



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:46 AM UTC

PDB ID : 4F9L / pdb_00004f9l
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

<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

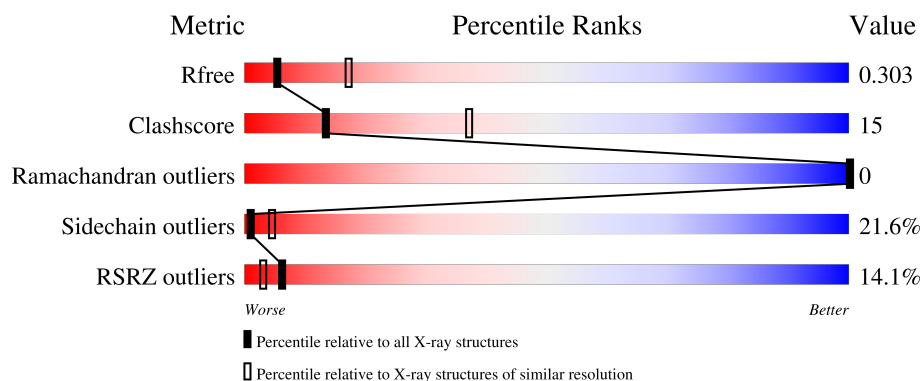
1 Overall quality at a glance

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}	180053	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (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 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	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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

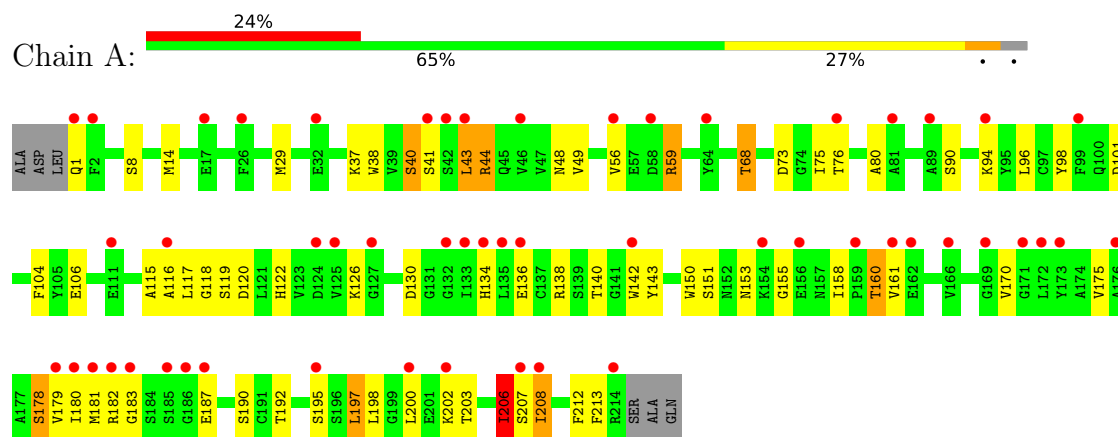


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

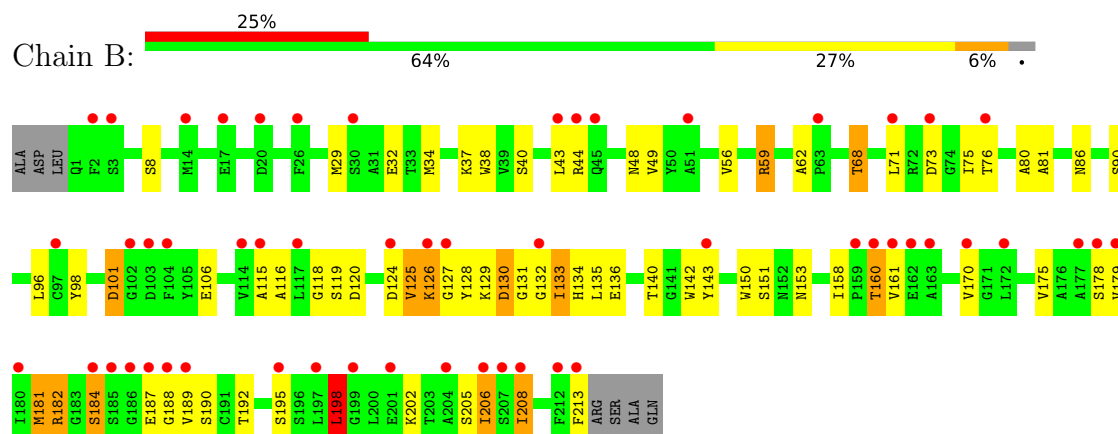
3 Residue-property plots [i](#)

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.

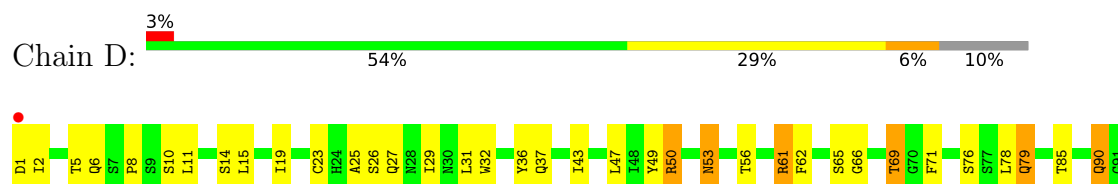
- Molecule 1: Butyrophilin subfamily 3 member A1

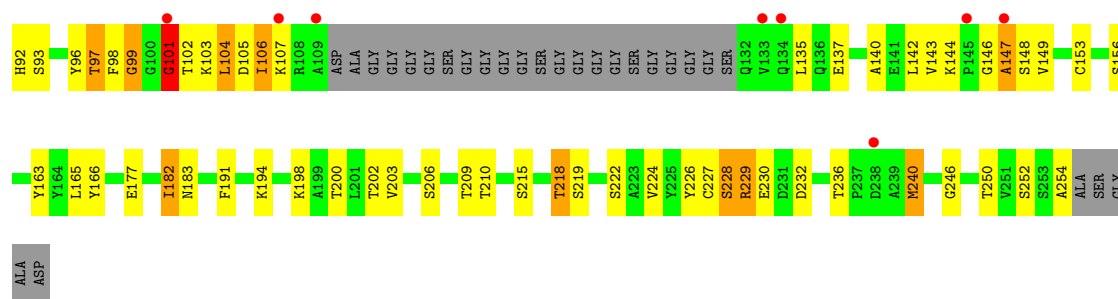


- Molecule 1: Butyrophilin subfamily 3 member A1

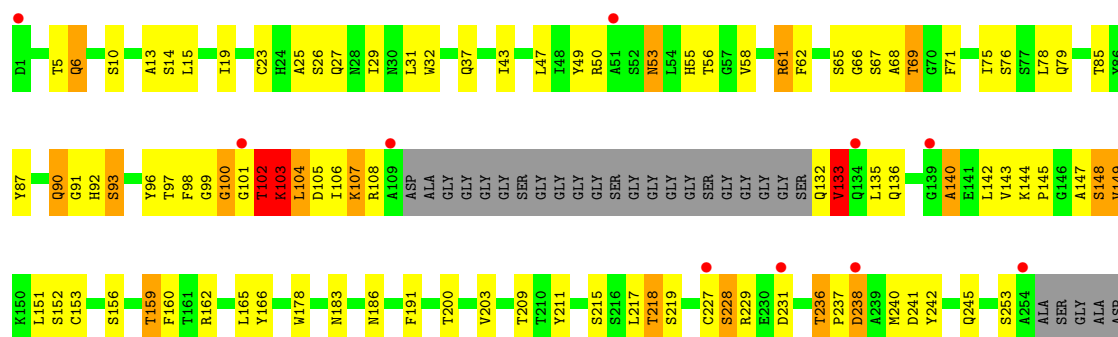


- Molecule 2: 20.1 anti-BTN3A1 antibody fragment





- Molecule 2: 20.1 anti-BTN3A1 antibody fragment



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) 99.7 (45.80-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.254 , 0.303 0.256 , 0.303	Depositor DCC
R_{free} test set	1330 reflections (5.14%)	wwPDB-VP
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 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	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.*

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: 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	0.47	0/1560	0.96	5/2131 (0.2%)
1	B	0.57	0/1555	0.98	5/2124 (0.2%)
2	C	0.59	3/1798 (0.2%)	0.96	7/2453 (0.3%)
2	D	0.58	2/1805 (0.1%)	1.00	8/2460 (0.3%)
All	All	0.56	5/6718 (0.1%)	0.98	25/9168 (0.3%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	103	LYS	C-O	-6.16	1.17	1.24
2	C	103	LYS	C-O	-5.53	1.17	1.24
2	C	100	GLY	CA-C	-5.47	1.46	1.52
2	D	104	LEU	C-O	-5.33	1.17	1.24
2	C	102	THR	C-O	-5.09	1.18	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	148	SER	N-CA-C	9.54	122.65	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	133	VAL	N-CA-C	8.63	121.28	109.80
2	D	101	GLY	CA-C-N	8.34	132.56	120.71
2	D	101	GLY	C-N-CA	8.34	132.56	120.71
2	C	107	LYS	N-CA-C	-8.15	100.38	110.41
2	D	99	GLY	N-CA-C	-8.07	100.17	112.51
2	D	107	LYS	N-CA-C	7.91	122.65	112.92
1	A	187	GLU	N-CA-C	-6.90	104.34	112.89
1	A	73	ASP	N-CA-C	6.83	119.57	111.71
1	B	73	ASP	N-CA-C	6.75	119.47	111.71
1	A	126	LYS	N-CA-C	6.53	119.72	111.69
2	C	140	ALA	N-CA-C	6.18	118.47	108.34
2	D	144	LYS	CA-C-N	6.07	127.42	119.84
2	D	144	LYS	C-N-CA	6.07	127.42	119.84
2	C	148	SER	N-CA-C	6.05	118.11	110.24
1	A	155	GLY	N-CA-C	5.72	120.83	111.27
1	B	184	SER	CB-CA-C	-5.56	110.15	116.54
2	D	147	ALA	N-CA-C	5.49	115.37	108.45
1	B	131	GLY	N-CA-C	-5.42	108.53	115.42
2	C	98	PHE	N-CA-C	-5.37	101.25	109.41
1	B	126	LYS	N-CA-C	5.36	117.20	111.36
1	B	198	LEU	N-CA-C	5.34	119.90	112.90
1	A	206	ILE	N-CA-C	5.32	117.42	108.81
2	C	96	TYR	N-CA-C	-5.28	103.06	110.50
2	C	160	PHE	N-CA-C	5.18	116.93	111.28

There are no chirality outliers.

All (11) planarity outliers are listed below:

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	38	0
1	B	1523	0	1421	50	0
2	C	1756	0	1651	58	0
2	D	1763	0	1670	50	0
3	A	14	0	13	0	0
3	B	14	0	13	5	0
All	All	6598	0	6187	187	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 15.

All (187) 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:HG3	2:C:61:ARG:NH1	1.87	0.89
2:C:61:ARG:HH11	2:C:61:ARG:CG	1.89	0.86
1:A:212:PHE:HZ	1:B:127:GLY:HA2	1.39	0.83
2:D:61:ARG:HH11	2:D:61:ARG:HG3	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:CG	1:B:182:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:ASP:OD1	2:C:106:ILE:N	2.21	0.73
2:D:50:ARG:HH11	2:D:50:ARG:HG2	1.51	0.73
1:A:206:ILE:HG13	1:A:207:SER:N	2.03	0.73
1:A:181:MET:HE1	1:A:207:SER:HA	1.72	0.71
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
2:C:32:TRP:HE3	2:C:238:ASP:OD1	1.79	0.66
1:B:71:LEU:HD12	1:B:81:ALA:HB3	1.76	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:D:228:SER:HB2	2:D:240:MET:HB2	1.80	0.64
2:C:58:VAL:HG13	2:C:62:PHE:HD2	1.62	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
1:B:86:ASN:CG	3:B:301:NAG:C1	2.71	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
1:B:188:GLY:C	1:B:189:VAL:HG13	2.25	0.60
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
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
2:C:55:HIS:NE2	2:C:241:ASP:OD2	2.37	0.58
1:B:150:TRP:H	1:B:160:THR:HG21	1.68	0.58
1:B:181:MET:SD	1:B:208:ILE:HG13	2.44	0.58
1:B:181:MET:O	1:B:181:MET:HG2	2.04	0.57
1:A:115:ALA:HB2	1:A:197:LEU:HD22	1.85	0.57
1:A:122:HIS:CE1	1:B:205:SER:HG	2.19	0.57
1:B:34:MET:HG2	1:B:101:ASP:HB2	1.86	0.57
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASP:O	1:B:135:LEU:HA	2.04	0.57
2:D:50:ARG:HH11	2:D:50:ARG:CG	2.16	0.57
1:B:48:ASN:HB2	1:B:68:THR:HG21	1.86	0.57
1:A:150:TRP:H	1:A:160:THR:HG21	1.70	0.57
2:D:226:TYR:CD1	2:D:246:GLY:HA3	2.40	0.57
1:B:86:ASN:ND2	3:B:301:NAG:C2	2.68	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
2:D:6:GLN:HE21	2:D:102:THR:H	1.53	0.56
1:A:101:ASP:OD1	1:A:101:ASP:C	2.49	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
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
1:B:125:VAL:HA	1:B:134:HIS:O	2.07	0.55
2:D:8:PRO:O	2:D:102:THR:HG23	2.07	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:130:ASP:C	1:B:132:GLY:H	2.15	0.54
2:C:6:GLN:OE1	2:C:99:GLY:O	2.25	0.53
1:B:133:ILE:HG21	1:B:208:ILE:HD12	1.90	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
2:C:65:SER:OG	2:C:66:GLY:N	2.41	0.52
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
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
2:C:136:GLN:HB3	2:C:153:CYS:SG	2.50	0.51
1:B:120:ASP:OD1	1:B:202:LYS:NZ	2.29	0.51
1:B:86:ASN:ND2	3:B:301:NAG:O5	2.30	0.50
2:D:90:GLN:HG2	2:D:92:HIS:H	1.77	0.50
2:C:61:ARG:HH11	2:C:61:ARG:CB	2.25	0.50
2:D:61:ARG:HG3	2:D:61:ARG:NH1	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:MET:HE1	1:A:198:LEU:HD21	1.93	0.49
1:A:130:ASP:HB3	1:A:180:ILE:HD13	1.93	0.49
1:A:1:GLN:HA	1:A:104:PHE:CZ	2.48	0.48
2:C:106:ILE:C	2:C:107:LYS:O	2.52	0.48
1:A:118:GLY:HA3	1:A:142:TRP:CE2	2.48	0.48
1:A:153:ASN:OD1	1:A:153:ASN:N	2.41	0.48
1:A:117:LEU:HD13	1:A:198:LEU:HD13	1.95	0.48
2:D:61:ARG:NH1	2:D:62:PHE:HE1	2.11	0.48
1:B:182:ARG:NH1	1:B:182:ARG:HG2	2.26	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:OD1	2:D:53:ASN:N	2.29	0.47
2:D:153:CYS:HB3	2:D:210:THR:CG2	2.45	0.47
2:C:106:ILE:O	2:C:107:LYS:O	2.32	0.47
1:B:118:GLY:HA3	1:B:142:TRP:CE2	2.50	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:D:49:TYR:O	2:D:50:ARG:CB	2.63	0.46
2:C:49:TYR:O	2:C:50:ARG:CB	2.64	0.46
2:C:67:SER:OG	2:C:68:ALA:N	2.48	0.45
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
1:B:188:GLY:C	1:B:189:VAL:CG1	2.89	0.45
1:A:116:ALA:HB3	1:A:143:TYR:H	1.82	0.45
2:D:29:ILE:HD11	2:D:71:PHE:CE2	2.52	0.45
2:C:78:LEU:HD23	2:C:106:ILE:HD11	1.98	0.45
2:D:29:ILE:O	2:D:32:TRP:HD1	2.00	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:D:85:THR:HG22	2:D:101:GLY:O	2.17	0.45
2:C:152:SER:HB3	2:C:211:TYR:CD2	2.52	0.45
1:B:116:ALA:HB3	1:B:143:TYR:H	1.83	0.44
1:A:14:MET:HA	1:A:14:MET:HE2	2.00	0.44
1:A:44:ARG:HA	1:A:44:ARG:HD3	1.47	0.44
2:C:85:THR:HA	2:C:103:LYS:HA	2.00	0.44
1:B:125:VAL:HG22	1:B:135:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:ARG:CG	2:D:50:ARG:NH1	2.74	0.44
2:C:62:PHE:HE1	2:C:75:ILE:HG23	1.78	0.44
2:C:183:ASN:OD1	1:B:62:ALA:HB1	2.17	0.44
1:B:125:VAL:HG22	1:B:135:LEU:CD2	2.47	0.44
1:B:153:ASN:OD1	1:B:153:ASN:N	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
1:B:126:LYS:HZ2	1:B:126:LYS:HG2	1.61	0.43
2:D:224:VAL:HG11	2:D:226:TYR:CZ	2.54	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:D:218:THR:OG1	2:D:219:SER:N	2.48	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:107:LYS:O	2:C:108:ARG:C	2.62	0.41
1:A:41:SER:OG	1:A:94:LYS:O	2.20	0.41
2:C:178:TRP:CD1	2:C:240:MET:HE1	2.55	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
2:C:144:LYS:HA	2:C:145:PRO:HD3	1.89	0.41
1:B:153:ASN:HB3	1:B:187:GLU:O	2.20	0.41
1:A:75:ILE:HD12	1:A:80:ALA:HB2	2.02	0.41
2:D:98:PHE:C	2:D:99:GLY:O	2.59	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
2:D:50:ARG:HG2	2:D:50:ARG:NH1	2.28	0.40
2:C:23:CYS:HB3	2:C:71:PHE:HB2	2.03	0.40
1:A:198:LEU:HB3	1:A:200:LEU:HG	2.03	0.40
2:D:177:GLU:OE2	2:D:194:LYS:NZ	2.37	0.40
2:C:62:PHE:HE1	2:C:75:ILE:CG2	2.34	0.40
2:D:166:TYR:O	2:D:227:CYS:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ASN:OD1	3:B:301:NAG:N2	2.54	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 [i](#)

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%)	121 (81%)	28 (19%)	1	7
1	B	146/178 (82%)	112 (77%)	34 (23%)	1	3
2	C	188/204 (92%)	146 (78%)	42 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	189/204 (93%)	148 (78%)	41 (22%)	1	4
All	All	672/764 (88%)	527 (78%)	145 (22%)	1	4

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	29	MET
1	A	38	TRP
1	A	40	SER
1	A	43	LEU
1	A	44	ARG
1	A	49	VAL
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
1	A	206	ILE
1	A	208	ILE
2	D	1	ASP
2	D	5	THR
2	D	10	SER
2	D	14	SER
2	D	15	LEU
2	D	19	ILE
2	D	26	SER
2	D	27	GLN

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Mol	Chain	Res	Type
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	90	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	222	SER
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
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

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Mol	Chain	Res	Type
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	90	GLN
2	C	93	SER
2	C	97	THR
2	C	102	THR
2	C	103	LYS
2	C	104	LEU
2	C	133	VAL
2	C	135	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	236	THR
2	C	245	GLN
2	C	253	SER
1	B	8	SER
1	B	29	MET
1	B	32	GLU
1	B	38	TRP
1	B	43	LEU
1	B	49	VAL
1	B	56	VAL
1	B	59	ARG
1	B	68	THR

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Mol	Chain	Res	Type
1	B	76	THR
1	B	90	SER
1	B	96	LEU
1	B	101	ASP
1	B	106	GLU
1	B	125	VAL
1	B	128	TYR
1	B	130	ASP
1	B	133	ILE
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

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

Mol	Chain	Res	Type
2	D	6	GLN
2	D	37	GLN
2	D	90	GLN
2	D	134	GLN
2	D	174	GLN
2	C	37	GLN
2	C	90	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 oligosaccharides 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	B	301	1	14,14,15	0.51	0	17,19,21	0.71	0
3	NAG	A	301	1	14,14,15	0.51	0	17,19,21	0.84	1 (5%)

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	B	301	1	-	4/6/23/26	0/1/1/1
3	NAG	A	301	1	-	2/6/23/26	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(°)	Ideal(°)
3	A	301	NAG	O5-C1-C2	-2.38	107.60	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	NAG	C8-C7-N2-C2
3	B	301	NAG	O7-C7-N2-C2
3	B	301	NAG	C4-C5-C6-O6
3	B	301	NAG	O5-C5-C6-O6
3	A	301	NAG	O5-C5-C6-O6
3	A	301	NAG	C4-C5-C6-O6

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 [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	214/220 (97%)	1.35	53 (24%) 2 1	55, 95, 157, 220	0
1	B	213/220 (96%)	1.44	54 (25%) 1 1	53, 96, 150, 210	0
2	C	232/259 (89%)	0.39	10 (4%) 40 21	46, 74, 106, 131	0
2	D	232/259 (89%)	0.27	9 (3%) 43 23	36, 66, 100, 144	0
All	All	891/958 (93%)	0.84	126 (14%) 6 3	36, 81, 143, 220	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	GLY	6.0
2	C	254	ALA	5.1
1	B	127	GLY	4.9
1	A	134	HIS	4.8
1	A	171	GLY	4.6
1	B	213	PHE	4.6
1	B	206	ILE	4.4
1	B	188	GLY	4.3
1	A	195	SER	4.2
1	B	185	SER	4.2
1	B	207	SER	4.0
1	B	184	SER	4.0
2	C	101	GLY	3.9
1	A	133	ILE	3.8
1	B	195	SER	3.8
1	B	187	GLU	3.7
1	A	2	PHE	3.5
1	A	161	VAL	3.5
1	A	185	SER	3.5
2	C	109	ALA	3.4
1	B	159	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	3	SER	3.4
1	B	208	ILE	3.4
1	B	71	LEU	3.4
1	A	214	ARG	3.4
1	B	170	VAL	3.4
2	D	107	LYS	3.3
2	C	238	ASP	3.3
1	A	169	GLY	3.3
1	A	208	ILE	3.2
1	B	199	GLY	3.2
1	A	135	LEU	3.1
1	B	172	LEU	3.0
1	B	132	GLY	3.0
1	A	166	VAL	3.0
1	A	179	VAL	3.0
1	A	200	LEU	3.0
1	B	186	GLY	3.0
1	A	181	MET	2.9
1	B	197	LEU	2.9
1	B	126	LYS	2.8
1	A	81	ALA	2.8
1	B	73	ASP	2.8
1	B	26	PHE	2.8
2	C	51	ALA	2.8
1	B	180	ILE	2.8
1	B	45	GLN	2.8
1	A	156	GLU	2.8
1	A	173	TYR	2.7
1	B	179	VAL	2.7
1	B	97	CYS	2.7
1	A	76	THR	2.7
1	A	42	SER	2.7
1	A	124	ASP	2.7
1	A	176	ALA	2.7
1	B	103	ASP	2.7
1	B	177	ALA	2.7
2	D	101	GLY	2.6
1	B	161	VAL	2.6
1	A	64	TYR	2.6
1	A	187	GLU	2.6
1	B	20	ASP	2.6
1	A	58	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	2	PHE	2.6
1	A	56	VAL	2.6
1	B	115	ALA	2.6
2	C	1	ASP	2.5
2	D	109	ALA	2.5
1	A	41	SER	2.5
1	B	44	ARG	2.5
1	A	111	GLU	2.5
1	A	116	ALA	2.5
1	A	142	TRP	2.5
1	B	162	GLU	2.5
2	C	227	CYS	2.5
1	A	154	LYS	2.5
1	A	159	PRO	2.5
1	B	63	PRO	2.5
2	D	145	PRO	2.5
1	A	186	GLY	2.4
1	B	51	ALA	2.4
1	B	30	SER	2.4
1	B	124	ASP	2.4
1	B	143	TYR	2.4
1	A	99	PHE	2.4
1	A	125	VAL	2.4
2	D	147	ALA	2.4
1	B	76	THR	2.4
1	B	189	VAL	2.4
2	D	133	VAL	2.4
2	C	134	GLN	2.4
1	B	17	GLU	2.4
1	B	160	THR	2.3
2	D	1	ASP	2.3
2	D	238	ASP	2.3
1	A	172	LEU	2.3
1	A	183	GLY	2.3
1	A	180	ILE	2.3
1	A	32	GLU	2.3
1	B	43	LEU	2.3
1	A	43	LEU	2.3
1	B	201	GLU	2.3
1	A	26	PHE	2.3
1	A	94	LYS	2.3
1	B	204	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	207	SER	2.2
1	B	178	SER	2.2
1	B	114	VAL	2.2
2	D	134	GLN	2.2
1	A	1	GLN	2.2
1	A	89	ALA	2.2
1	B	14	MET	2.1
1	B	163	ALA	2.1
2	C	231	ASP	2.1
2	C	139	GLY	2.1
1	A	202	LYS	2.1
1	A	46	VAL	2.1
1	B	212	PHE	2.1
1	B	117	LEU	2.1
1	A	132	GLY	2.1
1	A	17	GLU	2.1
1	A	136	GLU	2.1
1	B	104	PHE	2.0
1	A	162	GLU	2.0
1	B	102	GLY	2.0
1	A	182	ARG	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
3	NAG	A	301	14/15	0.19	0.24	79,122,136,137	0
3	NAG	B	301	14/15	0.44	0.21	83,118,145,160	0

6.5 Other polymers [i](#)

There are no such residues in this entry.