



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:46 PM UTC

PDB ID : 3LRS / pdb_00003lrs
Title : Structure of PG16, an antibody with broad and potent neutralization of HIV-1
Authors : Pancera, M.; Kwong, P.D.
Deposited on : 2010-02-11
Resolution : 2.37 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

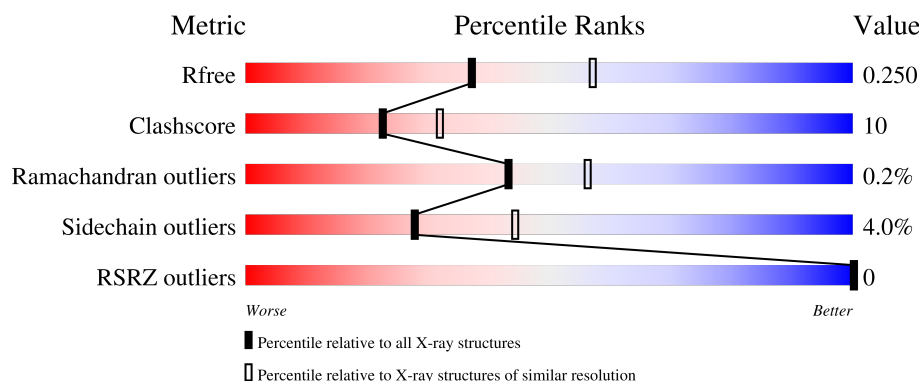
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	238	
1	C	238	
1	E	238	
1	H	238	
2	B	211	

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Mol	Chain	Length	Quality of chain
2	D	211	
2	F	211	
2	L	211	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	D	741	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13424 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 PG-16 Heavy Chain Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	220	Total	C	N	O	S	0	0	0
			1669	1057	284	319	9			
1	A	221	Total	C	N	O	S	0	0	0
			1675	1060	285	321	9			
1	C	228	Total	C	N	O	S	0	0	0
			1725	1089	294	333	9			
1	E	221	Total	C	N	O	S	0	0	0
			1680	1063	285	323	9			

- Molecule 2 is a protein called PG-16 Light Chain Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1558	969	264	320	5			
2	B	211	Total	C	N	O	S	0	0	0
			1558	969	264	320	5			
2	D	211	Total	C	N	O	S	0	0	0
			1557	969	264	319	5			
2	F	211	Total	C	N	O	S	0	0	0
			1557	969	264	319	5			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	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	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

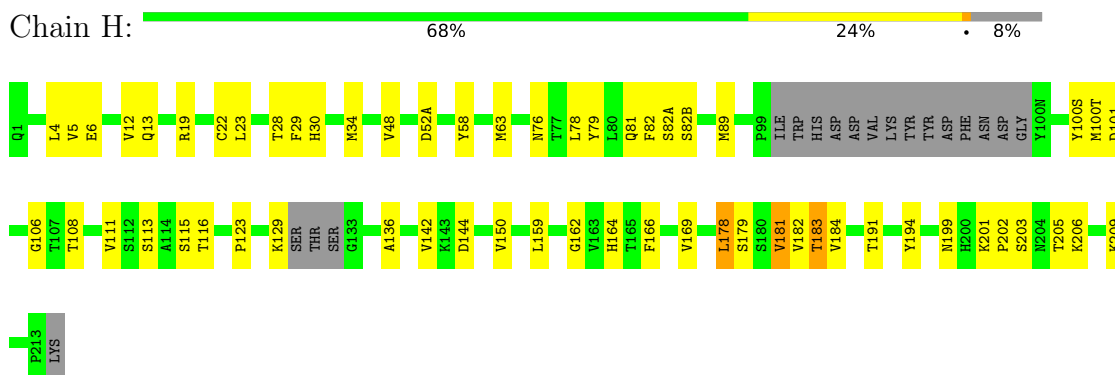
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	52	Total	O	0	0
			52	52		
4	L	46	Total	O	0	0
			46	46		
4	A	44	Total	O	0	0
			44	44		
4	B	38	Total	O	0	0
			38	38		
4	C	22	Total	O	0	0
			22	22		
4	D	73	Total	O	0	0
			73	73		
4	E	38	Total	O	0	0
			38	38		
4	F	76	Total	O	0	0
			76	76		

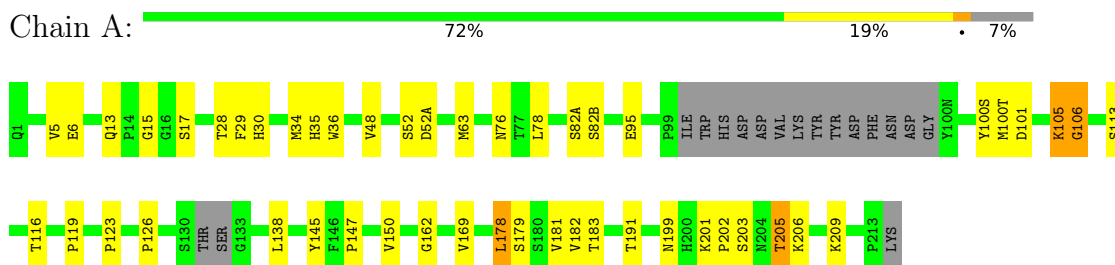
3 Residue-property plots

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.

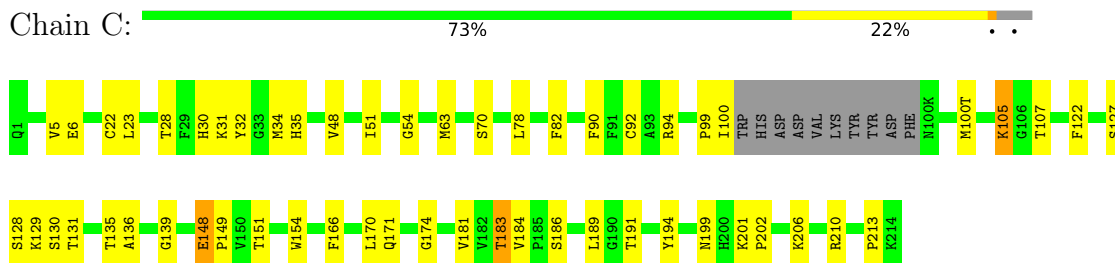
• Molecule 1: PG-16 Heavy Chain Fab



• Molecule 1: PG-16 Heavy Chain Fab

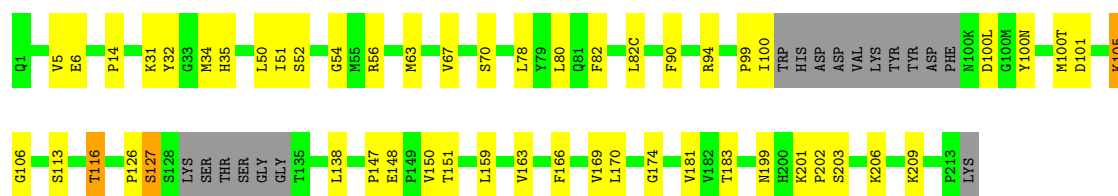


• Molecule 1: PG-16 Heavy Chain Fab



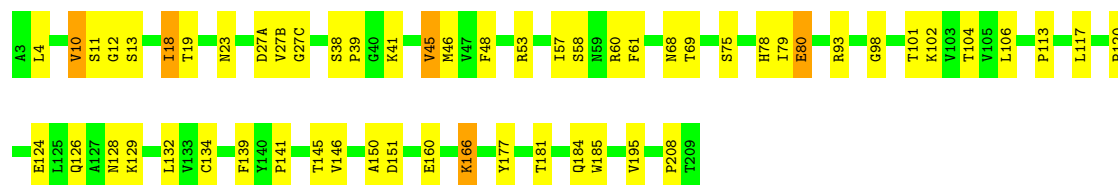
• Molecule 1: PG-16 Heavy Chain Fab





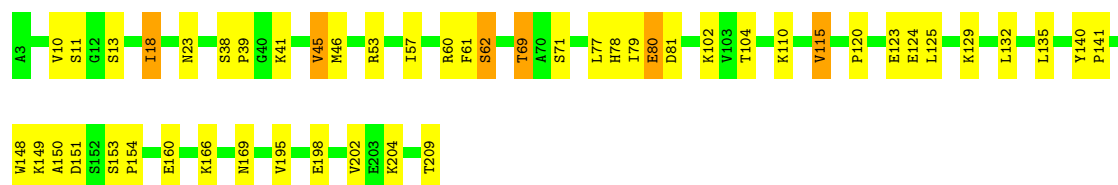
• Molecule 2: PG-16 Light Chain Fab

Chain L: 73% 25% .



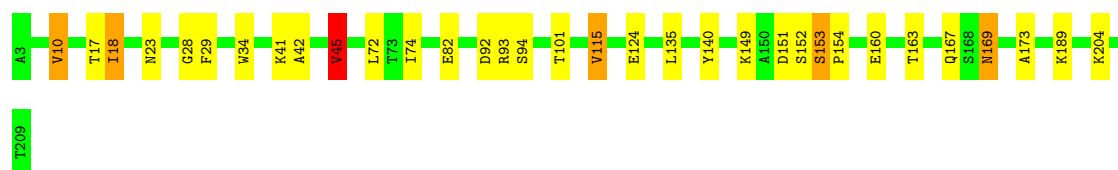
• Molecule 2: PG-16 Light Chain Fab

Chain B: 77% 20% .



• Molecule 2: PG-16 Light Chain Fab

Chain D: 84% 13% .



• Molecule 2: PG-16 Light Chain Fab

Chain F: 90% 9% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.32Å 165.09Å 81.36Å 90.00° 91.55° 90.00°	Depositor
Resolution (Å)	30.59 – 2.37 30.59 – 2.37	Depositor EDS
% Data completeness (in resolution range)	82.0 (30.59-2.37) 82.2 (30.59-2.37)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.211 , 0.260 0.197 , 0.250	Depositor DCC
R_{free} test set	3600 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.6	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13424	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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	0.48	0/1718	0.81	0/2332
1	C	0.51	0/1769	0.83	2/2402 (0.1%)
1	E	0.49	0/1723	0.82	4/2341 (0.2%)
1	H	0.49	0/1712	0.79	2/2324 (0.1%)
2	B	0.52	0/1595	0.83	0/2171
2	D	0.50	0/1594	0.83	2/2171 (0.1%)
2	F	0.52	0/1594	0.83	2/2171 (0.1%)
2	L	0.51	0/1595	0.80	0/2171
All	All	0.50	0/13300	0.82	12/18083 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	105	LYS	N-CA-C	-7.54	101.13	110.41
1	C	105	LYS	N-CA-C	-6.69	101.12	110.35
2	F	207	ALA	CA-C-N	5.91	127.23	119.84
2	F	207	ALA	C-N-CA	5.91	127.23	119.84
1	E	166	PHE	CA-C-N	5.76	125.78	119.90
1	E	166	PHE	C-N-CA	5.76	125.78	119.90
1	E	163	VAL	CB-CA-C	-5.63	104.62	111.88
2	D	169	ASN	N-CA-C	-5.32	103.00	110.50
1	C	92	CYS	N-CA-C	-5.24	101.17	109.76
1	H	166	PHE	CA-C-N	5.12	125.10	120.03
1	H	166	PHE	C-N-CA	5.12	125.10	120.03
2	D	45	VAL	CB-CA-C	-5.10	103.00	111.32

There are no chirality outliers.

There are no planarity outliers.

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	1675	0	1627	33	0
1	C	1725	0	1677	49	0
1	E	1680	0	1627	38	0
1	H	1669	0	1622	44	0
2	B	1558	0	1507	36	0
2	D	1557	0	1507	30	0
2	F	1557	0	1507	17	0
2	L	1558	0	1507	51	0
3	B	14	0	13	0	0
3	D	14	0	13	0	0
3	F	14	0	13	0	0
3	L	14	0	13	0	0
4	A	44	0	0	0	0
4	B	38	0	0	4	0
4	C	22	0	0	1	0
4	D	73	0	0	1	0
4	E	38	0	0	1	0
4	F	76	0	0	1	0
4	H	52	0	0	5	0
4	L	46	0	0	2	0
All	All	13424	0	12633	269	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 10.

All (269) 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:H:89:MET:HE2	1:H:108:THR:HG22	1.57	0.85
2:L:166:LYS:HE2	2:D:92:ASP:O	1.77	0.85
1:C:135:THR:CG2	1:C:183:THR:HG23	2.07	0.84
1:C:129:LYS:HB2	1:C:130:SER:C	2.03	0.83
2:F:18:ILE:HD12	2:F:77:LEU:HD11	1.59	0.82
1:H:89:MET:HE2	1:H:108:THR:CG2	2.15	0.77
1:E:99:PRO:O	1:E:100:ILE:HB	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:116:THR:HG22	1:H:203:SER:HB3	1.71	0.72
1:C:70:SER:O	1:C:78:LEU:HD12	1.90	0.71
2:D:18:ILE:CG2	2:D:74:ILE:HB	2.19	0.71
1:E:52:SER:HB3	1:E:56:ARG:HB3	1.74	0.68
1:E:70:SER:O	1:E:78:LEU:HD12	1.94	0.68
1:H:101:ASP:HA	2:L:45:VAL:HG21	1.76	0.67
1:C:181:VAL:HG11	2:D:135:LEU:CD1	2.24	0.67
2:L:11:SER:C	2:L:18:ILE:HD11	2.19	0.66
2:L:104:THR:HG23	4:L:214:HOH:O	1.96	0.66
1:A:178:LEU:HD12	1:A:178:LEU:C	2.20	0.66
1:C:129:LYS:HB3	1:C:131:THR:OG1	1.95	0.66
1:C:129:LYS:HB2	1:C:130:SER:CA	2.27	0.64
2:L:10:VAL:HG13	2:L:101:THR:HG21	1.79	0.64
1:C:186:SER:HA	1:C:189:LEU:HD23	1.80	0.64
1:C:129:LYS:HB3	1:C:131:THR:HG23	1.80	0.64
1:H:115:SER:HA	4:H:244:HOH:O	1.98	0.63
2:B:11:SER:C	2:B:18:ILE:HD11	2.23	0.63
1:H:100(T):MET:O	2:L:45:VAL:HG22	2.00	0.62
2:L:120:PRO:HD3	2:L:132:LEU:CD2	2.27	0.62
1:E:116:THR:HG21	1:E:202:PRO:O	2.00	0.62
2:B:209:THR:HA	4:B:227:HOH:O	1.98	0.61
1:C:129:LYS:HB3	1:C:131:THR:CG2	2.30	0.61
1:H:12:VAL:HG23	1:H:111:VAL:HG22	1.84	0.60
1:H:23:LEU:C	1:H:23:LEU:HD23	2.27	0.60
1:A:162:GLY:O	1:A:182:VAL:HA	2.02	0.60
2:D:18:ILE:HG22	2:D:74:ILE:O	2.02	0.60
1:H:48:VAL:HG22	1:H:63:MET:HE3	1.84	0.60
2:B:120:PRO:HD3	2:B:132:LEU:CD2	2.33	0.59
1:C:199:ASN:ND2	1:C:206:LYS:HE2	2.18	0.59
2:B:104:THR:HG21	2:B:141:PRO:HB3	1.85	0.59
2:D:41:LYS:HD3	2:D:42:ALA:H	1.68	0.58
1:A:13:GLN:OE1	1:A:113:SER:HA	2.03	0.58
1:C:135:THR:HG21	1:C:183:THR:HG23	1.83	0.58
2:L:78:HIS:HB3	2:L:80:GLU:OE2	2.04	0.58
1:H:178:LEU:HD12	1:H:178:LEU:C	2.28	0.58
2:L:185:TRP:CZ2	2:L:208:PRO:HA	2.39	0.58
2:L:60:ARG:HD2	2:L:75:SER:O	2.04	0.58
2:B:11:SER:O	2:B:18:ILE:HD11	2.03	0.58
2:L:46:MET:HA	2:L:57:ILE:HD13	1.85	0.58
1:A:178:LEU:HD12	1:A:179:SER:N	2.18	0.57
1:H:159:LEU:HD12	4:H:250:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:129:LYS:HE2	1:H:136:ALA:HA	1.86	0.56
1:A:101:ASP:HA	2:B:45:VAL:HG21	1.87	0.56
2:L:23:ASN:ND2	2:L:69:THR:HG21	2.20	0.56
1:C:6:GLU:OE1	1:C:105:LYS:O	2.24	0.56
1:E:199:ASN:ND2	1:E:206:LYS:HE2	2.21	0.56
1:E:35:HIS:CE1	1:E:50:LEU:HD13	2.41	0.55
2:L:10:VAL:HG13	2:L:101:THR:CG2	2.36	0.55
1:E:181:VAL:HG11	2:F:135:LEU:HD13	1.89	0.55
1:H:144:ASP:OD2	2:L:129:LYS:NZ	2.40	0.55
2:D:10:VAL:HG13	2:D:101:THR:HG21	1.89	0.55
1:A:145:TYR:CE1	1:A:150:VAL:HG23	2.42	0.54
2:B:115:VAL:HG13	2:B:202:VAL:HG11	1.89	0.54
1:A:169:VAL:HG21	2:B:160:GLU:HB3	1.89	0.54
1:A:6:GLU:CD	1:A:106:GLY:HA2	2.32	0.54
1:A:100(T):MET:O	2:B:45:VAL:HG22	2.08	0.54
1:A:5:VAL:HG23	1:A:5:VAL:O	2.07	0.54
1:E:32:TYR:CG	1:E:94:ARG:HD2	2.42	0.53
1:H:183:THR:HG22	1:H:183:THR:O	2.08	0.53
1:H:123:PRO:HG3	1:H:209:LYS:HD2	1.91	0.53
1:C:135:THR:HG23	1:C:183:THR:HG23	1.88	0.53
1:E:100(T):MET:O	2:F:45:VAL:HG22	2.08	0.53
1:E:82:PHE:HB3	1:E:82(C):LEU:HD11	1.91	0.53
1:E:169:VAL:HB	2:F:162:THR:HG22	1.89	0.53
1:C:34:MET:HB3	1:C:78:LEU:HD22	1.91	0.52
1:H:169:VAL:HG11	2:L:160:GLU:HB3	1.91	0.52
2:L:23:ASN:HA	2:L:69:THR:HG22	1.91	0.52
2:L:102:LYS:HE2	2:L:104:THR:HG22	1.90	0.52
1:E:181:VAL:HG11	2:F:135:LEU:CD1	2.39	0.52
2:F:120:PRO:HD3	2:F:132:LEU:HD23	1.90	0.52
1:A:199:ASN:ND2	1:A:206:LYS:HE2	2.24	0.52
2:B:38:SER:HB3	2:B:39:PRO:HD2	1.90	0.52
2:B:110:LYS:HD3	2:B:198:GLU:HG3	1.91	0.52
1:E:52:SER:HB3	1:E:56:ARG:HE	1.74	0.52
1:A:29:PHE:CD2	1:A:76:ASN:HA	2.44	0.52
2:D:115:VAL:HG23	2:D:204:LYS:HG3	1.91	0.52
2:D:17:THR:HG22	2:D:18:ILE:N	2.24	0.52
2:L:53:ARG:HD3	2:L:61:PHE:O	2.10	0.52
2:F:203:GLU:O	2:F:204:LYS:HD3	2.08	0.51
1:H:81:GLN:HG3	1:H:82:PHE:N	2.26	0.51
1:H:115:SER:C	4:H:218:HOH:O	2.54	0.51
1:A:181:VAL:HG11	2:B:135:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:SER:HB2	2:B:41:LYS:HD2	1.91	0.51
1:H:34:MET:HB3	1:H:78:LEU:HD22	1.93	0.51
2:B:125:LEU:HD23	2:B:129:LYS:O	2.10	0.51
2:B:46:MET:HA	2:B:57:ILE:HD13	1.93	0.50
1:H:162:GLY:O	1:H:182:VAL:HA	2.12	0.50
1:H:116:THR:HG22	1:H:203:SER:CB	2.42	0.49
1:C:129:LYS:CB	1:C:130:SER:C	2.81	0.49
1:E:82:PHE:CB	1:E:82(C):LEU:HD11	2.42	0.49
1:E:100(T):MET:O	2:F:45:VAL:CG2	2.59	0.49
2:F:3:ALA:N	4:F:339:HOH:O	2.44	0.49
1:H:100(S):TYR:CE1	1:H:101:ASP:HB3	2.48	0.49
1:C:127:SER:HA	1:C:128:SER:C	2.34	0.49
1:A:126:PRO:HG3	1:A:138:LEU:HB3	1.94	0.49
1:H:201:LYS:HB2	1:H:202:PRO:HD3	1.95	0.49
2:L:126:GLN:C	2:L:128:ASN:H	2.20	0.49
1:C:6:GLU:OE1	1:C:6:GLU:N	2.46	0.48
2:L:146:VAL:HG22	2:L:195:VAL:HG12	1.95	0.48
2:B:23:ASN:HA	2:B:69:THR:HG22	1.96	0.48
2:F:140:TYR:C	2:F:140:TYR:CD1	2.91	0.48
1:C:186:SER:HA	1:C:189:LEU:CD2	2.42	0.48
1:E:105:LYS:HD2	1:E:106:GLY:H	1.78	0.48
1:H:101:ASP:HA	2:L:45:VAL:CG2	2.42	0.48
1:A:34:MET:HB3	1:A:78:LEU:HD22	1.95	0.48
1:C:48:VAL:HG22	1:C:63:MET:HE3	1.96	0.48
1:E:126:PRO:O	1:E:127:SER:HB2	2.14	0.48
1:H:178:LEU:HD12	1:H:179:SER:N	2.29	0.47
2:L:10:VAL:CG1	2:L:101:THR:HG21	2.43	0.47
1:A:116:THR:HG22	1:A:203:SER:HB3	1.96	0.47
1:E:116:THR:HG22	1:E:203:SER:HB3	1.96	0.47
2:F:12:GLY:N	2:F:18:ILE:HD11	2.29	0.47
2:L:38:SER:HB2	2:L:41:LYS:HD2	1.97	0.47
2:L:27(C):GLY:HA3	2:L:68:ASN:OD1	2.15	0.47
2:B:53:ARG:HD3	2:B:61:PHE:O	2.15	0.47
1:C:28:THR:CG2	1:C:30:HIS:CE1	2.98	0.47
2:L:117:LEU:HD13	2:L:134:CYS:HB2	1.96	0.47
1:A:48:VAL:HG22	1:A:63:MET:HE3	1.96	0.47
1:C:201:LYS:N	1:C:202:PRO:CD	2.78	0.47
1:E:34:MET:HB3	1:E:78:LEU:HD22	1.96	0.47
2:L:12:GLY:N	2:L:18:ILE:HD11	2.29	0.47
1:E:6:GLU:OE1	1:E:105:LYS:O	2.33	0.47
1:C:107:THR:HG23	1:C:107:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:THR:HG22	2:D:18:ILE:H	1.80	0.46
2:D:140:TYR:CD1	2:D:140:TYR:C	2.93	0.46
1:A:105:LYS:O	1:A:106:GLY:O	2.32	0.46
1:C:129:LYS:HB2	1:C:130:SER:HA	1.97	0.46
2:L:23:ASN:ND2	2:L:69:THR:CG2	2.78	0.46
1:C:135:THR:HG21	1:C:183:THR:CG2	2.45	0.46
1:H:82(A):SER:O	1:H:82(B):SER:C	2.57	0.46
2:L:106:LEU:HD21	2:L:141:PRO:HG3	1.97	0.46
2:B:18:ILE:HD12	2:B:77:LEU:HD11	1.98	0.46
2:B:102:LYS:HE3	4:B:334:HOH:O	2.16	0.46
2:B:115:VAL:HG22	2:B:204:LYS:HG2	1.98	0.46
1:A:82(A):SER:O	1:A:82(B):SER:C	2.59	0.46
2:D:10:VAL:HG13	2:D:101:THR:CG2	2.44	0.46
1:C:166:PHE:HB3	4:D:311:HOH:O	2.15	0.46
2:D:18:ILE:O	2:D:18:ILE:HG23	2.16	0.46
1:E:63:MET:HE2	4:E:367:HOH:O	2.14	0.46
2:L:60:ARG:HB2	2:L:75:SER:O	2.16	0.46
2:B:60:ARG:NH2	2:B:81:ASP:OD2	2.46	0.46
2:L:38:SER:HB3	2:L:39:PRO:HD2	1.97	0.45
2:D:149:LYS:HE3	2:D:152:SER:O	2.15	0.45
1:E:201:LYS:N	1:E:202:PRO:CD	2.79	0.45
2:F:155:VAL:O	2:F:155:VAL:HG12	2.14	0.45
2:B:78:HIS:HB3	2:B:80:GLU:OE2	2.15	0.45
1:C:32:TYR:CG	1:C:94:ARG:HD2	2.51	0.45
1:C:82:PHE:HZ	1:C:90:PHE:CZ	2.33	0.45
2:B:78:HIS:HB2	2:B:80:GLU:HG2	1.98	0.45
1:C:6:GLU:CD	1:C:105:LYS:O	2.60	0.45
1:C:35:HIS:CG	1:C:100(T):MET:HE2	2.51	0.45
1:C:129:LYS:HB3	1:C:131:THR:CB	2.47	0.45
1:H:5:VAL:HG23	1:H:5:VAL:O	2.15	0.45
2:L:104:THR:HG21	4:L:229:HOH:O	2.16	0.45
2:D:115:VAL:CG2	2:D:204:LYS:HG3	2.46	0.45
1:H:169:VAL:HG21	2:L:177:TYR:CD2	2.51	0.45
1:A:100(S):TYR:CE1	1:A:101:ASP:HB3	2.52	0.45
1:C:51:ILE:HG12	1:C:54:GLY:HA2	1.99	0.45
1:H:6:GLU:CD	1:H:106:GLY:HA2	2.42	0.44
1:A:35:HIS:HE2	1:A:95:GLU:HB2	1.83	0.44
2:L:113:PRO:HB3	2:L:139:PHE:CD2	2.53	0.44
2:B:148:TRP:O	2:B:149:LYS:HG3	2.17	0.44
1:E:6:GLU:OE1	1:E:6:GLU:N	2.50	0.44
1:C:171:GLN:HG2	2:D:160:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:GLN:OE1	2:D:173:ALA:HB2	2.18	0.44
2:L:58:SER:OG	2:L:60:ARG:HG2	2.17	0.44
2:B:153:SER:HA	2:B:154:PRO:HD3	1.88	0.44
1:C:100(T):MET:O	2:D:45:VAL:CG2	2.66	0.44
2:F:120:PRO:HD3	2:F:132:LEU:CD2	2.48	0.44
1:E:82:PHE:HB3	1:E:82(C):LEU:CD1	2.48	0.44
1:C:139:GLY:HA2	1:C:154:TRP:CH2	2.53	0.43
1:H:4:LEU:HB3	1:H:22:CYS:SG	2.58	0.43
2:D:153:SER:HA	2:D:154:PRO:HD3	1.93	0.43
1:H:184:VAL:HG11	1:H:194:TYR:CE1	2.53	0.43
2:L:27(A):ASP:O	2:L:27(B):VAL:C	2.61	0.43
1:A:30:HIS:O	1:A:52(A):ASP:HB2	2.18	0.43
1:A:119:PRO:HD2	1:A:205:THR:HG21	1.99	0.43
1:H:89:MET:HE3	1:H:89:MET:HB2	1.92	0.43
2:D:167:GLN:O	2:D:169:ASN:O	2.36	0.43
1:H:116:THR:N	4:H:218:HOH:O	2.50	0.43
2:L:79:ILE:HD13	2:D:93:ARG:CZ	2.48	0.43
2:L:106:LEU:CD2	2:L:141:PRO:HG3	2.49	0.43
2:B:120:PRO:HD3	2:B:132:LEU:HD21	1.99	0.43
1:C:35:HIS:ND1	1:C:100(T):MET:HE2	2.34	0.43
2:L:195:VAL:O	2:L:195:VAL:HG23	2.18	0.42
2:D:93:ARG:O	2:D:94:SER:HB2	2.19	0.42
1:E:170:LEU:HD11	1:E:174:GLY:C	2.44	0.42
2:B:62:SER:HB3	4:B:238:HOH:O	2.19	0.42
1:H:29:PHE:CD2	1:H:76:ASN:HA	2.54	0.42
1:C:22:CYS:HB3	1:C:78:LEU:HB3	2.01	0.42
1:C:210:ARG:HG2	4:C:221:HOH:O	2.18	0.42
2:D:151:ASP:OD1	2:D:189:LYS:HB3	2.19	0.42
1:C:100:ILE:HD12	1:C:100:ILE:HA	1.95	0.42
1:C:136:ALA:HB3	1:C:189:LEU:HD21	2.00	0.42
1:E:147:PRO:C	1:E:148:GLU:O	2.62	0.42
2:F:181:THR:O	2:F:182:PRO:C	2.61	0.42
1:H:115:SER:N	4:H:218:HOH:O	2.53	0.42
1:C:184:VAL:HG11	1:C:194:TYR:CE1	2.55	0.42
1:A:145:TYR:CZ	1:A:150:VAL:HG23	2.54	0.42
1:C:127:SER:C	1:C:129:LYS:H	2.27	0.42
2:L:79:ILE:CD1	2:D:93:ARG:CZ	2.97	0.42
1:A:123:PRO:HG3	1:A:209:LYS:HD2	2.02	0.42
1:E:209:LYS:HD2	1:E:209:LYS:HA	1.91	0.42
1:C:82:PHE:HZ	1:C:90:PHE:CE1	2.38	0.42
1:C:100(T):MET:O	2:D:45:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:GLY:C	2:D:29:PHE:CD2	2.98	0.42
1:E:31:LYS:HD3	1:E:100(N):TYR:CZ	2.54	0.42
1:C:122:PHE:CE1	2:D:124:GLU:HA	2.55	0.42
1:E:82:PHE:HZ	1:E:90:PHE:CE1	2.38	0.42
1:E:99:PRO:O	1:E:100:ILE:CB	2.59	0.42
2:L:120:PRO:HD3	2:L:132:LEU:HD21	2.00	0.42
1:C:181:VAL:HG11	2:D:135:LEU:HD13	2.00	0.42
2:L:93:ARG:HG2	2:L:93:ARG:HH11	1.85	0.41
1:A:15:GLY:HA2	1:A:82(B):SER:HA	2.02	0.41
2:L:48:PHE:CD1	2:L:48:PHE:C	2.98	0.41
1:A:36:TRP:O	1:A:48:VAL:HB	2.20	0.41
2:B:45:VAL:O	2:B:57:ILE:CD1	2.68	0.41
2:B:140:TYR:HA	2:B:141:PRO:C	2.46	0.41
2:B:150:ALA:O	2:B:151:ASP:HB2	2.20	0.41
2:D:17:THR:CG2	2:D:18:ILE:N	2.83	0.41
1:H:169:VAL:HG21	2:L:177:TYR:CE2	2.56	0.41
2:L:80:GLU:CD	2:L:80:GLU:H	2.28	0.41
2:D:17:THR:CG2	2:D:18:ILE:H	2.33	0.41
1:E:105:LYS:HD2	1:E:106:GLY:N	2.35	0.41
2:L:12:GLY:HA3	2:L:18:ILE:HD12	2.01	0.41
1:A:101:ASP:HA	2:B:45:VAL:CG2	2.48	0.41
1:C:105:LYS:HA	1:C:105:LYS:HD2	1.74	0.41
1:C:148:GLU:HG3	1:C:149:PRO:HA	2.03	0.41
1:E:170:LEU:HD11	1:E:174:GLY:O	2.21	0.41
1:E:67:VAL:HB	1:E:80:LEU:HD11	2.03	0.41
1:H:13:GLN:OE1	1:H:113:SER:HA	2.20	0.41
1:H:199:ASN:ND2	1:H:206:LYS:HE2	2.35	0.41
1:C:99:PRO:O	1:C:100:ILE:HB	2.21	0.41
1:H:19:ARG:NH1	1:H:79:TYR:CE1	2.89	0.41
1:A:201:LYS:N	1:A:202:PRO:CD	2.84	0.41
2:B:13:SER:HB3	4:B:379:HOH:O	2.20	0.41
2:B:169:ASN:OD1	2:B:169:ASN:C	2.64	0.41
2:D:34:TRP:CE2	2:D:72:LEU:HB2	2.56	0.41
1:H:169:VAL:CG1	2:L:160:GLU:HB3	2.50	0.41
2:L:150:ALA:O	2:L:151:ASP:HB2	2.21	0.41
1:H:58:TYR:CD2	1:H:58:TYR:N	2.88	0.40
2:L:181:THR:OG1	2:L:184:GLN:HG3	2.21	0.40
1:A:52:SER:O	1:A:52(A):ASP:C	2.64	0.40
1:E:100(L):ASP:OD1	1:E:100(L):ASP:N	2.54	0.40
2:F:17:THR:HG22	2:F:18:ILE:N	2.36	0.40
1:E:51:ILE:HG12	1:E:54:GLY:HA2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:TYR:HA	2:F:141:PRO:C	2.46	0.40
1:H:164:HIS:HB2	1:H:181:VAL:HG23	2.04	0.40
2:L:4:LEU:O	2:L:98:GLY:HA2	2.22	0.40
2:L:45:VAL:O	2:L:57:ILE:HD11	2.21	0.40
1:A:100(T):MET:O	2:B:45:VAL:CG2	2.69	0.40
1:C:170:LEU:HD11	1:C:174:GLY:C	2.46	0.40
1:E:14:PRO:HG2	1:E:113:SER:HB2	2.03	0.40
1:E:101:ASP:HA	2:F:45:VAL:HG21	2.01	0.40
1:E:138:LEU:C	1:E:138:LEU:HD12	2.47	0.40
1:H:30:HIS:O	1:H:52(A):ASP:HB2	2.21	0.40
1:A:5:VAL:O	1:A:5:VAL:CG2	2.70	0.40
1:A:147:PRO:HD2	1:A:202:PRO:CB	2.52	0.40
1:H:142:VAL:HG11	1:H:150:VAL:HG11	2.03	0.40
2:L:124:GLU:HG2	2:L:129:LYS:O	2.21	0.40
2:B:124:GLU:HG2	2:B:129:LYS:C	2.47	0.40
2:B:166:LYS:HE2	2:B:166:LYS:HB3	1.92	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	215/238 (90%)	204 (95%)	10 (5%)	1 (0%)	24	34
1	C	224/238 (94%)	206 (92%)	17 (8%)	1 (0%)	30	40
1	E	215/238 (90%)	198 (92%)	16 (7%)	1 (0%)	24	34
1	H	214/238 (90%)	201 (94%)	13 (6%)	0	100	100
2	B	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
2	D	209/211 (99%)	197 (94%)	12 (6%)	0	100	100
2	F	209/211 (99%)	202 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	209/211 (99%)	197 (94%)	12 (6%)	0	100	100
All	All	1704/1796 (95%)	1606 (94%)	95 (6%)	3 (0%)	43	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	GLY
1	E	127	SER
1	C	213	PRO

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	186/202 (92%)	179 (96%)	7 (4%)	29	46
1	C	192/202 (95%)	185 (96%)	7 (4%)	31	49
1	E	187/202 (93%)	181 (97%)	6 (3%)	34	53
1	H	185/202 (92%)	179 (97%)	6 (3%)	34	53
2	B	178/178 (100%)	167 (94%)	11 (6%)	16	26
2	D	178/178 (100%)	170 (96%)	8 (4%)	24	39
2	F	178/178 (100%)	172 (97%)	6 (3%)	32	51
2	L	178/178 (100%)	170 (96%)	8 (4%)	24	39
All	All	1462/1520 (96%)	1403 (96%)	59 (4%)	28	44

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	28	THR
1	H	178	LEU
1	H	181	VAL
1	H	183	THR
1	H	191	THR

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Mol	Chain	Res	Type
1	H	205	THR
2	L	10	VAL
2	L	13	SER
2	L	18	ILE
2	L	19	THR
2	L	45	VAL
2	L	80	GLU
2	L	145	THR
2	L	166	LYS
1	A	17	SER
1	A	28	THR
1	A	105	LYS
1	A	178	LEU
1	A	183	THR
1	A	191	THR
1	A	205	THR
2	B	10	VAL
2	B	18	ILE
2	B	45	VAL
2	B	62	SER
2	B	69	THR
2	B	71	SER
2	B	79	ILE
2	B	80	GLU
2	B	115	VAL
2	B	123	GLU
2	B	195	VAL
1	C	5	VAL
1	C	23	LEU
1	C	31	LYS
1	C	148	GLU
1	C	151	THR
1	C	183	THR
1	C	191	THR
2	D	10	VAL
2	D	18	ILE
2	D	23	ASN
2	D	45	VAL
2	D	82	GLU
2	D	115	VAL
2	D	153	SER
2	D	163	THR

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Mol	Chain	Res	Type
1	E	5	VAL
1	E	116	THR
1	E	150	VAL
1	E	151	THR
1	E	159	LEU
1	E	183	THR
2	F	9	SER
2	F	10	VAL
2	F	18	ILE
2	F	45	VAL
2	F	115	VAL
2	F	122	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
1	H	100(R)	HIS
2	L	37	GLN
2	L	197	HIS
1	A	39	GLN
2	B	16	GLN
2	B	37	GLN
2	B	52	HIS
2	B	95	HIS
2	B	184	GLN
1	C	30	HIS
1	C	76	ASN
1	E	39	GLN
2	F	37	GLN
2	F	52	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	D	741	2	14,14,15	0.47	0	17,19,21	1.14	1 (5%)
3	NAG	F	741	2	14,14,15	0.55	0	17,19,21	0.95	2 (11%)
3	NAG	L	741	2	14,14,15	0.51	0	17,19,21	2.01	4 (23%)
3	NAG	B	741	2	14,14,15	0.57	0	17,19,21	2.00	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	741	2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	F	741	2	-	2/6/23/26	0/1/1/1
3	NAG	L	741	2	-	2/6/23/26	0/1/1/1
3	NAG	B	741	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	741	NAG	C1-O5-C5	7.08	121.67	112.19
3	L	741	NAG	O5-C1-C2	-5.06	103.46	111.29
3	L	741	NAG	C1-C2-N2	3.49	115.94	110.43
3	L	741	NAG	C1-O5-C5	3.01	116.22	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	741	NAG	C3-C4-C5	2.80	115.31	110.23
3	F	741	NAG	C2-N2-C7	-2.35	119.75	122.90
3	D	741	NAG	C1-O5-C5	2.23	115.17	112.19
3	B	741	NAG	O5-C1-C2	2.20	114.70	111.29
3	F	741	NAG	O5-C1-C2	-2.16	107.95	111.29
3	B	741	NAG	C4-C3-C2	-2.10	107.94	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	741	NAG	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	741	NAG	C8-C7-N2-C2
3	L	741	NAG	O7-C7-N2-C2
3	B	741	NAG	C8-C7-N2-C2
3	B	741	NAG	O7-C7-N2-C2
3	B	741	NAG	O5-C5-C6-O6
3	B	741	NAG	C4-C5-C6-O6
3	D	741	NAG	C8-C7-N2-C2
3	D	741	NAG	O7-C7-N2-C2
3	F	741	NAG	C8-C7-N2-C2
3	F	741	NAG	O7-C7-N2-C2

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	221/238 (92%)	-1.10	0 100 100	40, 64, 101, 144	0
1	C	228/238 (95%)	-0.98	0 100 100	36, 66, 119, 186	0
1	E	221/238 (92%)	-1.04	0 100 100	39, 65, 108, 170	0
1	H	220/238 (92%)	-1.06	0 100 100	39, 63, 100, 127	0
2	B	211/211 (100%)	-1.17	0 100 100	37, 58, 105, 130	0
2	D	211/211 (100%)	-1.16	0 100 100	36, 53, 91, 124	0
2	F	211/211 (100%)	-1.21	0 100 100	35, 53, 94, 109	0
2	L	211/211 (100%)	-1.09	0 100 100	38, 59, 106, 135	0
All	All	1734/1796 (96%)	-1.10	0 100 100	35, 60, 106, 186	0

There are no RSRZ outliers to report.

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	L	741	14/15	0.96	0.05	84,102,108,109	0
3	NAG	D	741	14/15	0.96	0.06	90,96,102,105	0
3	NAG	B	741	14/15	0.97	0.06	86,91,97,99	0
3	NAG	F	741	14/15	0.97	0.04	73,83,89,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.