



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:08 PM UTC

PDB ID : 8VC7 / pdb_00008vc7
Title : Crystal Structure of Human BTN2A1 ectodomain in complex with Antagonist 2A1.9 Fab
Authors : Ramesh, A.; Roy, S.; Adams, E.
Deposited on : 2023-12-13
Resolution : 2.76 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

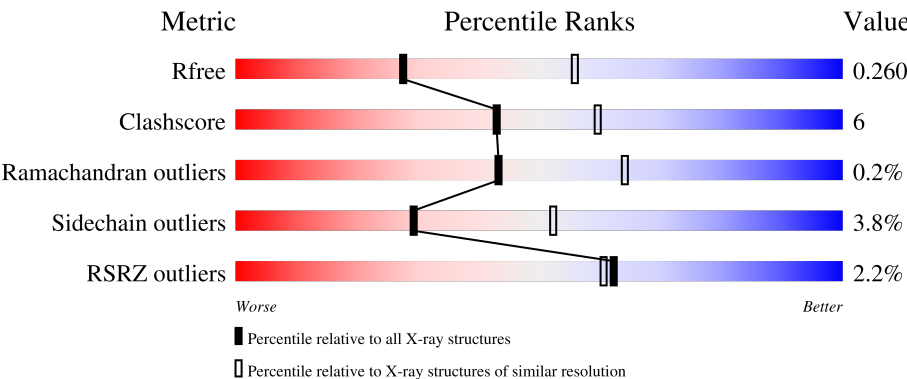
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	3% 82% 17% .
1	D	215	89% 10%
2	B	233	% 76% 15% 8%
2	J	233	% 80% 12% 8%
3	C	231	2% 72% 20% 7%

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Mol	Chain	Length	Quality of chain
3	E	231	5% 76% 15% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9797 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 Human IgG1 Fragment Antibody Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	214	Total	C	N	O	S	0	0	0
			1614	1003	271	334	6			
1	A	214	Total	C	N	O	S	0	0	0
			1596	992	268	330	6			

- Molecule 2 is a protein called Human IgG1 Fragment Antibody Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	215	Total	C	N	O	S	0	0	0
			1603	1017	263	317	6			
2	B	215	Total	C	N	O	S	0	0	0
			1606	1020	263	317	6			

- Molecule 3 is a protein called Butyrophilin subfamily 2 member A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	11	0	0
			1650	1039	288	312	11			
3	E	215	Total	C	N	O	S	11	0	0
			1658	1047	288	312	11			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ALA	-	expression tag	UNP Q7KYR7
C	-1	ASP	-	expression tag	UNP Q7KYR7
C	0	LEU	-	expression tag	UNP Q7KYR7
C	219	SER	CYS	engineered mutation	UNP Q7KYR7
C	220	GLY	-	expression tag	UNP Q7KYR7
C	221	SER	-	expression tag	UNP Q7KYR7
C	222	GLY	-	expression tag	UNP Q7KYR7
C	223	LEU	-	expression tag	UNP Q7KYR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	224	GLU	-	expression tag	UNP Q7KYR7
C	225	VAL	-	expression tag	UNP Q7KYR7
C	226	LEU	-	expression tag	UNP Q7KYR7
C	227	PHE	-	expression tag	UNP Q7KYR7
C	228	GLN	-	expression tag	UNP Q7KYR7
E	-2	ALA	-	expression tag	UNP Q7KYR7
E	-1	ASP	-	expression tag	UNP Q7KYR7
E	0	LEU	-	expression tag	UNP Q7KYR7
E	219	SER	CYS	engineered mutation	UNP Q7KYR7
E	220	GLY	-	expression tag	UNP Q7KYR7
E	221	SER	-	expression tag	UNP Q7KYR7
E	222	GLY	-	expression tag	UNP Q7KYR7
E	223	LEU	-	expression tag	UNP Q7KYR7
E	224	GLU	-	expression tag	UNP Q7KYR7
E	225	VAL	-	expression tag	UNP Q7KYR7
E	226	LEU	-	expression tag	UNP Q7KYR7
E	227	PHE	-	expression tag	UNP Q7KYR7
E	228	GLN	-	expression tag	UNP Q7KYR7

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

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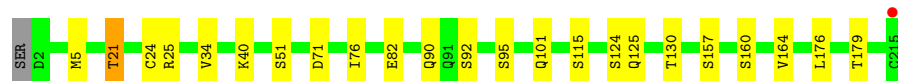
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

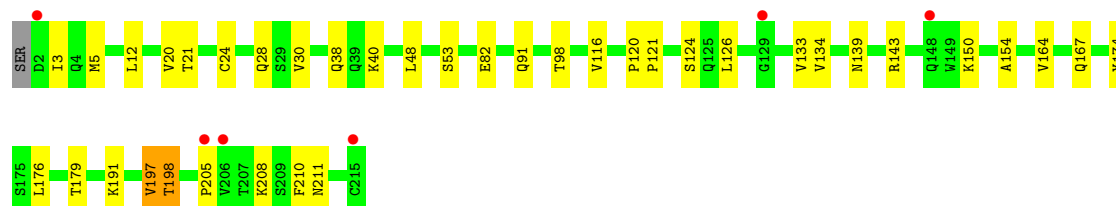
- Molecule 1: Human IgG1 Fragment Antibody Light Chain

Chain D: 



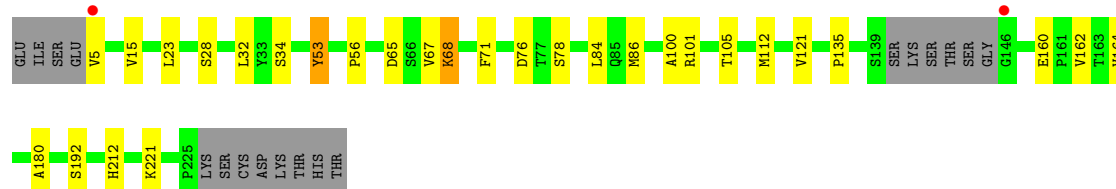
- Molecule 1: Human IgG1 Fragment Antibody Light Chain

Chain A: 



- Molecule 2: Human IgG1 Fragment Antibody Heavy Chain

Chain J: 



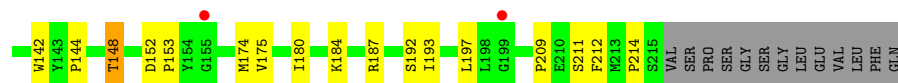
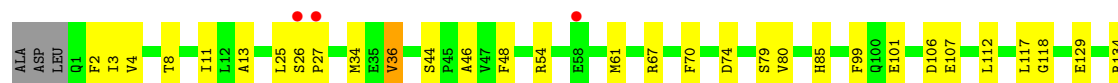
- Molecule 2: Human IgG1 Fragment Antibody Heavy Chain

Chain B: 

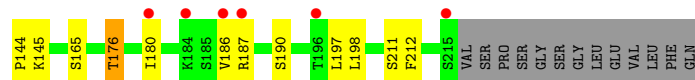
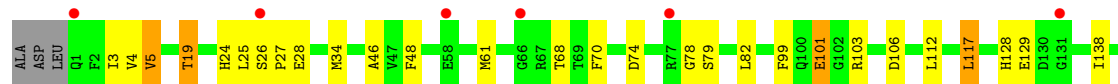
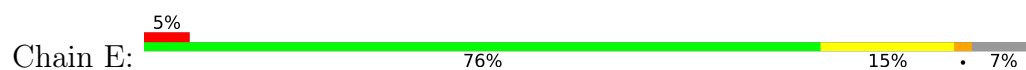




• Molecule 3: Butyrophilin subfamily 2 member A1



• Molecule 3: Butyrophilin subfamily 2 member A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.91Å 200.98Å 206.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.46 – 2.76 39.46 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.46-2.76) 91.1 (39.46-2.76)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5015	Depositor
R, R_{free}	0.218 , 0.261 0.218 , 0.260	Depositor DCC
R_{free} test set	1999 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9797	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9301e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.39	0/1628	0.65	0/2218
1	D	0.41	0/1646	0.63	0/2237
2	B	0.39	0/1649	0.65	0/2255
2	J	0.40	0/1646	0.66	0/2252
3	C	0.38	0/1686	0.60	0/2290
3	E	0.39	0/1695	0.61	0/2300
All	All	0.39	0/9950	0.63	0/13552

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
3	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	54	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	1596	0	1512	25	0
1	D	1614	0	1555	9	0
2	B	1606	0	1534	21	0
2	J	1603	0	1528	17	0
3	C	1650	0	1591	25	0
3	E	1658	0	1602	25	0
4	C	42	0	39	0	0
4	E	28	0	26	0	0
All	All	9797	0	9387	118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (118) 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)
3:E:3:ILE:HG12	3:E:26:SER:HB2	1.23	1.08
3:C:3:ILE:HG13	3:C:26:SER:HB3	1.52	0.91
3:E:3:ILE:H	3:E:26:SER:HB3	1.40	0.87
1:A:91:GLN:HE21	1:A:98:THR:HG22	1.44	0.83
1:D:21:THR:HG21	1:A:205:PRO:HD3	1.65	0.76
3:C:148:THR:HG21	3:C:175:VAL:HG11	1.65	0.76
1:A:143:ARG:HH21	1:A:164:VAL:HG21	1.51	0.76
1:A:164:VAL:HG22	1:A:176:LEU:HD12	1.66	0.75
1:A:167:GLN:HG3	1:A:174:TYR:CZ	2.27	0.70
1:A:139:ASN:HD21	2:B:176:HIS:CE1	2.10	0.69
1:A:3:ILE:O	1:A:98:THR:HG21	1.95	0.67
1:A:116:VAL:HG21	1:A:197:VAL:HG11	1.78	0.65
1:A:139:ASN:HD21	2:B:176:HIS:HE1	1.45	0.64
3:C:4:VAL:HG23	3:C:106:ASP:HB3	1.80	0.63
1:D:5:MET:HE3	1:D:24:CYS:SG	2.38	0.63
1:D:40:LYS:NZ	1:D:82:GLU:O	2.26	0.63
3:E:128:HIS:NE2	3:E:212:PHE:O	2.30	0.61
1:A:40:LYS:NZ	1:A:82:GLU:O	2.31	0.61
3:E:4:VAL:HG23	3:E:106:ASP:HB3	1.82	0.61
2:J:67:VAL:HG13	2:J:71:PHE:CG	2.36	0.60
1:D:164:VAL:HG22	1:D:176:LEU:HD12	1.84	0.60
2:J:32:LEU:HB3	2:J:56:PRO:HG2	1.85	0.59
2:B:222:LYS:HE2	2:B:224:GLU:HG2	1.83	0.59
3:C:2:PHE:HA	3:C:27:PRO:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:MET:HE3	1:A:24:CYS:SG	2.42	0.58
2:B:23:LEU:HG	2:B:86:MET:HE2	1.85	0.58
2:J:23:LEU:HG	2:J:86:MET:HE2	1.85	0.58
3:C:129:GLU:OE2	3:C:134:ARG:HD2	2.04	0.57
1:D:25:ARG:HG3	1:D:71:ASP:OD1	2.05	0.56
1:A:38:GLN:HB2	1:A:48:LEU:HD11	1.88	0.56
1:A:143:ARG:HB3	1:A:174:TYR:CD2	2.41	0.55
3:C:144:PRO:HD3	3:C:197:LEU:HD12	1.89	0.55
1:A:191:LYS:HD3	1:A:211:ASN:HB3	1.90	0.54
2:J:135:PRO:HD3	2:J:221:LYS:HE3	1.90	0.54
1:A:143:ARG:NH2	1:A:164:VAL:HG21	2.21	0.53
2:B:5:VAL:HA	2:B:28:SER:O	2.08	0.53
3:C:67:ARG:HD2	3:C:85:HIS:O	2.08	0.53
3:E:103:ARG:HG2	3:E:103:ARG:O	2.08	0.53
3:E:144:PRO:HD3	3:E:197:LEU:HD12	1.91	0.52
2:J:76:ASP:OD1	2:J:78:SER:OG	2.28	0.52
1:A:134:VAL:HG22	1:A:179:THR:HG23	1.93	0.51
3:E:3:ILE:H	3:E:26:SER:CB	2.19	0.51
3:E:34:MET:HE3	3:E:101:GLU:HB2	1.91	0.51
3:E:46:ALA:O	3:E:61:MET:HG3	2.11	0.51
1:D:125:GLN:HG2	1:D:130:THR:O	2.11	0.51
2:B:135:PRO:HD3	2:B:221:LYS:HE3	1.93	0.51
1:A:12:LEU:HD21	1:A:20:VAL:HG13	1.92	0.50
3:E:19:THR:HG21	3:E:112:LEU:HD21	1.93	0.49
2:B:76:ASP:OD1	2:B:78:SER:OG	2.30	0.49
1:A:3:ILE:HD13	1:A:30:VAL:HG12	1.95	0.49
3:C:34:MET:HE3	3:C:101:GLU:HB2	1.95	0.48
2:J:100:ALA:HB1	2:J:112:MET:HB3	1.96	0.48
2:J:67:VAL:HG13	2:J:71:PHE:CD2	2.49	0.48
3:E:129:GLU:OE1	3:E:180:ILE:HD11	2.14	0.48
3:C:11:ILE:HB	3:C:112:LEU:HD23	1.96	0.47
2:J:65:ASP:OD1	2:J:68:LYS:HE3	2.14	0.47
2:J:162:VAL:HG12	2:J:212:HIS:HB2	1.96	0.47
3:E:26:SER:OG	3:E:27:PRO:HD3	2.14	0.47
3:C:48:PHE:CZ	3:C:70:PHE:HB2	2.50	0.47
2:B:163:THR:HG22	2:B:211:ASN:O	2.15	0.47
3:E:5:VAL:HG13	3:E:24:HIS:CD2	2.49	0.47
2:B:163:THR:CG2	2:B:211:ASN:HB3	2.45	0.47
2:J:34:SER:HB2	3:C:44:SER:HB3	1.97	0.47
1:A:121:PRO:HD3	1:A:133:VAL:HG22	1.97	0.47
2:B:163:THR:HG23	2:B:211:ASN:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:68:THR:HB	3:E:82:LEU:HD11	1.97	0.46
1:A:198:THR:HG22	1:A:205:PRO:HG3	1.96	0.46
2:J:5:VAL:HA	2:J:28:SER:O	2.16	0.45
3:C:118:GLY:HA3	3:C:142:TRP:CE2	2.51	0.45
1:A:120:PRO:HB3	1:A:210:PHE:CE2	2.52	0.45
3:C:13:ALA:HB2	3:C:112:LEU:HD22	1.98	0.45
2:B:101:ARG:CZ	2:B:103:TYR:HB2	2.47	0.45
3:C:184:LYS:O	3:C:187:ARG:NH2	2.31	0.45
3:E:186:VAL:O	3:E:187:ARG:HB2	2.16	0.45
3:C:152:ASP:HB2	3:C:153:PRO:HD2	1.99	0.44
3:C:25:LEU:HD21	3:C:99:PHE:CG	2.52	0.44
3:C:174:MET:HE3	3:C:174:MET:HB2	1.77	0.44
3:E:24:HIS:HA	3:E:78:GLY:O	2.17	0.44
2:J:160:GLU:OE2	2:J:180:ALA:HB3	2.18	0.44
3:E:74:ASP:HB2	3:E:79:SER:HB3	2.00	0.44
2:J:86:MET:HE1	2:J:121:VAL:HG21	2.00	0.43
1:D:160:SER:HA	1:D:179:THR:O	2.17	0.43
3:C:74:ASP:HB2	3:C:79:SER:HB3	2.01	0.43
3:C:148:THR:HB	3:C:193:ILE:CD1	2.48	0.43
2:B:31:ASN:HD21	2:B:33:TYR:HB3	1.84	0.43
3:C:148:THR:HB	3:C:193:ILE:HD13	2.00	0.43
2:B:207:ILE:HG12	2:B:222:LYS:HB2	2.01	0.43
3:C:129:GLU:OE1	3:C:180:ILE:HD11	2.19	0.43
2:B:71:PHE:CE1	2:B:86:MET:HB3	2.54	0.42
3:E:138:ILE:HG22	3:E:176:THR:HB	2.00	0.42
1:D:34:VAL:HA	1:D:90:GLN:O	2.19	0.42
2:B:15:VAL:HG21	2:B:89:LEU:HD12	2.01	0.42
2:B:63:TYR:HB2	2:B:68:LYS:HG3	2.01	0.42
3:E:25:LEU:HD21	3:E:99:PHE:CD2	2.55	0.42
2:J:84:LEU:HD12	2:J:84:LEU:HA	1.89	0.42
2:B:100:ALA:HB1	2:B:112:MET:HB3	2.02	0.42
3:E:26:SER:CB	3:E:27:PRO:HD3	2.50	0.42
1:A:116:VAL:CG2	1:A:197:VAL:HG11	2.47	0.42
3:C:46:ALA:O	3:C:61:MET:HG3	2.19	0.41
1:A:116:VAL:O	1:A:208:LYS:HE3	2.20	0.41
2:J:53:TYR:C	2:J:53:TYR:CD1	2.98	0.41
3:E:117:LEU:HA	3:E:117:LEU:HD12	1.78	0.41
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.80	0.41
2:B:128:THR:HA	2:B:158:PHE:O	2.20	0.41
3:C:118:GLY:HA3	3:C:142:TRP:NE1	2.36	0.41
2:B:32:LEU:HB3	2:B:56:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:112:LEU:HD12	3:E:112:LEU:HA	1.67	0.41
3:C:209:PRO:HG2	3:C:212:PHE:CE2	2.56	0.41
2:J:71:PHE:CE1	2:J:86:MET:HB3	2.56	0.40
3:C:36:VAL:HG21	3:C:80:VAL:HG21	2.04	0.40
2:B:131:PRO:HB3	2:B:157:TYR:HB3	2.03	0.40
3:E:145:LYS:HG3	3:E:165:SER:OG	2.21	0.40
2:J:164:VAL:HG11	2:J:192:SER:CB	2.51	0.40
3:E:48:PHE:CZ	3:E:70:PHE:HB2	2.56	0.40
1:D:101:GLN:OE1	1:D:101:GLN:N	2.51	0.40
2:B:37:ILE:HD13	2:B:37:ILE:HA	1.93	0.40
1:A:150:LYS:HA	1:A:154:ALA:O	2.22	0.40
3:E:117:LEU:HD13	3:E:198:LEU:HD12	2.01	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	212/215 (99%)	206 (97%)	6 (3%)	0	100	100
1	D	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
2	B	211/233 (91%)	205 (97%)	5 (2%)	1 (0%)	24	43
2	J	211/233 (91%)	205 (97%)	6 (3%)	0	100	100
3	C	213/231 (92%)	207 (97%)	5 (2%)	1 (0%)	24	43
3	E	213/231 (92%)	204 (96%)	8 (4%)	1 (0%)	24	43
All	All	1272/1358 (94%)	1232 (97%)	37 (3%)	3 (0%)	43	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5	VAL

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Mol	Chain	Res	Type
3	C	214	PRO
3	E	28	GLU

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	180/190 (95%)	174 (97%)	6 (3%)	33	57
1	D	186/190 (98%)	178 (96%)	8 (4%)	26	47
2	B	175/195 (90%)	167 (95%)	8 (5%)	24	45
2	J	175/195 (90%)	170 (97%)	5 (3%)	37	61
3	C	177/199 (89%)	170 (96%)	7 (4%)	28	50
3	E	177/199 (89%)	170 (96%)	7 (4%)	28	50
All	All	1070/1168 (92%)	1029 (96%)	41 (4%)	29	52

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	21	THR
1	D	51	SER
1	D	76	ILE
1	D	92	SER
1	D	95	SER
1	D	115	SER
1	D	124	SER
1	D	157	SER
2	J	15	VAL
2	J	53	TYR
2	J	68	LYS
2	J	101	ARG
2	J	105	THR
3	C	8	THR
3	C	36	VAL
3	C	107	GLU

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Mol	Chain	Res	Type
3	C	117	LEU
3	C	148	THR
3	C	192	SER
3	C	211	SER
1	A	21	THR
1	A	28	GLN
1	A	53	SER
1	A	124	SER
1	A	197	VAL
1	A	198	THR
2	B	4	GLU
2	B	5	VAL
2	B	7	LEU
2	B	53	TYR
2	B	101	ARG
2	B	160	GLU
2	B	162	VAL
2	B	173	SER
3	E	5	VAL
3	E	19	THR
3	E	101	GLU
3	E	117	LEU
3	E	176	THR
3	E	190	SER
3	E	211	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	38	GLN
1	D	139	ASN
1	D	161	GLN
2	J	6	GLN
2	J	117	GLN
3	C	42	GLN
3	C	60	GLN
3	C	194	ASN
3	C	200	GLN
1	A	4	GLN
1	A	139	ASN
2	B	176	HIS
3	E	60	GLN

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Mol	Chain	Res	Type
3	E	90	GLN
3	E	111	HIS
3	E	194	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
4	NAG	C	303	3	14,14,15	0.73	0	17,19,21	1.87	3 (17%)
4	NAG	C	302	3	14,14,15	1.27	2 (14%)	17,19,21	3.21	7 (41%)
4	NAG	E	302	3	14,14,15	0.64	0	17,19,21	1.97	2 (11%)
4	NAG	C	301	3	14,14,15	0.98	1 (7%)	17,19,21	1.39	4 (23%)
4	NAG	E	301	3	14,14,15	1.19	1 (7%)	17,19,21	3.88	8 (47%)

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
4	NAG	C	303	3	-	2/6/23/26	0/1/1/1
4	NAG	C	302	3	-	2/6/23/26	0/1/1/1
4	NAG	E	302	3	-	0/6/23/26	0/1/1/1
4	NAG	C	301	3	-	3/6/23/26	0/1/1/1
4	NAG	E	301	3	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	302	NAG	C1-C2	3.15	1.56	1.52
4	E	301	NAG	C1-C2	3.06	1.56	1.52
4	C	301	NAG	C1-C2	2.04	1.55	1.52
4	C	302	NAG	O5-C5	-2.01	1.39	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	301	NAG	C2-N2-C7	11.00	137.63	122.90
4	C	302	NAG	C2-N2-C7	10.12	136.47	122.90
4	E	301	NAG	C1-O5-C5	8.54	123.63	112.19
4	E	302	NAG	C1-O5-C5	6.97	121.53	112.19
4	C	303	NAG	C1-O5-C5	6.75	121.23	112.19
4	C	302	NAG	C1-C2-N2	4.23	117.09	110.43
4	E	301	NAG	O5-C1-C2	3.89	117.31	111.29
4	C	302	NAG	O7-C7-N2	3.82	128.73	121.98
4	E	301	NAG	O7-C7-N2	3.27	127.76	121.98
4	C	301	NAG	C2-N2-C7	3.17	127.14	122.90
4	E	301	NAG	O5-C5-C6	-2.99	101.85	107.66
4	E	301	NAG	C4-C3-C2	2.98	115.39	111.02
4	C	302	NAG	C6-C5-C4	2.82	119.95	113.02
4	C	302	NAG	C4-C3-C2	2.76	115.07	111.02
4	C	301	NAG	O6-C6-C5	-2.55	102.64	111.33
4	C	302	NAG	O5-C5-C4	-2.41	104.97	110.83
4	C	301	NAG	C1-O5-C5	2.37	115.37	112.19
4	E	301	NAG	O7-C7-C8	-2.32	117.93	122.05
4	C	303	NAG	O3-C3-C2	-2.19	104.86	109.40
4	C	301	NAG	O4-C4-C5	2.17	114.67	109.32
4	E	301	NAG	O4-C4-C3	-2.14	105.34	110.38
4	C	302	NAG	O7-C7-C8	-2.13	118.27	122.05
4	C	303	NAG	O5-C5-C6	-2.01	103.75	107.66
4	E	302	NAG	C2-N2-C7	2.00	125.58	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	302	NAG	O5-C5-C6-O6
4	C	302	NAG	C4-C5-C6-O6
4	C	301	NAG	C8-C7-N2-C2
4	C	301	NAG	O7-C7-N2-C2
4	C	303	NAG	C8-C7-N2-C2
4	C	303	NAG	O7-C7-N2-C2
4	E	301	NAG	O5-C5-C6-O6
4	E	301	NAG	C4-C5-C6-O6
4	C	301	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	214/215 (99%)	0.04	6 (2%) 55 53	24, 34, 57, 87	0
1	D	214/215 (99%)	-0.21	1 (0%) 87 87	23, 33, 45, 83	0
2	B	215/233 (92%)	-0.23	2 (0%) 81 81	22, 33, 49, 68	0
2	J	215/233 (92%)	-0.26	2 (0%) 81 81	23, 32, 48, 69	0
3	C	215/231 (93%)	0.18	5 (2%) 61 59	22, 41, 59, 72	3 (1%)
3	E	215/231 (93%)	0.48	12 (5%) 30 30	28, 44, 71, 90	4 (1%)
All	All	1288/1358 (94%)	-0.00	28 (2%) 62 60	22, 36, 58, 90	7 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	215	SER	6.6
3	E	1	GLN	3.6
1	A	215	CYS	3.6
3	E	186	VAL	3.3
3	E	26	SER	2.9
1	D	215	CYS	2.8
2	B	146	GLY	2.8
3	E	180	ILE	2.8
3	C	155	GLY	2.7
3	E	187	ARG	2.6
3	E	66	GLY	2.5
3	C	26	SER	2.5
3	C	58	GLU	2.5
3	C	199	GLY	2.4
1	A	129	GLY	2.4
3	C	27	PRO	2.4
1	A	2	ASP	2.4
2	J	146	GLY	2.4
1	A	205	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	58	GLU	2.3
3	E	131	GLY	2.2
2	J	5	VAL	2.2
3	E	196	THR	2.1
3	E	77	ARG	2.1
2	B	161	PRO	2.1
3	E	184	LYS	2.0
1	A	148	GLN	2.0
1	A	206	VAL	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	302	14/15	0.50	0.22	60,70,78,81	0
4	NAG	E	301	14/15	0.51	0.19	47,70,78,80	0
4	NAG	C	301	14/15	0.56	0.17	54,64,71,79	0
4	NAG	E	302	14/15	0.88	0.12	39,53,57,66	0
4	NAG	C	303	14/15	0.89	0.10	46,49,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.