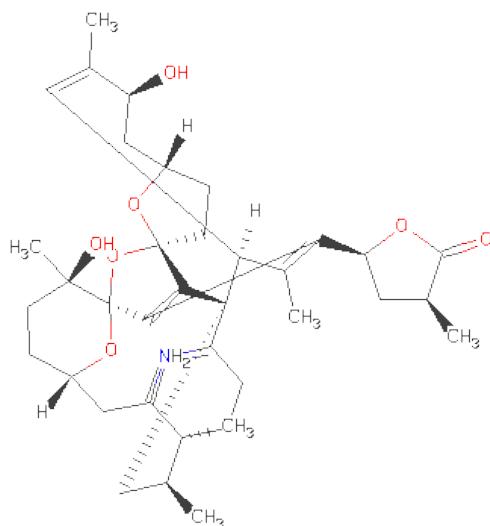
There are 3 unique types of molecules in this entry. The entry contains 18450 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SOLUBLE ACETYLCHOLINE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	4	0
			1724	1090	285	339	10			
1	B	213	Total	C	N	O	S	0	3	0
			1716	1082	286	339	9			
1	C	213	Total	C	N	O	S	0	3	0
			1702	1076	282	334	10			
1	D	211	Total	C	N	O	S	0	3	0
			1701	1074	286	332	9			
1	E	210	Total	C	N	O	S	0	3	0
			1698	1074	284	331	9			
1	F	208	Total	C	N	O	S	0	3	0
			1680	1062	280	329	9			
1	G	212	Total	C	N	O	S	0	3	0
			1710	1080	282	337	11			
1	H	211	Total	C	N	O	S	0	2	0
			1695	1071	282	333	9			
1	I	209	Total	C	N	O	S	0	5	0
			1703	1079	282	332	10			
1	J	212	Total	C	N	O	S	0	3	0
			1713	1081	285	337	10			

- Molecule 2 is 13-DESMETHYL SPIROLIDE C (three-letter code: SQX) (formula: C₄₂H₆₃NO₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			50	42	1	7		
2	B	1	Total	C	N	O	0	0
			50	42	1	7		
2	C	1	Total	C	N	O	0	0
			50	42	1	7		
2	D	1	Total	C	N	O	0	0
			50	42	1	7		
2	E	1	Total	C	N	O	0	0
			50	42	1	7		
2	F	1	Total	C	N	O	0	0
			50	42	1	7		
2	G	1	Total	C	N	O	0	0
			50	42	1	7		
2	H	1	Total	C	N	O	0	0
			50	42	1	7		
2	I	1	Total	C	N	O	0	0
			50	42	1	7		
2	J	1	Total	C	N	O	0	0
			50	42	1	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	95	Total	O	0	0
			95	95		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	99	Total 99	O 99	0	0
3	D	102	Total 102	O 102	0	0
3	E	79	Total 79	O 79	0	0
3	F	95	Total 95	O 95	0	0
3	G	78	Total 78	O 78	0	0
3	H	95	Total 95	O 95	0	0
3	I	108	Total 108	O 108	0	0
3	J	99	Total 99	O 99	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain A: 



• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain B: 



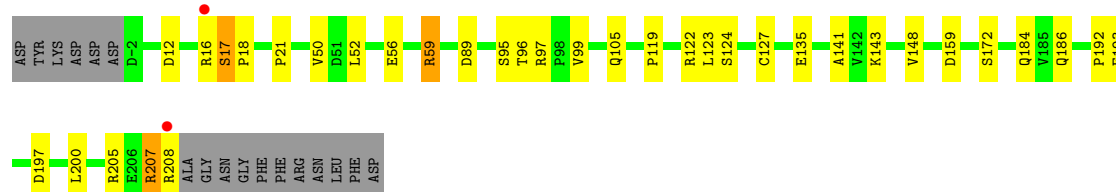
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain C: 



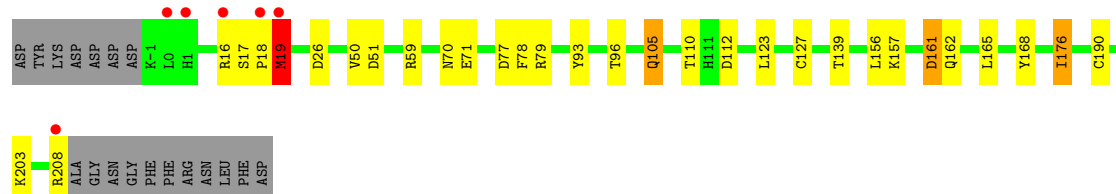
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain D: 



• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain E: 



- Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain F:



ASP

- Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain G:



- Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain H:



- Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain I:



- Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.63Å 131.75Å 125.59Å 90.00° 90.42° 90.00°	Depositor
Resolution (Å)	20.00 – 2.51 19.97 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.51) 96.7 (19.97-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.176 , 0.237 0.185 , 0.212	Depositor DCC
R_{free} test set	1705 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 22.0	EDS
Estimated twinning fraction	0.019 for -h,-l,-k 0.014 for -h,l,k 0.108 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 85215 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18450	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.43	0/1776	0.59	0/2420
1	B	0.44	0/1766	0.58	0/2406
1	C	0.44	0/1751	0.62	0/2386
1	D	0.46	0/1751	0.64	2/2386 (0.1%)
1	E	0.44	0/1748	0.60	0/2380
1	F	0.44	0/1729	0.60	0/2355
1	G	0.44	0/1760	0.60	0/2397
1	H	0.48	0/1742	0.60	0/2374
1	I	0.45	0/1760	0.63	0/2398
1	J	0.48	0/1763	0.60	0/2401
All	All	0.45	0/17546	0.61	2/23903 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	207[A]	ARG	C-N-CA	5.57	135.63	121.70
1	D	207[B]	ARG	C-N-CA	5.57	135.63	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	190	CYS	Peptide
1	G	190	CYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1724	0	1658	19	0
1	B	1716	0	1657	15	0
1	C	1702	0	1632	15	0
1	D	1701	0	1643	21	0
1	E	1698	0	1652	19	0
1	F	1680	0	1171	9	0
1	G	1710	0	0	4	0
1	H	1695	0	0	3	0
1	I	1703	0	0	2	0
1	J	1713	0	0	1	0
2	A	50	0	63	4	0
2	B	50	0	63	2	0
2	C	50	0	63	2	0
2	D	50	0	63	2	0
2	E	50	0	63	2	0
2	F	50	0	63	2	0
2	G	50	0	63	2	0
2	H	50	0	63	1	0
2	I	50	0	63	1	0
2	J	50	0	63	2	0
3	A	58	0	0	0	0
3	B	95	0	0	1	0
3	C	99	0	0	0	0
3	D	102	0	0	0	0
3	E	79	0	0	1	0
3	F	95	0	0	1	0
3	G	78	0	0	0	0
3	H	95	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	108	0	0	0	0
3	J	99	0	0	2	0
All	All	18450	0	10043	111	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (111) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:-3:ASP:H2	1:A:-1:LYS:N	1.73	0.86
1:C:207[A]:ARG:HH21	1:C:207[A]:ARG:HB3	1.45	0.81
1:E:168:TYR:CG	1:E:176:ILE:HD11	2.14	0.81
1:A:-3:ASP:H3	1:A:-2:ASP:HB2	1.45	0.80
1:D:17:SER:HB2	1:D:18:PRO:HA	1.62	0.80
1:B:59[B]:ARG:HB2	1:B:59[B]:ARG:HH11	1.51	0.76
2:J:301:SQX:H331	2:J:301:SQX:H192	1.69	0.74
2:D:301:SQX:H331	2:D:301:SQX:H192	1.67	0.74
2:E:301:SQX:H192	2:E:301:SQX:H331	1.70	0.73
1:E:18:PRO:HA	1:E:19:MET:HB2	1.71	0.72
1:E:105:GLN:HE21	1:E:105:GLN:HA	1.58	0.69
2:B:301:SQX:H331	2:B:301:SQX:H192	1.76	0.67
2:F:301:SQX:H192	2:F:301:SQX:H331	1.76	0.66
1:B:59[B]:ARG:HB2	1:B:59[B]:ARG:NH1	2.10	0.66
1:A:-3:ASP:N	1:A:-2:ASP:HB2	2.12	0.65
1:I:0:LEU:N	1:I:1:HIS:CB	2.63	0.62
1:A:-3:ASP:H2	1:A:-1:LYS:H	1.46	0.62
1:E:18:PRO:HA	1:E:19:MET:CB	2.29	0.62
1:D:172:SER:O	1:D:207[A]:ARG:HD2	1.98	0.62
1:E:17:SER:HB2	1:E:18:PRO:HD2	1.83	0.61
1:E:168:TYR:CD2	1:E:176:ILE:HD11	2.36	0.60
1:D:59[B]:ARG:NH1	1:D:159:ASP:OD1	2.33	0.60
2:I:301:SQX:H192	2:I:301:SQX:H331	1.84	0.60
1:D:143:LYS:NZ	1:D:184:GLN:HE22	2.01	0.59
1:D:122:ARG:HD2	1:E:96:THR:O	2.03	0.58
2:A:301:SQX:H192	2:A:301:SQX:H331	1.86	0.58
1:A:207:ARG:O	1:A:208:ARG:HB2	2.03	0.58
2:H:301:SQX:H331	2:H:301:SQX:H192	1.86	0.57
1:C:6:LEU:HD23	1:D:21:PRO:HB2	1.86	0.56
1:E:105:GLN:NE2	1:E:105:GLN:HA	2.19	0.56
1:C:50:VAL:HG21	1:C:127:CYS:SG	2.47	0.55
1:A:-3:ASP:N	1:A:-1:LYS:N	2.52	0.55
1:E:157:LYS:NZ	3:E:2052:HOH:O	2.39	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:59[B]:ARG:NH2	1:B:159:ASP:OD2	2.40	0.54
1:A:-3:ASP:N	1:A:-1:LYS:H	2.05	0.54
1:A:12:ASP:HA	1:A:16:ARG:HG2	1.88	0.54
1:C:122:ARG:HD2	1:D:96:THR:O	2.07	0.54
2:G:301:SQX:H331	2:G:301:SQX:H192	1.89	0.54
1:F:50:VAL:HG21	1:F:127:CYS:SG	2.48	0.54
1:B:93:TYR:HB3	2:B:301:SQX:H72C	1.90	0.53
1:F:184:GLN:NE2	1:F:197:ASP:OD1	2.41	0.53
1:D:184:GLN:NE2	1:D:197:ASP:OD1	2.37	0.52
1:B:105:GLN:HE21	1:B:105:GLN:HA	1.75	0.52
1:A:93:TYR:HB3	2:A:301:SQX:H72C	1.92	0.52
1:A:172:SER:O	1:A:207:ARG:HD3	2.09	0.52
1:C:5:ASN:HD22	1:C:73:GLY:HA3	1.75	0.52
1:F:122:ARG:HD2	1:G:96:THR:O	2.10	0.52
1:C:77:ASP:OD1	1:C:79:ARG:NH2	2.41	0.51
1:F:74:ASN:ND2	3:F:2026:HOH:O	2.42	0.51
1:D:89:ASP:OD2	1:D:148:VAL:HG22	2.11	0.50
1:D:143:LYS:HZ3	1:D:184:GLN:HE22	1.58	0.50
1:E:165:LEU:HD22	1:E:176:ILE:HD13	1.94	0.49
1:D:135:GLU:O	1:D:205:ARG:NH2	2.45	0.49
2:C:301:SQX:H192	2:C:301:SQX:H331	1.95	0.48
1:B:105:GLN:NE2	1:B:105:GLN:HA	2.28	0.48
1:G:171:SER:O	1:H:48:ASN:ND2	2.47	0.47
1:D:17:SER:CB	1:D:18:PRO:HA	2.37	0.47
1:C:5:ASN:ND2	1:C:73:GLY:HA3	2.29	0.47
1:D:12:ASP:HA	1:D:16:ARG:HB2	1.96	0.47
1:C:79:ARG:NH1	2:D:301:SQX:H531	2.29	0.47
1:E:161:ASP:HB3	1:E:162:GLN:HE21	1.81	0.46
1:A:195:TYR:CZ	2:A:301:SQX:H802	2.51	0.46
1:D:56:GLU:O	1:D:119:PRO:HD2	2.16	0.46
1:A:-1:LYS:HG3	1:B:27:ASP:OD2	2.16	0.45
1:I:155:ASP:OD2	1:I:157:LYS:NZ	2.49	0.45
1:D:105:GLN:HE21	1:D:105:GLN:HA	1.81	0.45
1:C:-4:ASP:O	1:C:-3:ASP:CB	2.65	0.45
1:B:7:MET:HG3	1:C:21:PRO:HG3	1.99	0.45
1:C:105:GLN:HE21	1:C:105:GLN:HA	1.82	0.45
1:A:195:TYR:OH	2:A:301:SQX:H802	2.16	0.45
1:E:110:THR:HG22	1:E:112:ASP:H	1.82	0.45
1:J:74:ASN:ND2	3:J:2026:HOH:O	2.50	0.45
1:F:99:VAL:HG11	1:F:121:GLN:OE1	2.18	0.44
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.57	0.44
1:E:17:SER:HB2	1:E:18:PRO:CD	2.46	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:139:THR:HG23	1:E:203[A]:LYS:HG2	1.99	0.44
1:A:50:VAL:HG21	1:A:127:CYS:SG	2.58	0.44
1:C:8:ARG:NH2	1:C:71:GLU:O	2.41	0.44
1:H:97[B]:ARG:NH2	3:H:2042:HOH:O	2.49	0.44
1:A:187[B]:HIS:N	1:A:187[B]:HIS:ND1	2.66	0.44
1:A:188[C]:TYR:HB3	1:A:190:CYS:HB3	1.99	0.43
1:C:191:CYS:SG	2:C:301:SQX:H801	2.59	0.43
1:B:74:ASN:ND2	3:B:2030:HOH:O	2.45	0.43
1:C:207[A]:ARG:HH21	1:C:207[A]:ARG:CB	2.24	0.43
1:D:141:ALA:HA	1:D:200:LEU:O	2.19	0.43
1:B:110:THR:HG22	1:B:111:HIS:N	2.32	0.42
1:D:50:VAL:HG21	1:D:127:CYS:SG	2.59	0.42
1:E:78:PHE:C	1:E:79:ARG:HD2	2.38	0.42
1:C:175:GLU:OE1	1:C:207[B]:ARG:HD3	2.20	0.42
1:D:97[B]:ARG:HD3	1:D:124:SER:CB	2.49	0.42
1:F:95:SER:HB3	1:F:123:LEU:HD11	2.01	0.42
1:B:141:ALA:HA	1:B:200:LEU:O	2.20	0.42
1:G:156:LEU:O	1:G:183:ARG:NE	2.53	0.42
2:F:301:SQX:H331	2:F:301:SQX:H12	1.84	0.41
1:H:103:SER:OG	1:H:120:ALA:N	2.54	0.41
1:F:79:ARG:HD2	1:F:108:VAL:HG22	2.01	0.41
1:A:122:ARG:HD2	1:B:96:THR:O	2.20	0.41
1:A:52:LEU:O	1:A:122:ARG:HA	2.21	0.41
1:E:93:TYR:HB3	2:E:301:SQX:H72C	2.02	0.41
1:E:77:ASP:OD1	1:E:79:ARG:NH2	2.43	0.41
1:D:95:SER:HB3	1:D:123:LEU:HD11	2.03	0.41
1:A:104:PRO:HG2	1:B:89:ASP:HB2	2.03	0.41
1:B:110:THR:CG2	1:B:111:HIS:N	2.84	0.41
1:F:61:LYS:HA	1:F:114:SER:HA	2.03	0.41
1:B:59[B]:ARG:CB	1:B:59[B]:ARG:NH1	2.83	0.41
1:G:-1:LYS:O	1:G:2:SER:N	2.53	0.41
1:F:118:ILE:HD12	2:G:301:SQX:H352	2.02	0.41
1:D:192:PRO:HD2	1:D:193:GLU:OE1	2.21	0.41
2:J:301:SQX:H4	3:J:2018:HOH:O	2.21	0.40
1:D:105:GLN:HA	1:D:105:GLN:NE2	2.36	0.40
1:E:51:ASP:HA	1:E:123:LEU:O	2.20	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	214/228 (94%)	210 (98%)	3 (1%)	1 (0%)	38	60
1	B	214/228 (94%)	211 (99%)	3 (1%)	0	100	100
1	C	213/228 (93%)	203 (95%)	9 (4%)	1 (0%)	38	60
1	D	212/228 (93%)	208 (98%)	3 (1%)	1 (0%)	38	60
1	E	211/228 (92%)	206 (98%)	4 (2%)	1 (0%)	38	60
1	F	208/228 (91%)	201 (97%)	7 (3%)	0	100	100
1	G	213/228 (93%)	209 (98%)	3 (1%)	1 (0%)	38	60
1	H	211/228 (92%)	206 (98%)	5 (2%)	0	100	100
1	I	212/228 (93%)	207 (98%)	4 (2%)	1 (0%)	38	60
1	J	213/228 (93%)	209 (98%)	2 (1%)	2 (1%)	25	42
All	All	2121/2280 (93%)	2070 (98%)	43 (2%)	8 (0%)	43	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	1	HIS
1	C	-3	ASP
1	D	17	SER
1	A	-2	ASP
1	E	19	MET
1	J	17	SER
1	G	0	LEU
1	J	18	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	197/206 (96%)	193 (98%)	4 (2%)	68	89
1	B	196/206 (95%)	194 (99%)	2 (1%)	85	97
1	C	192/206 (93%)	191 (100%)	1 (0%)	94	99
1	D	193/206 (94%)	187 (97%)	6 (3%)	52	79
1	E	194/206 (94%)	183 (94%)	11 (6%)	29	50
1	F	192/206 (93%)	187 (97%)	5 (3%)	59	84
1	G	196/206 (95%)	188 (96%)	8 (4%)	41	67
1	H	193/206 (94%)	186 (96%)	7 (4%)	47	73
1	I	195/206 (95%)	193 (99%)	2 (1%)	85	97
1	J	196/206 (95%)	185 (94%)	11 (6%)	30	51
All	All	1944/2060 (94%)	1887 (97%)	57 (3%)	56	81

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	167	SER
1	A	190	CYS
1	A	191	CYS
1	B	17	SER
1	B	127	CYS
1	C	91	THR
1	D	52	LEU
1	D	59[A]	ARG
1	D	59[B]	ARG
1	D	99	VAL
1	D	186	GLN
1	D	208	ARG
1	E	16	ARG
1	E	19	MET
1	E	26	ASP
1	E	59	ARG
1	E	70	ASN
1	E	71	GLU
1	E	105	GLN
1	E	156	LEU
1	E	161	ASP
1	E	176	ILE
1	E	208	ARG

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Mol	Chain	Res	Type
1	F	11	SER
1	F	79	ARG
1	F	97[A]	ARG
1	F	97[B]	ARG
1	F	135	GLU
1	G	-2	ASP
1	G	0	LEU
1	G	19	MET
1	G	26	ASP
1	G	127	CYS
1	G	136	GLU
1	G	156	LEU
1	G	186	GLN
1	H	16	ARG
1	H	17	SER
1	H	79	ARG
1	H	91	THR
1	H	99	VAL
1	H	161	ASP
1	H	167	SER
1	I	186[A]	GLN
1	I	186[B]	GLN
1	J	0	LEU
1	J	16	ARG
1	J	17	SER
1	J	19	MET
1	J	33	LEU
1	J	71	GLU
1	J	91	THR
1	J	132	VAL
1	J	135	GLU
1	J	178	SER
1	J	193	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	199	ASN
1	B	105	GLN
1	C	3	GLN
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	105	GLN
1	C	111	HIS
1	C	187	HIS
1	D	3	GLN
1	D	105	GLN
1	D	121	GLN
1	D	184	GLN
1	D	186	GLN
1	D	199	ASN
1	E	105	GLN
1	E	162	GLN
1	E	184	GLN
1	F	15	ASN
1	F	70	ASN
1	F	74	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 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	SQX	A	301	-	56,56,56	1.02	2 (3%)	74,88,88	1.57	12 (16%)
2	SQX	B	301	-	56,56,56	1.01	2 (3%)	74,88,88	1.54	11 (14%)
2	SQX	C	301	-	56,56,56	1.03	2 (3%)	74,88,88	1.82	15 (20%)
2	SQX	D	301	-	56,56,56	1.05	1 (1%)	74,88,88	1.48	12 (16%)
2	SQX	E	301	-	56,56,56	1.05	1 (1%)	74,88,88	1.68	12 (16%)
2	SQX	F	301	-	56,56,56	1.04	1 (1%)	74,88,88	1.55	12 (16%)
2	SQX	G	301	-	56,56,56	1.06	2 (3%)	74,88,88	1.50	12 (16%)
2	SQX	H	301	-	56,56,56	1.00	1 (1%)	74,88,88	1.65	13 (17%)
2	SQX	I	301	-	56,56,56	1.08	2 (3%)	74,88,88	1.55	13 (17%)
2	SQX	J	301	-	56,56,56	1.10	2 (3%)	74,88,88	1.63	13 (17%)

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	SQX	A	301	-	-	0/24/122/122	0/1/7/7
2	SQX	B	301	-	-	0/24/122/122	0/1/7/7
2	SQX	C	301	-	-	0/24/122/122	0/1/7/7
2	SQX	D	301	-	-	0/24/122/122	0/1/7/7
2	SQX	E	301	-	-	0/24/122/122	0/1/7/7
2	SQX	F	301	-	-	0/24/122/122	0/1/7/7
2	SQX	G	301	-	-	0/24/122/122	0/1/7/7
2	SQX	H	301	-	-	0/24/122/122	0/1/7/7
2	SQX	I	301	-	-	0/24/122/122	0/1/7/7
2	SQX	J	301	-	-	0/24/122/122	0/1/7/7

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	SQX	O1-C5	6.51	1.45	1.35
2	J	301	SQX	O1-C5	6.41	1.45	1.35
2	E	301	SQX	O1-C5	6.32	1.45	1.35
2	A	301	SQX	O1-C5	6.22	1.45	1.35
2	D	301	SQX	O1-C5	6.03	1.44	1.35
2	G	301	SQX	O1-C5	5.99	1.44	1.35
2	F	301	SQX	O1-C5	5.94	1.44	1.35
2	H	301	SQX	O1-C5	5.93	1.44	1.35
2	C	301	SQX	O1-C5	5.88	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	SQX	O1-C5	5.84	1.44	1.35
2	G	301	SQX	C13-C8	2.85	1.36	1.33
2	C	301	SQX	O1-C2	-2.45	1.42	1.45
2	J	301	SQX	C2-C8	-2.26	1.50	1.51
2	I	301	SQX	C13-C8	2.21	1.36	1.33
2	B	301	SQX	C13-C8	2.14	1.36	1.33
2	A	301	SQX	C13-C8	2.00	1.36	1.33

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	SQX	O1-C2-C3	6.52	108.03	104.14
2	E	301	SQX	O1-C2-C3	6.37	107.94	104.14
2	J	301	SQX	O1-C2-C3	6.36	107.93	104.14
2	H	301	SQX	C29-C30-N31	-6.26	105.60	112.32
2	C	301	SQX	C2-O1-C5	-6.21	105.42	110.24
2	H	301	SQX	O1-C2-C3	5.90	107.66	104.14
2	E	301	SQX	C2-O1-C5	-5.84	105.71	110.24
2	A	301	SQX	O1-C2-C3	5.20	107.24	104.14
2	D	301	SQX	C29-C30-N31	-5.06	106.89	112.32
2	G	301	SQX	O1-C2-C3	4.98	107.11	104.14
2	I	301	SQX	O1-C2-C3	4.95	107.09	104.14
2	F	301	SQX	O1-C2-C3	4.86	107.04	104.14
2	B	301	SQX	C2-O1-C5	-4.54	106.72	110.24
2	J	301	SQX	C2-O1-C5	-4.53	106.73	110.24
2	B	301	SQX	C30-N31-C32	4.51	132.77	118.76
2	B	301	SQX	O1-C2-C3	4.34	106.73	104.14
2	G	301	SQX	C30-N31-C32	4.32	132.16	118.76
2	E	301	SQX	C30-N31-C32	4.30	132.13	118.76
2	H	301	SQX	C30-N31-C32	4.25	131.96	118.76
2	I	301	SQX	C2-O1-C5	-4.25	106.95	110.24
2	J	301	SQX	C30-N31-C32	4.23	131.89	118.76
2	I	301	SQX	C30-N31-C32	4.22	131.86	118.76
2	C	301	SQX	C29-C30-N31	-4.20	107.81	112.32
2	F	301	SQX	C30-N31-C32	4.13	131.59	118.76
2	C	301	SQX	C30-N31-C32	3.99	131.14	118.76
2	F	301	SQX	C29-C30-N31	-3.94	108.09	112.32
2	A	301	SQX	O47-C48-C37	3.93	109.83	105.98
2	I	301	SQX	C29-C30-N31	-3.93	108.10	112.32
2	D	301	SQX	C30-N31-C32	3.93	130.95	118.76
2	A	301	SQX	C30-N31-C32	3.90	130.87	118.76
2	A	301	SQX	C29-C30-N31	-3.77	108.27	112.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	SQX	C2-O1-C5	-3.74	107.34	110.24
2	F	301	SQX	C2-O1-C5	-3.70	107.37	110.24
2	A	301	SQX	C2-O1-C5	-3.70	107.37	110.24
2	B	301	SQX	C29-C30-N31	-3.60	108.46	112.32
2	H	301	SQX	C2-O1-C5	-3.57	107.47	110.24
2	C	301	SQX	C3-C4-C5	-3.56	99.33	102.51
2	C	301	SQX	O1-C5-C4	3.55	114.41	110.37
2	E	301	SQX	O1-C5-C4	3.48	114.33	110.37
2	G	301	SQX	C2-O1-C5	-3.47	107.55	110.24
2	I	301	SQX	C37-C36-C38	-3.46	117.60	120.89
2	G	301	SQX	O47-C48-C37	3.39	109.30	105.98
2	D	301	SQX	O1-C2-C3	3.34	106.13	104.14
2	B	301	SQX	O1-C5-C4	3.31	114.13	110.37
2	C	301	SQX	C37-C36-C38	-3.29	117.76	120.89
2	E	301	SQX	O6-C5-C4	-3.28	123.97	128.53
2	A	301	SQX	C4-C3-C2	3.19	107.95	102.63
2	A	301	SQX	O6-C5-C4	-3.18	124.11	128.53
2	B	301	SQX	O6-C5-C4	-3.14	124.17	128.53
2	J	301	SQX	C29-C30-N31	-3.13	108.96	112.32
2	H	301	SQX	C37-C36-C38	-3.11	117.93	120.89
2	I	301	SQX	O6-C5-C4	-3.05	124.29	128.53
2	D	301	SQX	C49-C50-C51	3.04	115.77	112.98
2	J	301	SQX	O47-C48-C37	3.03	108.95	105.98
2	A	301	SQX	O1-C5-C4	3.00	113.78	110.37
2	E	301	SQX	C29-C30-N31	-2.98	109.12	112.32
2	G	301	SQX	C29-C30-N31	-2.94	109.17	112.32
2	B	301	SQX	O48-C23-C80	2.92	108.05	104.44
2	D	301	SQX	C37-C36-C38	-2.91	118.12	120.89
2	F	301	SQX	C19-C16-C17	2.86	120.86	115.30
2	F	301	SQX	C50-C49-C48	2.81	115.37	110.25
2	J	301	SQX	C14-C13-C8	-2.79	118.21	123.84
2	B	301	SQX	C37-C36-C38	-2.75	118.27	120.89
2	H	301	SQX	C55-C42-C43	2.73	107.23	103.20
2	J	301	SQX	C19-C16-C17	2.72	120.58	115.30
2	G	301	SQX	C4-C3-C2	2.70	107.13	102.63
2	J	301	SQX	O48-C23-C80	2.68	107.76	104.44
2	C	301	SQX	O48-C23-C80	2.66	107.73	104.44
2	G	301	SQX	O48-C23-C80	2.63	107.70	104.44
2	E	301	SQX	C19-C16-C17	2.61	120.37	115.30
2	A	301	SQX	C19-C16-C17	2.58	120.31	115.30
2	I	301	SQX	C55-C42-C43	2.58	107.01	103.20
2	I	301	SQX	C4-C3-C2	2.55	106.89	102.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	SQX	C19-C16-C17	2.53	120.21	115.30
2	I	301	SQX	C14-C13-C8	-2.53	118.75	123.84
2	D	301	SQX	C55-C42-C43	2.49	106.88	103.20
2	H	301	SQX	C4-C3-C2	2.44	106.71	102.63
2	D	301	SQX	C34-C35-C36	-2.45	110.11	114.52
2	E	301	SQX	C4-C3-C2	2.43	106.68	102.63
2	C	301	SQX	C14-C13-C8	-2.43	118.95	123.84
2	G	301	SQX	O6-C5-C4	-2.41	125.19	128.53
2	E	301	SQX	C55-C42-C43	2.40	106.74	103.20
2	C	301	SQX	O6-C5-C4	-2.40	125.20	128.53
2	G	301	SQX	O1-C5-C4	2.39	113.09	110.37
2	A	301	SQX	C55-C42-C43	2.39	106.73	103.20
2	F	301	SQX	C4-C3-C2	2.38	106.59	102.63
2	J	301	SQX	O6-C5-C4	-2.37	125.24	128.53
2	I	301	SQX	O48-C23-C80	2.37	107.37	104.44
2	B	301	SQX	C4-C3-C2	2.36	106.57	102.63
2	J	301	SQX	C55-C42-C43	2.34	106.65	103.20
2	F	301	SQX	C9-C10-C27	2.33	115.90	112.16
2	G	301	SQX	C55-C42-C43	2.32	106.62	103.20
2	C	301	SQX	C2-C8-C13	-2.30	119.87	122.37
2	C	301	SQX	O47-C48-C37	2.30	108.23	105.98
2	H	301	SQX	C14-C13-C8	-2.30	119.22	123.84
2	F	301	SQX	O1-C5-C4	2.28	112.96	110.37
2	A	301	SQX	O48-C23-C80	2.26	107.24	104.44
2	F	301	SQX	O6-C5-C4	-2.23	125.44	128.53
2	G	301	SQX	C50-C49-C48	2.22	114.29	110.25
2	C	301	SQX	C4-C3-C2	2.22	106.33	102.63
2	E	301	SQX	C3-C4-C5	-2.20	100.54	102.51
2	D	301	SQX	C4-C3-C2	2.20	106.30	102.63
2	E	301	SQX	C50-C49-C48	2.19	114.25	110.25
2	H	301	SQX	O1-C5-C4	2.18	112.86	110.37
2	J	301	SQX	O1-C5-C4	2.16	112.83	110.37
2	B	301	SQX	C18-C21-C81	-2.15	110.88	114.43
2	I	301	SQX	C19-C16-C17	2.14	119.45	115.30
2	C	301	SQX	C55-C42-C43	2.13	106.35	103.20
2	F	301	SQX	O1-C2-C8	-2.13	105.95	109.20
2	A	301	SQX	C37-C36-C38	-2.13	118.87	120.89
2	H	301	SQX	O48-C23-C80	2.12	107.06	104.44
2	H	301	SQX	C43-O44-C23	2.11	115.46	107.83
2	I	301	SQX	O1-C5-C4	2.10	112.76	110.37
2	D	301	SQX	C14-C13-C8	-2.09	119.63	123.84
2	B	301	SQX	C3-C4-C5	-2.08	100.64	102.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	SQX	C19-C16-C17	2.08	119.35	115.30
2	J	301	SQX	O1-C2-C8	-2.08	106.02	109.20
2	H	301	SQX	O6-C5-C4	-2.07	125.65	128.53
2	F	301	SQX	O48-C23-C80	2.07	107.00	104.44
2	C	301	SQX	C42-C55-C23	2.07	105.61	103.22
2	I	301	SQX	C3-C4-C5	-2.04	100.68	102.51
2	J	301	SQX	C4-C3-C2	2.04	106.03	102.63
2	H	301	SQX	C49-C48-C37	-2.03	108.92	112.40
2	D	301	SQX	O48-C23-C80	2.02	106.94	104.44
2	E	301	SQX	C14-C13-C8	-2.02	119.78	123.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	212/228 (92%)	-0.06	6 (2%)	50	53	32, 49, 81, 104	0
1	B	213/228 (93%)	-0.26	3 (1%)	72	74	30, 43, 66, 91	0
1	C	213/228 (93%)	-0.27	1 (0%)	88	90	26, 41, 78, 102	0
1	D	211/228 (92%)	-0.24	2 (0%)	81	82	27, 42, 79, 93	0
1	E	210/228 (92%)	-0.22	6 (2%)	49	51	30, 44, 77, 96	0
1	F	208/228 (91%)	-0.29	3 (1%)	72	74	28, 42, 80, 96	0
1	G	212/228 (92%)	-0.17	6 (2%)	50	53	31, 44, 84, 111	0
1	H	211/228 (92%)	-0.34	0	100	100	30, 41, 72, 88	0
1	I	209/228 (91%)	-0.39	2 (0%)	79	81	29, 40, 62, 70	0
1	J	212/228 (92%)	-0.32	4 (1%)	64	66	28, 39, 74, 100	0
All	All	2111/2280 (92%)	-0.25	33 (1%)	68	71	26, 42, 78, 111	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	ALA	5.7
1	E	19	MET	5.3
1	A	19[A]	MET	4.9
1	G	19	MET	4.6
1	E	0	LEU	4.3
1	J	1	HIS	4.3
1	G	-3	ASP	3.6
1	J	-3	ASP	3.5
1	E	18	PRO	3.5
1	A	188[B]	TYR	3.4
1	G	-2	ASP	3.3
1	G	1	HIS	3.3
1	G	18	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	1	HIS	2.9
1	B	-3	ASP	2.9
1	I	0	LEU	2.8
1	F	0	LEU	2.8
1	B	0	LEU	2.7
1	J	208	ARG	2.6
1	E	1	HIS	2.5
1	A	-2	ASP	2.5
1	A	208	ARG	2.5
1	D	208	ARG	2.5
1	F	18	PRO	2.3
1	J	16	ARG	2.2
1	A	191	CYS	2.2
1	D	16	ARG	2.2
1	A	189	SER	2.1
1	I	208	ARG	2.1
1	E	16	ARG	2.1
1	E	208	ARG	2.1
1	F	16	ARG	2.1
1	G	14	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SQX	F	301	50/50	0.13	0.98	33,39,41,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SQX	D	301	50/50	0.14	0.87	33,36,37,38	0
2	SQX	C	301	50/50	0.13	0.50	31,38,41,42	0
2	SQX	J	301	50/50	0.12	0.12	31,35,39,41	0
2	SQX	E	301	50/50	0.12	0.11	36,39,41,43	0
2	SQX	B	301	50/50	0.13	-0.06	37,42,45,45	0
2	SQX	G	301	50/50	0.12	-0.17	37,44,46,47	0
2	SQX	A	301	50/50	0.14	-0.37	46,50,53,54	0
2	SQX	I	301	50/50	0.12	-0.41	34,38,41,44	0
2	SQX	H	301	50/50	0.11	-0.59	32,37,39,40	0

6.5 Other polymers

There are no such residues in this entry.