



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:59 am GMT

PDB ID : 3EW2
Title : Crystal structure of rhizavidin-biotin complex
Authors : Livnah, O.; Meir, A.
Deposited on : 2008-10-14
Resolution : 2.30 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 : trunk28620
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) : recalc28949

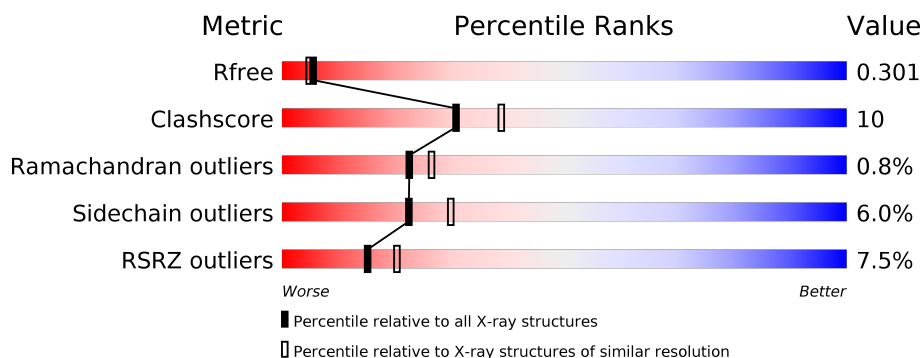
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	135	<div> <div style="width: 63%;"></div> <div style="width: 19%;"></div> <div style="width: 16%;"></div> </div>
1	B	135	<div>4%</div> <div> <div style="width: 76%;"></div> <div style="width: 13%;"></div> <div style="width: 10%;"></div> </div>
1	C	135	<div>5%</div> <div> <div style="width: 75%;"></div> <div style="width: 15%;"></div> <div style="width: 8%;"></div> </div>
1	D	135	<div>16%</div> <div> <div style="width: 43%;"></div> <div style="width: 22%;"></div> <div style="width: 5%;"></div> <div style="width: 30%;"></div> </div>
1	E	135	<div>%</div> <div> <div style="width: 83%;"></div> <div style="width: 5%;"></div> <div style="width: 12%;"></div> </div>
1	F	135	<div>12%</div> <div> <div style="width: 61%;"></div> <div style="width: 23%;"></div> <div style="width: 12%;"></div> </div>

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Mol	Chain	Length	Quality of chain
1	G	135	<div><div></div><div>6%</div><div>60%</div><div>21%</div><div>•</div><div>19%</div></div>

2 Entry composition [i](#)

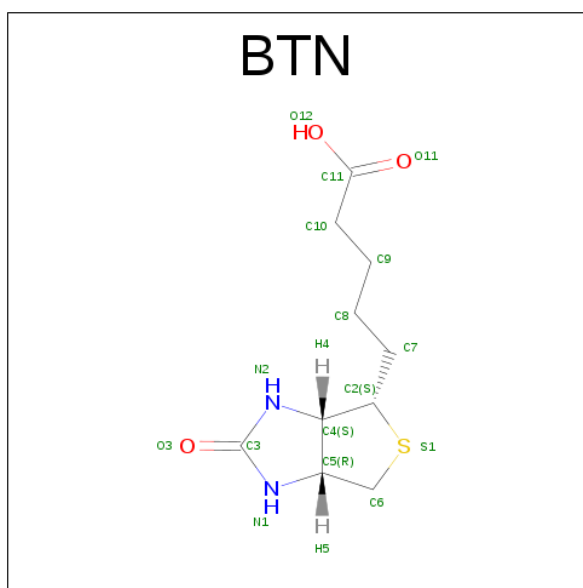
There are 3 unique types of molecules in this entry. The entry contains 6236 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 rhizavidin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			854	523	147	181	3			
1	B	121	Total	C	N	O	S	0	0	0
			904	554	154	193	3			
1	C	124	Total	C	N	O	S	0	0	0
			932	573	159	197	3			
1	D	95	Total	C	N	O	S	0	0	0
			707	438	121	145	3			
1	E	119	Total	C	N	O	S	0	0	0
			885	541	152	189	3			
1	F	119	Total	C	N	O	S	0	0	0
			896	549	155	189	3			
1	G	110	Total	C	N	O	S	0	0	0
			824	505	143	173	3			

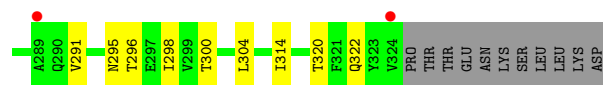
- Molecule 2 is BIOTIN (three-letter code: BTN) (formula: $C_{10}H_{16}N_2O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	B	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	C	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	D	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	E	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	F	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	G	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	30	Total	O	0	0
			30	30		
3	C	19	Total	O	0	0
			19	19		
3	D	5	Total	O	0	0
			5	5		
3	E	24	Total	O	0	0
			24	24		
3	F	13	Total	O	0	0
			13	13		
3	G	11	Total	O	0	0
			11	11		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	45.65Å 130.03Å 237.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 47.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.30) 98.7 (47.51-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.213 , 0.304 0.212 , 0.301	Depositor DCC
R_{free} test set	1607 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.900	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6236	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: BTN

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	0.86	0/874	0.83	0/1195
1	B	0.91	0/925	0.89	1/1264 (0.1%)
1	C	0.72	0/954	0.70	0/1302
1	D	0.59	0/723	0.67	0/984
1	E	0.84	0/905	0.79	0/1237
1	F	0.67	0/914	0.79	1/1244 (0.1%)
1	G	0.62	0/843	0.70	0/1151
All	All	0.76	0/6138	0.77	2/8377 (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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	132	LEU	CA-CB-CG	5.82	128.68	115.30
1	B	257	LEU	CA-CB-CG	5.45	127.83	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	80	ASN	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	854	0	765	15	0
1	B	904	0	809	13	0
1	C	932	0	837	22	0
1	D	707	0	632	27	0
1	E	885	0	796	3	0
1	F	896	0	813	32	0
1	G	824	0	738	16	0
2	A	16	0	15	2	0
2	B	16	0	15	0	0
2	C	16	0	15	0	0
2	D	16	0	15	2	0
2	E	16	0	15	0	0
2	F	16	0	15	4	0
2	G	16	0	15	0	0
3	A	20	0	0	2	0
3	B	30	0	0	2	1
3	C	19	0	0	0	0
3	D	5	0	0	0	0
3	E	24	0	0	0	0
3	F	13	0	0	0	0
3	G	11	0	0	0	0
All	All	6236	0	5495	121	1

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 10.

All (121) 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:F:26:THR:HB	1:F:44:ARG:HH12	1.30	0.95
1:G:295:ASN:ND2	1:G:322:GLN:OE1	2.01	0.93
1:D:285:TRP:HD1	1:D:300:THR:HG1	1.07	0.91
1:C:6:PHE:HB3	1:C:96:THR:HG21	1.54	0.90
1:F:26:THR:HB	1:F:44:ARG:NH1	1.91	0.85
1:C:26:THR:HG22	1:C:42:VAL:HB	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:GLY:O	1:C:60:ARG:NH1	2.13	0.82
1:C:35:GLY:C	1:C:60:ARG:HH12	1.81	0.81
1:F:113:ALA:O	1:F:114:ILE:HG13	1.81	0.80
1:C:90:GLN:HE21	1:C:99:VAL:HG21	1.49	0.77
1:D:220:GLN:HG2	1:D:225:SER:O	1.89	0.71
1:C:6:PHE:CB	1:C:96:THR:HG21	2.21	0.71
1:B:315:GLU:OE2	1:F:132:LEU:HD21	1.91	0.70
1:D:242:VAL:HG12	1:D:252:ASN:HA	1.73	0.69
1:B:208:ASP:HB3	1:B:210:SER:OG	1.93	0.68
1:C:97:GLU:HG2	1:C:122:GLN:HE21	1.58	0.67
1:F:103:ASN:O	1:G:286:THR:HG21	1.93	0.67
1:B:287:GLY:HA3	1:B:299:VAL:O	1.95	0.67
1:D:248:THR:HB	2:D:700:BTN:H92	1.77	0.67
1:D:298:ILE:HG22	1:D:300:THR:HG22	1.77	0.66
1:F:45:ALA:O	1:F:48:THR:OG1	2.14	0.66
1:A:74:ASN:O	1:A:75:SER:CB	2.42	0.65
1:F:131:SER:O	1:F:132:LEU:HB3	1.95	0.65
1:D:250:CYS:HB3	1:D:255:TYR:CE1	2.32	0.64
1:D:226:THR:HG21	1:D:244:ARG:HH11	1.64	0.62
1:B:228:ILE:HD13	1:F:74:ASN:HB2	1.82	0.62
1:F:26:THR:CB	1:F:44:ARG:HH12	2.09	0.59
1:C:60:ARG:HA	1:C:60:ARG:HH11	1.68	0.59
1:C:118:GLN:HG3	1:F:34:PHE:CD2	2.38	0.59
1:C:9:PHE:HD2	1:C:12:ILE:HD11	1.67	0.58
1:B:257:LEU:HD23	1:B:257:LEU:C	2.24	0.58
1:D:242:VAL:HG13	1:D:253:SER:N	2.19	0.58
1:B:212:ILE:HG22	3:B:1118:HOH:O	2.03	0.58
1:D:272:TRP:CZ2	2:D:700:BTN:H82	2.39	0.58
1:D:242:VAL:CG1	1:D:252:ASN:HA	2.34	0.56
1:C:6:PHE:HB3	1:C:96:THR:CG2	2.32	0.56
1:F:132:LEU:HD22	1:F:132:LEU:O	2.06	0.56
1:D:221:ASN:N	1:D:225:SER:OG	2.39	0.55
1:A:92:ASN:HB2	1:A:95:ASN:HB2	1.89	0.54
1:A:72:TRP:HB2	1:A:81:SER:HB3	1.88	0.54
1:F:113:ALA:O	1:F:114:ILE:CG1	2.56	0.54
1:G:291:VAL:HA	1:G:296:THR:HA	1.89	0.53
1:F:34:PHE:N	1:F:34:PHE:CD2	2.76	0.53
1:F:55:TYR:OH	1:F:77:GLU:HB3	2.09	0.53
1:C:90:GLN:HE21	1:C:99:VAL:CG2	2.20	0.53
1:G:217:SER:HB2	1:G:219:TRP:HE1	1.74	0.52
1:F:57:LEU:C	1:F:57:LEU:HD23	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:TRP:HD1	1:G:281:SER:HG	1.54	0.52
1:C:9:PHE:CD2	1:C:12:ILE:HD11	2.44	0.51
1:G:291:VAL:HG23	1:G:295:ASN:O	2.11	0.51
1:B:264:THR:O	1:B:264:THR:CG2	2.57	0.51
1:D:250:CYS:N	1:D:279:CYS:SG	2.84	0.51
1:F:25:SER:CB	2:F:900:BTN:O3	2.59	0.51
1:B:264:THR:O	1:B:264:THR:HG23	2.10	0.50
1:D:226:THR:CG2	1:D:244:ARG:HH11	2.24	0.50
1:E:13:ALA:O	1:E:14:SER:HB2	2.10	0.50
1:C:62:ASN:ND2	1:D:281:SER:H	2.11	0.49
1:B:212:ILE:CG2	3:B:1118:HOH:O	2.60	0.49
1:A:26:THR:HG21	3:A:1087:HOH:O	2.12	0.48
1:D:308:GLY:N	1:D:311:GLY:O	2.40	0.48
1:G:298:ILE:HG22	1:G:300:THR:HG22	1.95	0.48
1:B:213:ALA:HA	1:B:231:VAL:O	2.13	0.48
1:B:237:VAL:O	1:B:258:THR:HA	2.14	0.48
1:C:35:GLY:C	1:C:60:ARG:NH1	2.57	0.48
1:F:22:GLN:HE22	1:F:119:ASP:HA	1.79	0.48
1:A:21:ASN:HA	1:A:120:THR:O	2.14	0.47
1:A:124:VAL:HG12	1:A:127:THR:H	1.79	0.47
1:D:231:VAL:HG22	1:D:237:VAL:HG22	1.96	0.47
1:D:218:SER:HA	1:D:228:ILE:HG22	1.96	0.46
1:D:224:GLY:HA3	1:D:244:ARG:O	2.15	0.46
1:G:237:VAL:CG2	1:G:261:VAL:HG13	2.46	0.46
1:F:132:LEU:O	1:F:132:LEU:HD13	2.15	0.46
1:A:87:GLY:HA3	1:A:99:VAL:O	2.16	0.46
1:C:57:LEU:C	1:C:57:LEU:HD23	2.36	0.46
1:G:228:ILE:O	1:G:239:GLY:HA3	2.16	0.46
1:F:55:TYR:HH	1:F:77:GLU:HB3	1.82	0.45
1:F:21:ASN:HB3	1:F:121:PHE:CD2	2.51	0.45
1:D:255:TYR:CE2	1:D:273:ASN:N	2.85	0.45
1:G:221:ASN:HA	1:G:320:THR:O	2.16	0.45
1:A:32:ASP:OD2	1:A:36:ASN:HB2	2.17	0.45
1:G:248:THR:O	1:G:251:GLN:NE2	2.49	0.45
1:C:21:ASN:HA	1:C:120:THR:O	2.16	0.44
1:D:249:GLY:O	1:D:250:CYS:C	2.54	0.44
1:F:19:TRP:CZ3	1:F:123:TYR:HB2	2.52	0.44
1:G:268:PHE:CE2	1:G:285:TRP:CE3	3.05	0.44
1:C:58:THR:HG22	1:D:260:ARG:HG2	1.99	0.44
1:E:87:GLY:HA3	1:E:99:VAL:O	2.17	0.44
1:C:26:THR:HB	1:C:44:ARG:HH12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASN:O	1:A:51:GLN:HA	2.18	0.43
1:F:32:ASP:C	1:F:34:PHE:H	2.20	0.43
1:F:102:TRP:CD2	2:F:900:BTN:H61	2.53	0.43
1:B:297:GLU:HB2	1:B:321:PHE:O	2.17	0.43
1:C:6:PHE:C	1:C:6:PHE:CD2	2.91	0.43
1:F:103:ASN:OD1	1:F:116:GLN:HG2	2.18	0.43
1:F:48:THR:HB	2:F:900:BTN:H92	2.00	0.43
1:F:37:VAL:CG2	1:F:61:VAL:HG13	2.48	0.43
1:C:50:CYS:N	1:C:79:CYS:SG	2.92	0.42
1:D:255:TYR:HE2	1:D:273:ASN:N	2.16	0.42
1:F:19:TRP:HB3	1:F:121:PHE:HB3	2.01	0.42
1:A:30:GLN:HG2	3:A:1088:HOH:O	2.19	0.42
1:A:48:THR:HB	2:A:400:BTN:H92	2.02	0.42
1:A:97:GLU:OE2	1:A:122:GLN:NE2	2.53	0.42
1:A:102:TRP:CD2	2:A:400:BTN:H61	2.55	0.42
1:F:78:ASN:OD1	1:F:78:ASN:C	2.58	0.41
1:B:272:TRP:HD1	1:B:281:SER:HG	1.65	0.41
1:F:26:THR:HG22	1:F:42:VAL:HB	2.02	0.41
1:A:89:ALA:HA	1:A:97:GLU:O	2.20	0.41
1:C:90:GLN:NE2	1:C:99:VAL:HG21	2.27	0.41
1:D:234:PHE:CZ	1:E:14:SER:HA	2.55	0.41
1:D:302:TRP:CE2	1:D:317:GLY:HA3	2.55	0.41
1:G:268:PHE:CE2	1:G:285:TRP:CD2	3.09	0.41
1:D:232:ASP:OD2	1:D:236:ASN:HB2	2.20	0.41
1:F:43:ASN:ND2	2:F:900:BTN:H92	2.35	0.41
1:A:17:SER:O	1:A:28:ILE:HD12	2.21	0.41
1:D:267:ALA:HB2	1:D:286:THR:HG23	2.03	0.41
1:G:274:ASN:O	1:G:275:SER:CB	2.69	0.41
1:D:226:THR:HG23	1:D:242:VAL:O	2.21	0.41
1:G:304:LEU:O	1:G:314:ILE:HA	2.21	0.41
1:G:272:TRP:CD1	1:G:281:SER:OG	2.72	0.40
1:F:22:GLN:NE2	1:F:119:ASP:HA	2.37	0.40
1:F:50:CYS:N	1:F:79:CYS:SG	2.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1091:HOH:O	3:B:1091:HOH:O[4_565]	1.69	0.51

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	112/135 (83%)	107 (96%)	4 (4%)	1 (1%)	20	23
1	B	119/135 (88%)	115 (97%)	4 (3%)	0	100	100
1	C	122/135 (90%)	119 (98%)	3 (2%)	0	100	100
1	D	89/135 (66%)	79 (89%)	8 (9%)	2 (2%)	8	6
1	E	117/135 (87%)	111 (95%)	5 (4%)	1 (1%)	20	23
1	F	114/135 (84%)	103 (90%)	9 (8%)	2 (2%)	10	9
1	G	108/135 (80%)	104 (96%)	4 (4%)	0	100	100
All	All	781/945 (83%)	738 (94%)	37 (5%)	6 (1%)	22	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	110	SER
1	D	247	GLY
1	F	80	ASN
1	A	127	THR
1	F	114	ILE
1	D	273	ASN

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	92/111 (83%)	87 (95%)	5 (5%)	26	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	98/111 (88%)	94 (96%)	4 (4%)	35	48
1	C	101/111 (91%)	96 (95%)	5 (5%)	28	39
1	D	74/111 (67%)	66 (89%)	8 (11%)	7	8
1	E	96/111 (86%)	94 (98%)	2 (2%)	59	76
1	F	98/111 (88%)	88 (90%)	10 (10%)	8	10
1	G	88/111 (79%)	83 (94%)	5 (6%)	24	32
All	All	647/777 (83%)	608 (94%)	39 (6%)	22	30

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	61	VAL
1	A	75	SER
1	A	96	THR
1	A	126	THR
1	B	257	LEU
1	B	264	THR
1	B	292	ASN
1	B	296	THR
1	C	6	PHE
1	C	26	THR
1	C	64	THR
1	C	95	ASN
1	C	96	THR
1	D	218	SER
1	D	220	GLN
1	D	228	ILE
1	D	244	ARG
1	D	257	LEU
1	D	286	THR
1	D	300	THR
1	D	315	GLU
1	E	96	THR
1	E	101	SER
1	F	26	THR
1	F	34	PHE
1	F	51	GLN
1	F	57	LEU
1	F	110	SER

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Mol	Chain	Res	Type
1	F	118	GLN
1	F	126	THR
1	F	130	LYS
1	F	131	SER
1	F	132	LEU
1	G	217	SER
1	G	226	THR
1	G	233	SER
1	G	238	SER
1	G	242	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	30	GLN
1	B	292	ASN
1	C	20	GLN
1	C	80	ASN
1	C	90	GLN
1	C	92	ASN
1	C	95	ASN
1	C	122	GLN
1	D	240	GLN
1	D	246	GLN
1	D	303	ASN
1	E	20	GLN
1	E	46	GLN
1	F	51	GLN
1	F	92	ASN
1	F	95	ASN
1	F	118	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

7 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	BTN	A	400	-	14,17,17	3.50	2 (14%)	19,23,23	2.42	5 (26%)
2	BTN	B	500	-	14,17,17	3.50	2 (14%)	19,23,23	2.43	5 (26%)
2	BTN	C	600	-	14,17,17	3.50	2 (14%)	19,23,23	2.43	5 (26%)
2	BTN	D	700	-	14,17,17	3.50	2 (14%)	19,23,23	2.43	5 (26%)
2	BTN	E	800	-	14,17,17	3.50	2 (14%)	19,23,23	2.43	5 (26%)
2	BTN	F	900	-	14,17,17	3.49	2 (14%)	19,23,23	2.43	5 (26%)
2	BTN	G	350	-	14,17,17	3.36	3 (21%)	19,23,23	1.93	5 (26%)

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	BTN	A	400	-	-	0/5/28/28	0/2/2/2
2	BTN	B	500	-	-	0/5/28/28	0/2/2/2
2	BTN	C	600	-	-	0/5/28/28	0/2/2/2
2	BTN	D	700	-	-	0/5/28/28	0/2/2/2
2	BTN	E	800	-	-	0/5/28/28	0/2/2/2
2	BTN	F	900	-	-	0/5/28/28	0/2/2/2
2	BTN	G	350	-	-	0/5/28/28	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	BTN	C2-S1	-9.67	1.67	1.82
2	C	600	BTN	C2-S1	-9.66	1.67	1.82
2	E	800	BTN	C2-S1	-9.64	1.67	1.82
2	F	900	BTN	C2-S1	-9.64	1.67	1.82
2	B	500	BTN	C2-S1	-9.63	1.67	1.82
2	D	700	BTN	C2-S1	-9.62	1.67	1.82
2	G	350	BTN	C2-S1	-8.00	1.70	1.82
2	G	350	BTN	C3-N1	-2.58	1.31	1.35
2	A	400	BTN	O3-C3	8.44	1.41	1.23
2	C	600	BTN	O3-C3	8.45	1.41	1.23
2	F	900	BTN	O3-C3	8.45	1.41	1.23
2	E	800	BTN	O3-C3	8.45	1.41	1.23
2	B	500	BTN	O3-C3	8.47	1.41	1.23
2	D	700	BTN	O3-C3	8.49	1.41	1.23
2	G	350	BTN	O3-C3	8.85	1.42	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	350	BTN	C6-C5-N1	-4.82	108.28	113.15
2	G	350	BTN	C2-C4-C5	-3.77	105.66	108.78
2	C	600	BTN	C6-C5-N1	-3.53	109.58	113.15
2	E	800	BTN	C6-C5-N1	-3.49	109.62	113.15
2	B	500	BTN	C6-C5-N1	-3.48	109.62	113.15
2	F	900	BTN	C6-C5-N1	-3.47	109.63	113.15
2	D	700	BTN	C6-C5-N1	-3.45	109.66	113.15
2	A	400	BTN	C6-C5-N1	-3.44	109.67	113.15
2	C	600	BTN	C2-C4-N2	-3.00	110.35	113.13
2	D	700	BTN	C2-C4-N2	-2.99	110.36	113.13
2	F	900	BTN	C2-C4-N2	-2.97	110.37	113.13
2	A	400	BTN	C2-C4-N2	-2.97	110.38	113.13
2	E	800	BTN	C2-C4-N2	-2.95	110.40	113.13
2	B	500	BTN	C2-C4-N2	-2.95	110.40	113.13
2	G	350	BTN	C8-C7-C2	-2.28	109.31	113.80
2	G	350	BTN	O3-C3-N1	-2.13	122.98	125.90
2	E	800	BTN	N2-C3-N1	2.10	110.47	108.85
2	B	500	BTN	N2-C3-N1	2.11	110.48	108.85
2	C	600	BTN	N2-C3-N1	2.12	110.49	108.85
2	F	900	BTN	N2-C3-N1	2.13	110.49	108.85
2	A	400	BTN	N2-C3-N1	2.15	110.50	108.85
2	D	700	BTN	N2-C3-N1	2.16	110.51	108.85
2	G	350	BTN	C4-C2-S1	3.68	108.81	105.21
2	A	400	BTN	C5-C6-S1	5.45	110.16	106.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	BTN	C5-C6-S1	5.47	110.17	106.24
2	F	900	BTN	C5-C6-S1	5.48	110.18	106.24
2	B	500	BTN	C5-C6-S1	5.50	110.20	106.24
2	D	700	BTN	C5-C6-S1	5.51	110.20	106.24
2	E	800	BTN	C5-C6-S1	5.52	110.21	106.24
2	D	700	BTN	C4-C2-S1	6.37	111.45	105.21
2	C	600	BTN	C4-C2-S1	6.37	111.45	105.21
2	B	500	BTN	C4-C2-S1	6.38	111.46	105.21
2	A	400	BTN	C4-C2-S1	6.38	111.46	105.21
2	E	800	BTN	C4-C2-S1	6.38	111.47	105.21
2	F	900	BTN	C4-C2-S1	6.42	111.50	105.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	BTN	2	0
2	D	700	BTN	2	0
2	F	900	BTN	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

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	114/135 (84%)	0.14	0 100 100	26, 36, 59, 73	0
1	B	121/135 (89%)	0.20	6 (4%) 30 36	24, 34, 61, 71	0
1	C	124/135 (91%)	0.31	7 (5%) 25 32	27, 44, 69, 73	1 (0%)
1	D	95/135 (70%)	1.37	21 (22%) 1 1	46, 72, 86, 89	0
1	E	119/135 (88%)	0.13	2 (1%) 70 76	23, 37, 59, 76	0
1	F	119/135 (88%)	0.75	16 (13%) 4 5	35, 54, 75, 80	0
1	G	110/135 (81%)	0.58	8 (7%) 16 21	35, 55, 82, 91	1 (0%)
All	All	802/945 (84%)	0.47	60 (7%) 15 20	23, 46, 77, 91	2 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	246	GLN	7.5
1	B	212	ILE	6.6
1	G	254	PRO	6.3
1	D	242	VAL	5.4
1	D	252	ASN	5.0
1	G	230	GLN	4.6
1	C	10	SER	4.3
1	D	317	GLY	4.3
1	D	220	GLN	4.2
1	D	226	THR	4.1
1	D	255	TYR	4.1
1	D	276	THR	4.0
1	E	110	SER	3.9
1	F	132	LEU	3.9
1	D	306	TYR	3.7
1	D	288	TYR	3.6
1	F	94	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	118	GLN	3.5
1	D	254	PRO	3.4
1	E	109	GLY	3.4
1	C	110	SER	3.3
1	F	108	GLY	3.3
1	F	34	PHE	3.2
1	F	110	SER	3.1
1	B	310	SER	3.1
1	F	91	VAL	3.1
1	F	98	ILE	3.0
1	C	7	LYS	2.9
1	G	216	SER	2.9
1	D	253	SER	2.9
1	D	316	GLN	2.9
1	D	275	SER	2.8
1	D	309	GLY	2.8
1	G	289	ALA	2.8
1	F	14	SER	2.7
1	F	31	VAL	2.7
1	D	304	LEU	2.6
1	F	33	SER	2.6
1	F	104	LEU	2.6
1	G	264	THR	2.6
1	G	244	ARG	2.6
1	F	106	TYR	2.6
1	D	285	TRP	2.5
1	B	294	ASN	2.5
1	D	269	SER	2.5
1	B	213	ALA	2.4
1	G	324	VAL	2.4
1	B	309	GLY	2.4
1	B	311	GLY	2.4
1	C	6	PHE	2.4
1	F	109	GLY	2.3
1	F	44	ARG	2.2
1	C	34	PHE	2.2
1	C	65	PHE	2.2
1	D	223	SER	2.1
1	G	234	PHE	2.1
1	F	15	ALA	2.1
1	F	95	ASN	2.0
1	D	251	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	289	ALA	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 [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. 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	BTN	A	400	16/16	0.94	0.19	1.80	27,31,38,38	0
2	BTN	E	800	16/16	0.94	0.15	1.20	27,30,38,38	0
2	BTN	F	900	16/16	0.90	0.20	1.15	43,47,55,57	0
2	BTN	D	700	16/16	0.81	0.20	0.20	66,68,71,72	0
2	BTN	B	500	16/16	0.94	0.12	-0.31	24,28,35,36	0
2	BTN	G	350	16/16	0.96	0.12	-0.51	27,35,37,39	0
2	BTN	C	600	16/16	0.95	0.12	-0.53	26,32,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.