W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 10:13 am GMT

PDB ID	:	4F9L
Title	:	Crystal Structure of the Human BTN3A1 Ectodomain in Complex with the 20.1 Single Chain Antibody
Authors	:	Palakodeti, A.; Sandstrom, A.; Sundaresan, L.; Harly, C.; Nedellec, S.; Olive, D.; Scotet, E.; Bonneville, M.; Adams, E.J.
Deposited on	:	2012-05-18
Resolution	:	3.14 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 (i) symbol.

The following versions of software and data (see references (i)) 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 ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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.
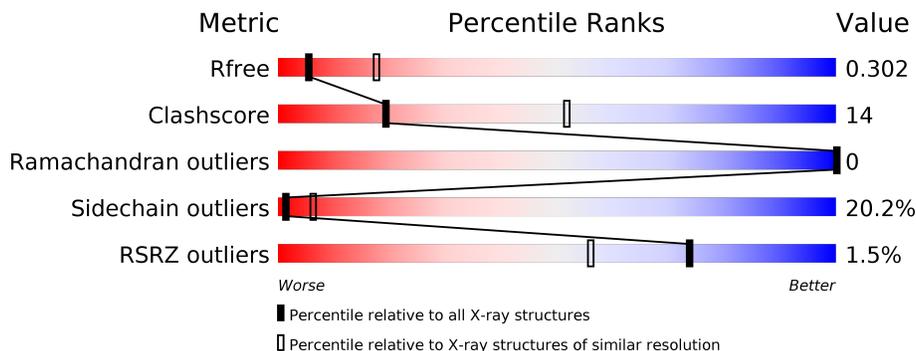
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1234 (3.18-3.10)
Clashscore	112137	1345 (3.18-3.10)
Ramachandran outliers	110173	1301 (3.18-3.10)
Sidechain outliers	110143	1301 (3.18-3.10)
RSRZ outliers	101464	1240 (3.18-3.10)

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 <=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	220	
1	B	220	
2	C	259	
2	D	259	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6598 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 Butyrophilin subfamily 3 member A1.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1528	963	262	295	8			
1	B	213	Total	C	N	O	S	0	0	0
			1523	963	264	289	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	EXPRESSION TAG	UNP O00481
A	-1	ASP	-	EXPRESSION TAG	UNP O00481
A	0	LEU	-	EXPRESSION TAG	UNP O00481
B	-2	ALA	-	EXPRESSION TAG	UNP O00481
B	-1	ASP	-	EXPRESSION TAG	UNP O00481
B	0	LEU	-	EXPRESSION TAG	UNP O00481

- Molecule 2 is a protein called 20.1 anti-BTN3A1 antibody fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	232	Total	C	N	O	S	0	0	0
			1763	1112	294	352	5			
2	C	232	Total	C	N	O	S	0	0	0
			1756	1106	292	353	5			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
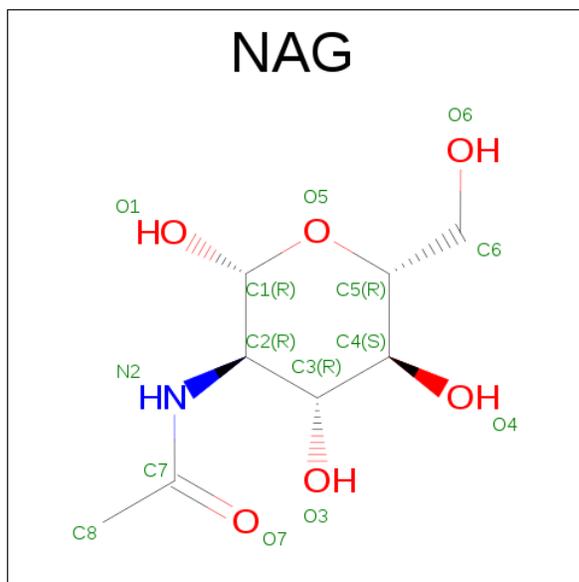
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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 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: Butyrophilin subfamily 3 member A1
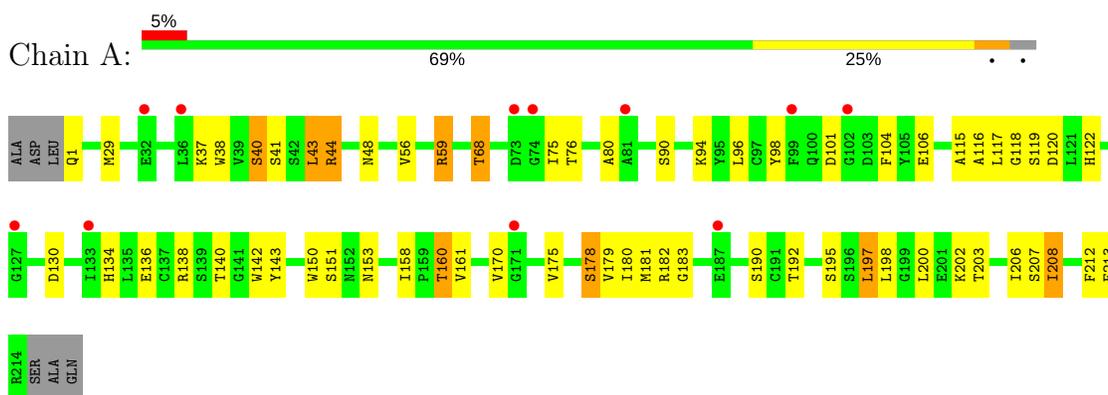
- Molecule 1: Butyrophilin subfamily 3 member A1

- Molecule 2: 20.1 anti-BTN3A1 antibody fragment

• Molecule 2: 20.1 anti-BTN3A1 antibody fragment

Chain C:

54%   30%   5%   10%

D1 T5 Q6 S10 A13 S14 L15 I19 C23 H24 A25 S26 Q27 N28 I29 N30 L31 W32 Q37 I43 L47 I48 Y49 R50 N53 L54 H55 T56 G57 V58 R61 F62 S65 G66 S67 A68 T69 G70 F71 I75 S76 S77 L78 Q79 T85 Y86 Y87

Q90 G91 H92 S93 G99 G100 G101 T102 K103 L104 D105 I106 K107 R108 A109 ASP ALA GLY GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER Q132 V133 Q134 L135 Q136 A140 E141 L142 V143 K144 P145 G146 A147 S148 V149 K150 L151 S152 C153

S156 T159 R162 L165 Y166 N183 N186 F191 T200 V203 T209 T210 Y211 S215 S216 L217 T218 S219 C227 S228 R229 E230 D231 T236 P237 D238 D241 Y242 Q245 S253 A254 ALA SER GLY ALA ASP

4　Data and refinement statistics　ⓘ

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	165.14Å　165.14Å　53.81Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	45.80　–　3.14 45.80　–　3.14	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.80-3.14) 99.8 (45.80-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.254　,　0.303 0.255　,　0.302	Depositor DCC
R_{free} test set	1325 reflections (5.13%)	DCC
Wilson B-factor (Å^2)	75.2	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 58.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6598	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG

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	0.38	0/1560	0.60	0/2131
1	B	0.41	0/1555	0.64	1/2124 (0.0%)
2	C	0.45	0/1798	0.63	1/2453 (0.0%)
2	D	0.47	0/1805	0.63	2/2460 (0.1%)
All	All	0.43	0/6718	0.62	4/9168 (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
2	C	0	5
2	D	0	5
All	All	0	11

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	ASP	CB-CG-OD1	5.84	123.55	118.30
2	D	99	GLY	N-CA-C	-5.17	100.17	113.10
2	C	102	THR	CA-CB-CG2	-5.14	105.20	112.40
2	D	61	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Mol	Chain	Res	Type	Group
1	A	183	GLY	Peptide
2	C	101	GLY	Peptide
2	C	132	GLN	Peptide
2	C	133	VAL	Peptide
2	C	140	ALA	Peptide
2	C	238	ASP	Peptide
2	D	101	GLY	Peptide
2	D	106	ILE	Peptide
2	D	140	ALA	Peptide
2	D	146	GLY	Peptide
2	D	147	ALA	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	1528	0	1419	37	0
1	B	1523	0	1421	51	0
2	C	1756	0	1651	56	0
2	D	1763	0	1670	49	0
3	A	14	0	13	0	0
3	B	14	0	13	5	0
All	All	6598	0	6187	184	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 14.

All (184) 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:86:ASN:HD21	3:B:301:NAG:C1	1.14	1.55
1:A:212:PHE:CZ	1:B:127:GLY:HA2	1.95	1.00
2:C:166:TYR:HB2	2:C:228:SER:HB2	1.39	0.99
2:C:85:THR:HG23	2:C:102:THR:O	1.66	0.94
2:C:61:ARG:HH11	2:C:61:ARG:HG3	1.33	0.91
2:C:61:ARG:NH1	2:C:61:ARG:HG3	1.87	0.89
2:C:61:ARG:CG	2:C:61:ARG:HH11	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PHE:HZ	1:B:127:GLY:HA2	1.39	0.83
2:D:61:ARG:HG3	2:D:61:ARG:HH11	1.44	0.80
1:B:129:LYS:HE3	1:B:134:HIS:ND1	1.97	0.80
2:D:226:TYR:CE1	2:D:246:GLY:HA3	2.17	0.79
1:B:182:ARG:HH11	1:B:182:ARG:CG	1.94	0.79
1:A:48:ASN:HD22	1:A:68:THR:HG22	1.49	0.78
1:B:48:ASN:HD22	1:B:68:THR:HG22	1.49	0.77
1:B:182:ARG:HH11	1:B:182:ARG:HG3	1.49	0.77
1:A:181:MET:SD	1:A:208:ILE:HG13	2.24	0.77
2:C:231:ASP:OD2	2:C:238:ASP:HB2	1.85	0.76
1:B:188:GLY:O	1:B:189:VAL:HG13	1.86	0.76
2:C:85:THR:CG2	2:C:102:THR:O	2.32	0.76
1:A:182:ARG:HA	1:A:213:PHE:CE1	2.22	0.75
2:C:91:GLY:O	1:B:59:ARG:NH2	2.21	0.73
2:C:105:ASP:OD1	2:C:106:ILE:N	2.21	0.73
2:D:50:ARG:HG2	2:D:50:ARG:HH11	1.51	0.73
1:A:206:ILE:HG13	1:A:207:SER:N	2.03	0.73
1:B:182:ARG:CG	1:B:182:ARG:NH1	2.52	0.71
2:D:153:CYS:O	2:D:209:THR:HG23	1.91	0.70
1:B:135:LEU:HD13	1:B:206:ILE:HG21	1.73	0.69
2:D:49:TYR:CZ	2:D:53:ASN:HB2	2.28	0.69
2:D:90:GLN:HE21	2:D:93:SER:H	1.40	0.68
1:B:188:GLY:O	1:B:189:VAL:CG1	2.41	0.68
2:C:90:GLN:HE21	2:C:93:SER:H	1.41	0.67
1:B:71:LEU:HD12	1:B:81:ALA:HB3	1.76	0.66
2:C:32:TRP:HE3	2:C:238:ASP:OD1	1.79	0.66
1:B:115:ALA:HB1	1:B:198:LEU:HD22	1.76	0.66
2:C:87:TYR:CD2	2:C:100:GLY:HA2	2.32	0.64
2:C:159:THR:HG23	2:C:162:ARG:HD3	1.79	0.64
2:C:58:VAL:HG13	2:C:62:PHE:HD2	1.62	0.64
2:D:228:SER:HB2	2:D:240:MET:HB2	1.80	0.64
2:D:229:ARG:NH1	2:D:230:GLU:O	2.31	0.63
2:D:11:LEU:HD23	2:D:104:LEU:HD13	1.79	0.62
2:C:53:ASN:OD1	2:C:53:ASN:N	2.27	0.62
2:C:62:PHE:CE1	2:C:75:ILE:HG23	2.34	0.62
2:C:49:TYR:O	2:C:50:ARG:HB2	1.99	0.61
2:C:136:GLN:NE2	2:C:242:TYR:O	2.34	0.61
2:C:142:LEU:HD22	2:C:149:VAL:HG21	1.83	0.60
1:A:122:HIS:ND1	1:B:205:SER:OG	2.23	0.60
2:D:90:GLN:NE2	2:D:93:SER:O	2.35	0.59
1:A:40:SER:OG	1:A:43:LEU:O	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:MET:SD	1:A:208:ILE:CG1	2.90	0.59
1:A:181:MET:O	1:A:213:PHE:HE1	1.86	0.59
1:A:48:ASN:HB2	1:A:68:THR:HG21	1.85	0.58
1:B:150:TRP:H	1:B:160:THR:HG21	1.68	0.58
2:C:55:HIS:NE2	2:C:241:ASP:OD2	2.37	0.58
1:B:181:MET:SD	1:B:208:ILE:HG13	2.44	0.58
1:B:181:MET:HG2	1:B:181:MET:O	2.04	0.57
1:B:86:ASN:CG	3:B:301:NAG:C1	2.71	0.57
1:A:115:ALA:HB2	1:A:197:LEU:HD22	1.85	0.57
1:B:34:MET:HG2	1:B:101:ASP:HB2	1.86	0.57
1:A:122:HIS:CE1	1:B:205:SER:HG	2.19	0.57
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.86	0.57
1:B:124:ASP:O	1:B:135:LEU:HA	2.04	0.57
1:B:48:ASN:HB2	1:B:68:THR:HG21	1.86	0.57
2:D:50:ARG:CG	2:D:50:ARG:HH11	2.16	0.57
1:A:150:TRP:H	1:A:160:THR:HG21	1.70	0.57
1:B:86:ASN:ND2	3:B:301:NAG:C2	2.68	0.57
2:D:226:TYR:CD1	2:D:246:GLY:HA3	2.40	0.57
1:A:203:THR:HB	1:B:120:ASP:OD2	2.05	0.57
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.86	0.57
1:A:120:ASP:OD1	1:A:202:LYS:NZ	2.30	0.56
2:C:218:THR:OG1	2:C:219:SER:N	2.38	0.56
1:B:188:GLY:C	1:B:189:VAL:HG13	2.25	0.56
2:D:6:GLN:HE21	2:D:102:THR:H	1.53	0.56
2:C:136:GLN:HG2	2:C:227:CYS:SG	2.47	0.55
2:C:87:TYR:HD2	2:C:100:GLY:HA2	1.72	0.55
1:B:124:ASP:O	1:B:136:GLU:N	2.35	0.55
1:B:125:VAL:HA	1:B:134:HIS:O	2.07	0.55
2:C:49:TYR:CZ	2:C:53:ASN:HB2	2.41	0.55
2:C:90:GLN:NE2	2:C:93:SER:O	2.39	0.55
2:D:8:PRO:O	2:D:102:THR:HG23	2.07	0.54
2:C:65:SER:OG	2:C:66:GLY:N	2.41	0.54
2:C:58:VAL:CG1	2:C:62:PHE:HD2	2.19	0.54
2:C:166:TYR:HB2	2:C:228:SER:CB	2.26	0.54
1:B:133:ILE:HG21	1:B:208:ILE:HD12	1.90	0.53
2:C:6:GLN:OE1	2:C:99:GLY:O	2.25	0.53
1:A:136:GLU:OE1	1:A:138:ARG:NH1	2.39	0.53
2:D:78:LEU:HD23	2:D:106:ILE:HD11	1.90	0.53
2:D:65:SER:OG	2:D:66:GLY:N	2.42	0.53
1:A:182:ARG:HA	1:A:213:PHE:HE1	1.72	0.52
1:A:59:ARG:NH2	2:D:92:HIS:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:104:LEU:HD12	2:C:105:ASP:N	2.25	0.52
2:D:61:ARG:NH2	2:D:79:GLN:HB2	2.25	0.52
1:A:212:PHE:CE2	1:B:127:GLY:HA2	2.42	0.51
2:C:90:GLN:HG2	2:C:92:HIS:H	1.76	0.51
2:D:2:ILE:O	2:D:97:THR:HG21	2.10	0.51
1:B:120:ASP:OD1	1:B:202:LYS:NZ	2.29	0.51
2:C:136:GLN:HB3	2:C:153:CYS:SG	2.50	0.51
1:A:101:ASP:OD1	1:A:101:ASP:C	2.49	0.51
1:A:181:MET:HE1	1:A:208:ILE:H	1.76	0.51
1:B:86:ASN:ND2	3:B:301:NAG:O5	2.30	0.50
1:A:206:ILE:CG1	1:A:207:SER:N	2.75	0.50
2:D:90:GLN:HG2	2:D:92:HIS:H	1.77	0.50
2:C:61:ARG:CB	2:C:61:ARG:HH11	2.25	0.50
1:B:130:ASP:C	1:B:132:GLY:H	2.15	0.49
2:D:61:ARG:NH1	2:D:61:ARG:HG3	2.23	0.49
1:A:130:ASP:HB3	1:A:180:ILE:HD13	1.93	0.49
1:A:41:SER:OG	1:A:94:LYS:O	2.20	0.48
1:A:1:GLN:HA	1:A:104:PHE:CZ	2.48	0.48
1:A:118:GLY:HA3	1:A:142:TRP:CE2	2.48	0.48
1:A:153:ASN:N	1:A:153:ASN:OD1	2.41	0.48
1:A:117:LEU:HD13	1:A:198:LEU:HD13	1.95	0.48
1:B:182:ARG:HG2	1:B:182:ARG:NH1	2.26	0.48
2:D:61:ARG:NH1	2:D:62:PHE:HE1	2.11	0.48
2:D:25:ALA:O	2:D:69:THR:HG22	2.13	0.48
1:B:184:SER:HB2	1:B:213:PHE:CE2	2.49	0.48
1:A:134:HIS:NE2	1:A:178:SER:OG	2.33	0.48
2:C:25:ALA:O	2:C:69:THR:HG22	2.13	0.47
2:C:147:ALA:O	2:C:217:LEU:HD12	2.15	0.47
2:D:226:TYR:CD1	2:D:246:GLY:CA	2.98	0.47
2:D:53:ASN:N	2:D:53:ASN:OD1	2.29	0.47
2:D:153:CYS:HB3	2:D:210:THR:CG2	2.45	0.47
1:B:118:GLY:HA3	1:B:142:TRP:CE2	2.50	0.47
2:C:106:ILE:O	2:C:107:LYS:O	2.32	0.47
2:C:67:SER:OG	2:C:68:ALA:N	2.48	0.47
1:B:115:ALA:CB	1:B:198:LEU:HD22	2.45	0.46
1:A:37:LYS:HB3	1:A:98:TYR:HB2	1.96	0.46
2:D:153:CYS:HB3	2:D:210:THR:HG23	1.97	0.46
2:C:49:TYR:O	2:C:50:ARG:CB	2.64	0.46
2:D:49:TYR:O	2:D:50:ARG:CB	2.63	0.46
2:C:153:CYS:O	2:C:209:THR:HG23	2.15	0.45
2:D:182:ILE:HG13	2:D:183:ASN:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ALA:HB3	1:A:143:TYR:H	1.82	0.45
2:C:78:LEU:HD23	2:C:106:ILE:HD11	1.98	0.45
2:D:29:ILE:HD11	2:D:71:PHE:CE2	2.52	0.45
2:D:29:ILE:O	2:D:32:TRP:HD1	2.00	0.45
2:C:106:ILE:C	2:C:107:LYS:O	2.52	0.45
2:C:32:TRP:CE3	2:C:238:ASP:OD1	2.65	0.45
1:A:119:SER:HB3	1:A:140:THR:H	1.82	0.45
2:C:152:SER:HB3	2:C:211:TYR:CD2	2.52	0.45
2:D:85:THR:HG22	2:D:101:GLY:O	2.17	0.45
2:D:218:THR:OG1	2:D:219:SER:N	2.48	0.44
1:B:116:ALA:HB3	1:B:143:TYR:H	1.83	0.44
1:A:44:ARG:HA	1:A:44:ARG:HD3	1.47	0.44
1:B:125:VAL:HG22	1:B:135:LEU:HD23	1.99	0.44
2:C:85:THR:HA	2:C:103:LYS:HA	2.00	0.44
2:C:183:ASN:OD1	1:B:62:ALA:HB1	2.17	0.44
2:C:62:PHE:HE1	2:C:75:ILE:HG23	1.78	0.44
2:D:50:ARG:NH1	2:D:50:ARG:CG	2.74	0.44
1:B:125:VAL:HG22	1:B:135:LEU:CD2	2.47	0.44
1:B:153:ASN:N	1:B:153:ASN:OD1	2.40	0.44
2:D:96:TYR:N	2:D:96:TYR:CD1	2.86	0.44
1:B:119:SER:HB3	1:B:140:THR:H	1.83	0.44
2:D:163:TYR:HB3	2:D:229:ARG:HD3	2.00	0.43
2:D:198:LYS:HA	2:D:198:LYS:HD3	1.88	0.43
2:D:36:TYR:OH	2:D:240:MET:HG2	2.19	0.43
2:D:61:ARG:HH21	2:D:79:GLN:HB2	1.83	0.43
2:D:153:CYS:O	2:D:209:THR:CG2	2.64	0.43
2:D:165:LEU:HB2	2:D:182:ILE:HG23	2.00	0.43
2:D:224:VAL:HG11	2:D:226:TYR:CZ	2.54	0.42
1:B:126:LYS:HZ2	1:B:126:LYS:HG2	1.55	0.42
1:B:75:ILE:HD12	1:B:80:ALA:HB2	2.02	0.42
2:C:13:ALA:O	2:C:106:ILE:HA	2.19	0.42
2:C:61:ARG:HH11	2:C:61:ARG:HB2	1.83	0.42
2:C:29:ILE:O	2:C:32:TRP:HD1	2.02	0.42
2:D:252:SER:OG	2:D:254:ALA:O	2.37	0.42
2:C:29:ILE:HD11	2:C:71:PHE:CE2	2.55	0.42
2:D:229:ARG:HD2	2:D:230:GLU:N	2.35	0.41
2:C:236:THR:OG1	2:C:237:PRO:HD2	2.20	0.41
2:C:102:THR:CG2	2:C:103:LYS:N	2.74	0.41
1:B:153:ASN:HB3	1:B:187:GLU:O	2.20	0.41
2:C:144:LYS:HA	2:C:145:PRO:HD3	1.89	0.41
1:B:197:LEU:HG	1:B:198:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:HD12	1:A:80:ALA:HB2	2.02	0.41
1:B:37:LYS:HB3	1:B:98:TYR:HB2	2.03	0.41
1:B:40:SER:O	1:B:44:ARG:HA	2.21	0.41
1:A:181:MET:O	1:A:213:PHE:CE1	2.70	0.41
1:B:188:GLY:C	1:B:189:VAL:CG1	2.89	0.40
2:C:23:CYS:HB3	2:C:71:PHE:HB2	2.03	0.40
2:D:50:ARG:NH1	2:D:50:ARG:HG2	2.28	0.40
1:A:198:LEU:HB3	1:A:200:LEU:HG	2.03	0.40
2:C:62:PHE:HE1	2:C:75:ILE:CG2	2.34	0.40
2:D:177:GLU:OE2	2:D:194:LYS:NZ	2.37	0.40
1:B:86:ASN:OD1	3:B:301:NAG:N2	2.54	0.40
2:D:166:TYR:O	2:D:227:CYS:HA	2.22	0.40
2:D:23:CYS:HB3	2:D:71:PHE:HB2	2.04	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	212/220 (96%)	210 (99%)	2 (1%)	0	100	100
1	B	211/220 (96%)	205 (97%)	6 (3%)	0	100	100
2	C	228/259 (88%)	209 (92%)	19 (8%)	0	100	100
2	D	228/259 (88%)	214 (94%)	14 (6%)	0	100	100
All	All	879/958 (92%)	838 (95%)	41 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	149/178 (84%)	124 (83%)	25 (17%)	2	10
1	B	146/178 (82%)	114 (78%)	32 (22%)	1	5
2	C	188/204 (92%)	149 (79%)	39 (21%)	1	6
2	D	189/204 (93%)	149 (79%)	40 (21%)	1	5
All	All	672/764 (88%)	536 (80%)	136 (20%)	1	6

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	MET
1	A	38	TRP
1	A	40	SER
1	A	43	LEU
1	A	44	ARG
1	A	56	VAL
1	A	59	ARG
1	A	68	THR
1	A	76	THR
1	A	90	SER
1	A	96	LEU
1	A	106	GLU
1	A	151	SER
1	A	158	ILE
1	A	160	THR
1	A	161	VAL
1	A	170	VAL
1	A	175	VAL
1	A	178	SER
1	A	179	VAL
1	A	190	SER
1	A	192	THR
1	A	195	SER
1	A	197	LEU

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Mol	Chain	Res	Type
1	A	208	ILE
2	D	1	ASP
2	D	5	THR
2	D	6	GLN
2	D	10	SER
2	D	14	SER
2	D	15	LEU
2	D	19	ILE
2	D	26	SER
2	D	27	GLN
2	D	31	LEU
2	D	43	ILE
2	D	50	ARG
2	D	53	ASN
2	D	56	THR
2	D	61	ARG
2	D	69	THR
2	D	76	SER
2	D	79	GLN
2	D	97	THR
2	D	105	ASP
2	D	135	LEU
2	D	137	GLU
2	D	142	LEU
2	D	143	VAL
2	D	149	VAL
2	D	156	SER
2	D	182	ILE
2	D	191	PHE
2	D	200	THR
2	D	202	THR
2	D	203	VAL
2	D	206	SER
2	D	215	SER
2	D	218	THR
2	D	228	SER
2	D	229	ARG
2	D	232	ASP
2	D	236	THR
2	D	240	MET
2	D	250	THR
2	C	5	THR

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Mol	Chain	Res	Type
2	C	6	GLN
2	C	10	SER
2	C	14	SER
2	C	15	LEU
2	C	19	ILE
2	C	26	SER
2	C	27	GLN
2	C	31	LEU
2	C	43	ILE
2	C	53	ASN
2	C	56	THR
2	C	61	ARG
2	C	69	THR
2	C	76	SER
2	C	79	GLN
2	C	102	THR
2	C	104	LEU
2	C	133	VAL
2	C	135	LEU
2	C	136	GLN
2	C	142	LEU
2	C	143	VAL
2	C	148	SER
2	C	149	VAL
2	C	151	LEU
2	C	156	SER
2	C	159	THR
2	C	165	LEU
2	C	186	ASN
2	C	191	PHE
2	C	200	THR
2	C	203	VAL
2	C	215	SER
2	C	218	THR
2	C	228	SER
2	C	229	ARG
2	C	245	GLN
2	C	253	SER
1	B	8	SER
1	B	29	MET
1	B	32	GLU
1	B	38	TRP

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Mol	Chain	Res	Type
1	B	43	LEU
1	B	56	VAL
1	B	59	ARG
1	B	68	THR
1	B	76	THR
1	B	90	SER
1	B	96	LEU
1	B	101	ASP
1	B	106	GLU
1	B	128	TYR
1	B	130	ASP
1	B	151	SER
1	B	158	ILE
1	B	160	THR
1	B	161	VAL
1	B	170	VAL
1	B	175	VAL
1	B	178	SER
1	B	179	VAL
1	B	181	MET
1	B	182	ARG
1	B	190	SER
1	B	192	THR
1	B	195	SER
1	B	198	LEU
1	B	206	ILE
1	B	208	ILE
1	B	210	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	6	GLN
2	D	90	GLN
2	D	134	GLN
2	D	136	GLN
2	D	174	GLN
2	C	170	GLN
1	B	86	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	NAG	A	301	1	14,14,15	0.51	0	15,19,21	0.92	1 (6%)
3	NAG	B	301	1	14,14,15	0.51	0	15,19,21	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	301	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	NAG	O5-C1-C2	-2.78	107.60	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	NAG	5	0

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	214/220 (97%)	0.40	11 (5%)	29	13	55, 95, 157, 220	0
1	B	213/220 (96%)	0.30	2 (0%)	84	71	53, 96, 150, 210	0
2	C	232/259 (89%)	-0.17	0	100	100	46, 74, 106, 131	0
2	D	232/259 (89%)	-0.19	0	100	100	36, 66, 100, 144	0
All	All	891/958 (93%)	0.07	13 (1%)	74	56	36, 81, 143, 220	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	ALA	3.4
1	A	127	GLY	3.4
1	B	163	ALA	3.4
1	A	32	GLU	3.2
1	A	99	PHE	3.1
1	A	36	LEU	2.7
1	A	171	GLY	2.5
1	A	74	GLY	2.3
1	B	185	SER	2.3
1	A	102	GLY	2.3
1	A	133	ILE	2.1
1	A	187	GLU	2.1
1	A	73	ASP	2.1

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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	B	301	14/15	0.61	0.30	-	83,118,145,160	0
3	NAG	A	301	14/15	0.64	0.26	-	79,122,136,137	0

6.5 Other polymers ⓘ

There are no such residues in this entry.