Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:17 PM BST

PDB ID	:	3RPI
Title	:	Crystal Structure of Fab from 3BNC60, Highly Potent anti-HIV Antibody
Authors	:	Diskin, R.; Bjorkman, P.J.
Deposited on	:	2011-04-26
Resolution	:	2.65 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 following versions of software and data (see references ⓘ) were used in the production of this report:

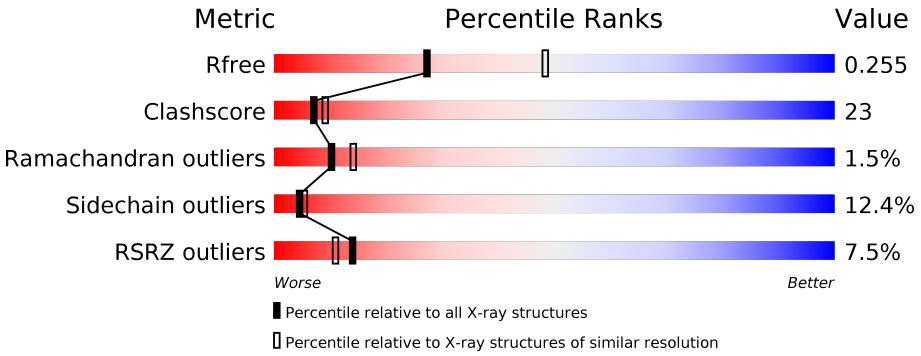
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.65 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}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 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 <=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	B	206	11% 53% 39% 5%
1	L	206	12% 51% 43%
2	A	229	2% 60% 29% 7%
2	H	229	5% 58% 29% 6% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6650 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.

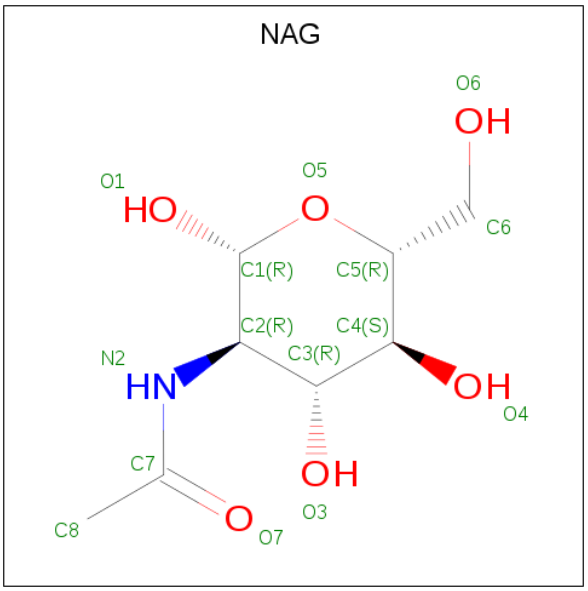
- Molecule 1 is a protein called Light chain from highly potent anti-HIV neutralizing antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	203	Total	C	N	O	S	0	0	0
			1600	1002	279	314	5			
1	B	203	Total	C	N	O	S	0	0	0
			1600	1002	279	314	5			

- Molecule 2 is a protein called Heavy chain from highly potent anti-HIV neutralizing antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total	C	N	O	S	0	0	0
			1638	1040	285	308	5			
2	A	212	Total	C	N	O	S	0	0	0
			1638	1040	285	308	5			

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



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

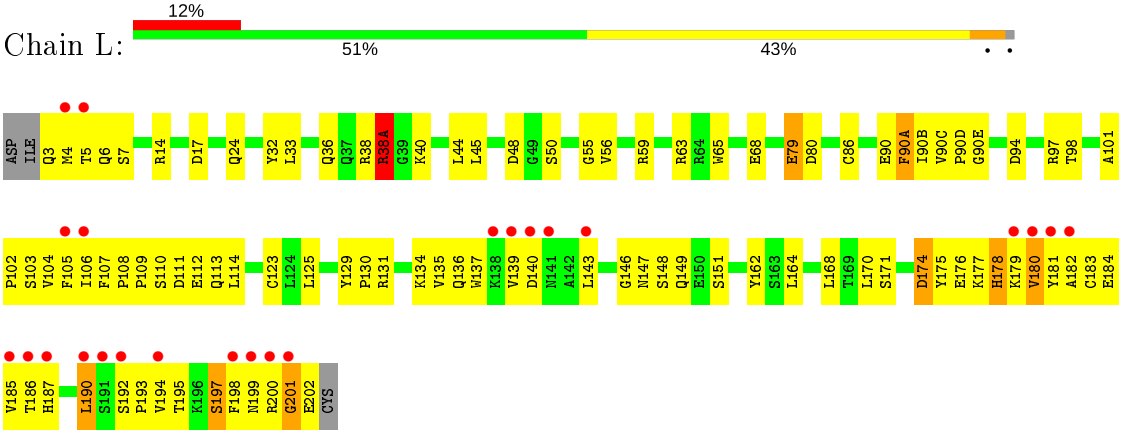
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	48	Total O 48 48	0	0
4	H	25	Total O 25 25	0	0
4	A	31	Total O 31 31	0	0
4	B	42	Total O 42 42	0	0

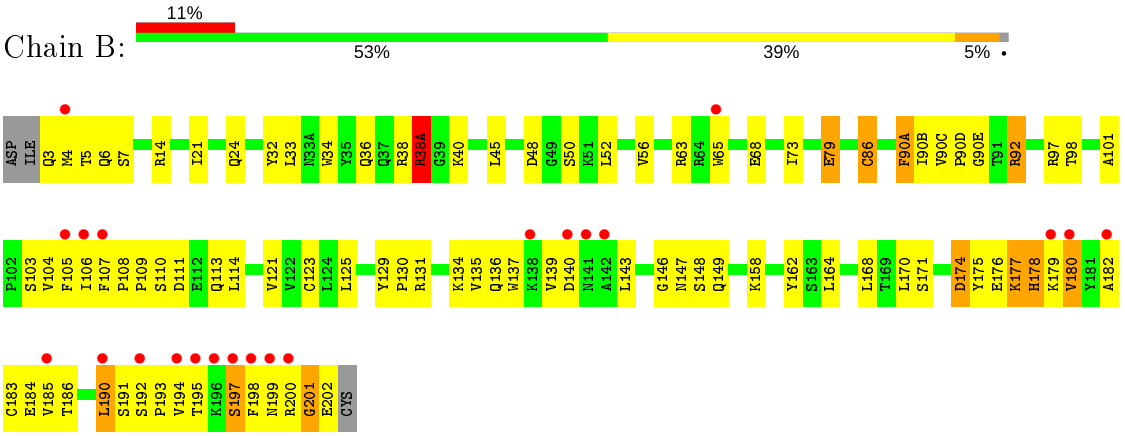
3 Residue-property plots (i)

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.

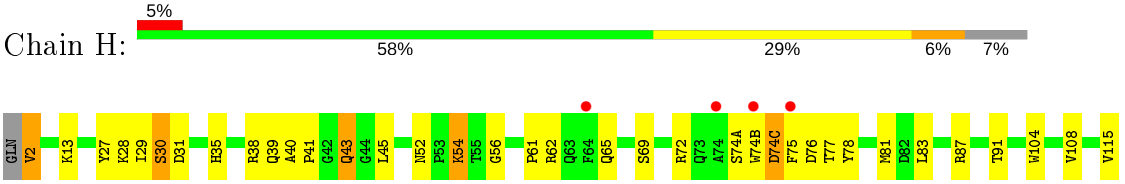
• Molecule 1: Light chain from highly potent anti-HIV neutralizing antibody

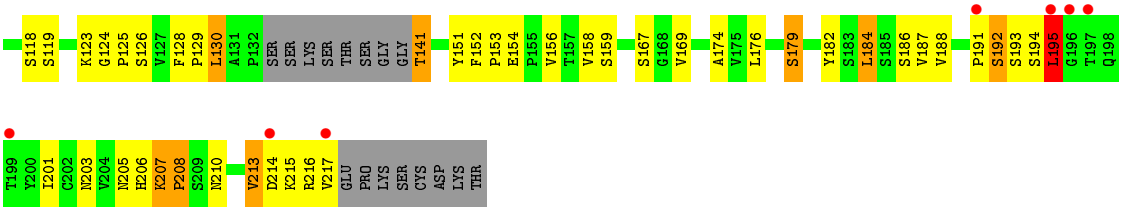


• Molecule 1: Light chain from highly potent anti-HIV neutralizing antibody



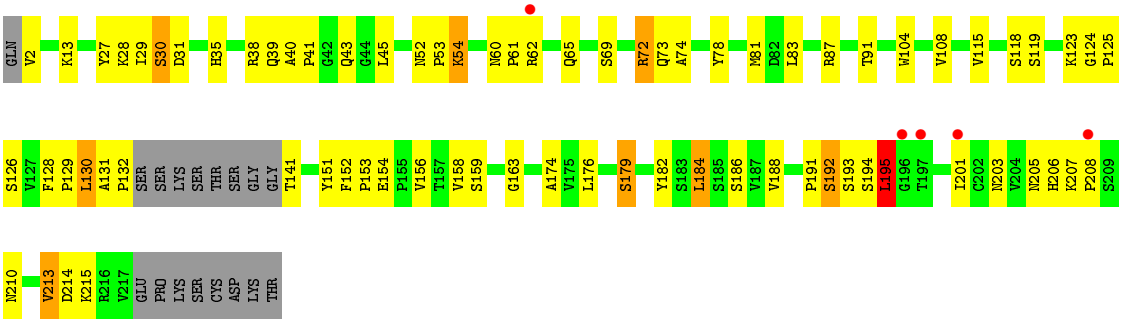
• Molecule 2: Heavy chain from highly potent anti-HIV neutralizing antibody





• Molecule 2: Heavy chain from highly potent anti-HIV neutralizing antibody

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.62Å 155.68Å 74.76Å 90.00° 110.40° 90.00°	Depositor
Resolution (Å)	39.17 – 2.65 39.17 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.7 (39.17-2.65) 93.7 (39.17-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.208 , 0.258 0.204 , 0.255	Depositor DCC
R_{free} test set	1918 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 75.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6650	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	B	0.59	2/1634 (0.1%)	0.72	2/2217 (0.1%)
1	L	0.56	0/1634	0.72	1/2217 (0.0%)
2	A	0.49	0/1687	0.61	0/2304
2	H	0.49	0/1687	0.61	0/2304
All	All	0.53	2/6642 (0.0%)	0.66	3/9042 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	86	CYS	CB-SG	-7.01	1.70	1.82
1	B	34	TRP	CB-CG	-5.02	1.41	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	177	LYS	CD-CE-NZ	6.07	125.66	111.70
1	B	158	LYS	CD-CE-NZ	-6.05	97.79	111.70
1	B	177	LYS	CD-CE-NZ	5.60	124.58	111.70

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	B	1600	0	1560	87	0
1	L	1600	0	1560	99	0
2	A	1638	0	1570	55	0
2	H	1638	0	1570	61	0
3	B	14	0	13	1	0
3	L	14	0	13	1	0
4	A	31	0	0	3	0
4	B	42	0	0	5	0
4	H	25	0	0	4	0
4	L	48	0	0	21	0
All	All	6650	0	6286	292	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 23.

All (292) 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:90(C):VAL:HG13	1:B:90(D):PRO:HD2	1.47	0.95
2:H:167:SER:OG	4:H:242:HOH:O	1.83	0.94
1:L:90(C):VAL:HG13	1:L:90(D):PRO:HD2	1.49	0.94
1:L:56:VAL:CA	4:L:245:HOH:O	2.15	0.94
1:L:50:SER:O	4:L:30:HOH:O	1.85	0.94
1:L:102:PRO:HD3	1:L:187:HIS:HD2	1.34	0.92
1:L:17:ASP:OD2	4:L:247:HOH:O	1.90	0.87
2:A:62:ARG:NH1	4:A:243:HOH:O	2.07	0.87
1:L:90(D):PRO:HG2	4:L:236:HOH:O	1.73	0.86
1:B:6:GLN:HB2	1:B:90(C):VAL:HG11	1.58	0.84
1:L:97:ARG:NH1	1:L:98:THR:O	2.11	0.84
1:B:97:ARG:NH1	1:B:98:THR:O	2.12	0.83
1:L:79:GLU:OE2	4:L:216:HOH:O	1.95	0.83
1:L:6:GLN:HB2	1:L:90(C):VAL:HG11	1.62	0.82
1:L:55:GLY:C	4:L:245:HOH:O	2.17	0.82
1:L:102:PRO:HD3	1:L:187:HIS:CD2	2.17	0.80
1:B:140:ASP:OD2	1:B:178:HIS:HB3	1.83	0.78
1:L:56:VAL:C	4:L:245:HOH:O	2.20	0.78
1:B:135:VAL:HA	1:B:185:VAL:HG12	1.65	0.77
1:L:135:VAL:HA	1:L:185:VAL:HG12	1.66	0.76
1:L:140:ASP:OD2	1:L:178:HIS:HB3	1.85	0.76
1:B:97:ARG:HH11	1:B:97:ARG:HG3	1.49	0.76
1:L:97:ARG:HH11	1:L:97:ARG:HG3	1.51	0.76
1:L:44:LEU:O	4:L:206:HOH:O	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ALA:HB2	1:B:197:SER:HB3	1.71	0.73
2:H:27:TYR:CE1	2:H:29:ILE:HA	2.22	0.73
2:A:27:TYR:CE1	2:A:29:ILE:HA	2.24	0.73
1:L:55:GLY:O	4:L:245:HOH:O	2.06	0.72
1:B:90(D):PRO:O	4:B:228:HOH:O	2.08	0.71
1:L:111:ASP:HA	1:L:114:LEU:HD13	1.72	0.71
1:B:111:ASP:HA	1:B:114:LEU:HD13	1.73	0.71
2:A:125:PRO:HB3	2:A:151:TYR:HB3	1.72	0.71
1:L:36:GLN:HB2	1:L:45:LEU:HD11	1.71	0.71
1:L:94:ASP:OD2	4:L:229:HOH:O	2.08	0.71
2:A:163:GLY:O	4:A:252:HOH:O	2.09	0.70
1:L:182:ALA:HB2	1:L:197:SER:HB3	1.72	0.70
1:B:90(C):VAL:CG1	1:B:90(D):PRO:HD2	2.22	0.70
2:H:216:ARG:O	4:H:230:HOH:O	2.08	0.70
1:L:90(A):PHE:HD1	1:L:90(B):ILE:N	1.89	0.70
1:L:56:VAL:N	4:L:245:HOH:O	2.19	0.70
1:L:200:ARG:HH11	1:L:200:ARG:HA	1.55	0.70
2:H:56:GLY:O	4:H:229:HOH:O	2.10	0.69
1:B:191:SER:O	4:B:243:HOH:O	2.09	0.69
1:B:90(A):PHE:HD1	1:B:90(B):ILE:N	1.90	0.69
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.74	0.69
1:B:200:ARG:HH11	1:B:200:ARG:HA	1.57	0.69
1:L:3:GLN:N	4:L:242:HOH:O	2.26	0.68
2:A:141:THR:HA	2:A:191:PRO:HA	1.76	0.68
2:H:141:THR:HA	2:H:191:PRO:HA	1.74	0.68
2:H:81:MET:HE1	2:H:83:LEU:HG	1.76	0.67
1:L:131:ARG:HB3	1:L:162:TYR:CE2	2.30	0.67
1:B:36:GLN:HB2	1:B:45:LEU:HD11	1.75	0.66
2:A:60:ASN:OD1	4:A:231:HOH:O	2.14	0.66
1:L:90(C):VAL:CG1	1:L:90(D):PRO:HD2	2.24	0.66
1:L:125:LEU:HD11	1:L:185:VAL:HG11	1.78	0.65
1:B:6:GLN:CB	1:B:90(C):VAL:HG11	2.26	0.65
2:H:179:SER:HA	2:A:179:SER:HA	1.80	0.64
2:H:129:PRO:HD3	2:H:215:LYS:NZ	2.13	0.63
1:B:114:LEU:H	1:B:114:LEU:HD12	1.64	0.63
2:A:130:LEU:HD12	1:B:107:PHE:HB3	1.80	0.63
1:B:125:LEU:HD11	1:B:185:VAL:HG11	1.80	0.63
1:L:6:GLN:CB	1:L:90(C):VAL:HG11	2.28	0.63
1:L:174:ASP:O	1:L:178:HIS:CD2	2.52	0.63
1:L:149:GLN:NE2	2:H:176:LEU:O	2.32	0.62
1:L:114:LEU:H	1:L:114:LEU:HD12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:131:ARG:HB3	1:L:162:TYR:CD2	2.35	0.62
1:L:107:PHE:HB3	2:H:130:LEU:HD12	1.82	0.61
2:A:123:LYS:HG2	2:A:124:GLY:O	2.01	0.61
1:B:174:ASP:O	1:B:178:HIS:CD2	2.52	0.61
1:B:182:ALA:CB	1:B:197:SER:HB3	2.30	0.61
2:A:2:VAL:HG22	2:A:108:VAL:HG21	1.83	0.61
1:B:97:ARG:HG3	1:B:97:ARG:NH1	2.16	0.61
1:L:182:ALA:CB	1:L:197:SER:HB3	2.31	0.60
2:A:129:PRO:HD3	2:A:215:LYS:NZ	2.17	0.59
1:B:32:TYR:CZ	1:B:48:ASP:HB2	2.37	0.59
2:A:141:THR:N	2:A:192:SER:H	2.00	0.59
1:B:3:GLN:N	4:B:226:HOH:O	2.36	0.59
2:A:81:MET:HE1	2:A:83:LEU:HG	1.84	0.59
2:H:141:THR:N	2:H:192:SER:H	2.00	0.59
2:A:62:ARG:HA	2:A:65:GLN:HG2	1.84	0.58
2:H:201:ILE:O	2:H:201:ILE:HG23	2.03	0.58
2:H:123:LYS:HG2	2:H:124:GLY:O	2.04	0.58
2:H:62:ARG:HA	2:H:65:GLN:HG2	1.84	0.58
1:L:90:GLU:HB2	4:L:238:HOH:O	2.04	0.58
1:B:182:ALA:HB1	1:B:195:THR:HG21	1.86	0.58
2:A:201:ILE:HG23	2:A:201:ILE:O	2.05	0.57
1:B:131:ARG:HB2	1:B:162:TYR:CD2	2.39	0.57
2:H:213:VAL:CG2	2:H:214:ASP:N	2.68	0.57
2:A:28:LYS:HG2	2:A:31:ASP:OD2	2.04	0.57
1:L:32:TYR:CZ	1:L:48:ASP:HB2	2.40	0.57
2:H:2:VAL:HG22	2:H:108:VAL:HG21	1.87	0.57
1:L:182:ALA:HB1	1:L:195:THR:HG21	1.87	0.56
1:L:170:LEU:HD11	1:L:175:TYR:HB2	1.87	0.56
2:A:213:VAL:CG2	2:A:214:ASP:N	2.68	0.56
2:A:29:ILE:HG21	2:A:78:TYR:CD2	2.40	0.56
1:L:110:SER:O	1:L:114:LEU:HD12	2.05	0.56
1:B:110:SER:O	1:B:114:LEU:HD12	2.05	0.56
2:H:152:PHE:CE1	2:H:153:PRO:HB3	2.41	0.56
1:B:106:ILE:HD12	1:B:183:CYS:HB2	1.88	0.56
1:B:147:ASN:OD1	1:B:168:LEU:HD12	2.07	0.55
1:L:108:PRO:HB3	1:L:198:PHE:CE1	2.41	0.55
2:A:72:ARG:HG2	2:A:73:GLN:N	2.19	0.55
1:L:149:GLN:OE1	1:L:149:GLN:HA	2.07	0.55
1:L:147:ASN:OD1	1:L:168:LEU:HD12	2.06	0.55
2:H:28:LYS:HG2	2:H:31:ASP:OD2	2.06	0.55
1:B:33:LEU:HD11	1:B:86:CYS:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ARG:HH12	1:B:131:ARG:CD	2.20	0.54
1:L:164:LEU:HD23	1:L:164:LEU:C	2.28	0.54
1:L:4:MET:HA	1:L:24:GLN:O	2.07	0.54
1:L:90(A):PHE:HD1	1:L:90(A):PHE:C	2.11	0.54
1:L:106:ILE:HD12	1:L:183:CYS:HB2	1.90	0.54
1:L:90:GLU:N	4:L:238:HOH:O	2.07	0.54
1:B:170:LEU:HD11	1:B:175:TYR:HB2	1.89	0.54
1:B:4:MET:HA	1:B:24:GLN:O	2.08	0.53
1:B:182:ALA:HB1	1:B:195:THR:CG2	2.39	0.53
1:L:113:GLN:HB2	2:H:128:PHE:CD1	2.43	0.53
2:H:201:ILE:HG12	2:H:214:ASP:OD1	2.09	0.53
1:L:129:TYR:CG	1:L:130:PRO:HA	2.43	0.53
2:A:201:ILE:HG12	2:A:214:ASP:OD1	2.09	0.53
2:A:152:PHE:CE1	2:A:153:PRO:HB3	2.44	0.53
1:L:182:ALA:HB1	1:L:195:THR:CG2	2.39	0.53
1:L:90(A):PHE:CD1	1:L:90(A):PHE:C	2.82	0.53
2:A:125:PRO:CB	2:A:151:TYR:HB3	2.39	0.52
1:B:129:TYR:CG	1:B:130:PRO:HA	2.44	0.52
1:L:113:GLN:HG3	2:H:128:PHE:CZ	2.44	0.52
1:B:101:ALA:HB1	1:B:190:LEU:HD22	1.92	0.52
2:H:74(A):SER:HB3	2:H:77:THR:O	2.09	0.52
1:L:97:ARG:HG3	1:L:97:ARG:NH1	2.19	0.52
2:H:40:ALA:HB1	2:H:41:PRO:HD2	1.92	0.52
1:L:4:MET:HE1	1:L:90(A):PHE:HB3	1.91	0.52
1:B:146:GLY:O	1:B:147:ASN:CG	2.49	0.52
1:B:90(A):PHE:CD1	1:B:90(A):PHE:C	2.83	0.51
1:B:90(A):PHE:HD1	1:B:90(A):PHE:C	2.14	0.51
1:B:174:ASP:HA	1:B:177:LYS:HD2	1.93	0.51
2:A:176:LEU:O	1:B:149:GLN:NE2	2.44	0.51
1:B:149:GLN:HA	1:B:149:GLN:OE1	2.10	0.51
2:A:213:VAL:HG23	2:A:214:ASP:N	2.26	0.51
2:H:118:SER:OG	2:H:152:PHE:CZ	2.59	0.51
2:A:205:ASN:OD1	2:A:206:HIS:N	2.44	0.50
1:B:186:THR:HG22	1:B:193:PRO:HB3	1.94	0.50
1:B:164:LEU:C	1:B:164:LEU:HD23	2.31	0.50
2:A:154:GLU:OE2	2:A:174:ALA:HB3	2.10	0.50
1:B:131:ARG:HB2	1:B:162:TYR:CE2	2.46	0.50
2:H:205:ASN:OD1	2:H:206:HIS:N	2.44	0.50
2:H:125:PRO:CB	2:H:151:TYR:HB3	2.41	0.50
1:L:131:ARG:NH1	4:L:235:HOH:O	2.44	0.50
1:B:104:VAL:O	1:B:105:PHE:CD1	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLN:HG3	1:B:3:GLN:O	2.11	0.50
2:H:154:GLU:OE2	2:H:174:ALA:HB3	2.12	0.49
2:A:118:SER:OG	2:A:152:PHE:CZ	2.61	0.49
2:A:176:LEU:HD13	2:A:182:TYR:CE1	2.47	0.49
2:H:81:MET:CE	2:H:83:LEU:HG	2.41	0.49
1:L:146:GLY:O	1:L:147:ASN:CG	2.50	0.49
2:A:158:VAL:HG11	2:A:186:SER:CB	2.43	0.49
2:H:213:VAL:HG23	2:H:214:ASP:N	2.28	0.49
1:L:179:LYS:HE2	1:L:199:ASN:ND2	2.27	0.49
1:B:179:LYS:HE2	1:B:199:ASN:ND2	2.27	0.49
1:L:3:GLN:O	1:L:3:GLN:HG3	2.12	0.49
1:L:90:GLU:CB	4:L:238:HOH:O	2.58	0.48
1:L:101:ALA:HB1	1:L:190:LEU:HD22	1.94	0.48
1:B:90(C):VAL:CG1	1:B:90(D):PRO:CD	2.91	0.48
1:L:186:THR:HG22	1:L:193:PRO:HB3	1.96	0.48
1:B:140:ASP:HA	1:B:180:VAL:HG13	1.95	0.48
2:H:158:VAL:HG11	2:H:186:SER:CB	2.44	0.47
2:A:184:LEU:HD12	2:A:184:LEU:C	2.35	0.47
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.97	0.47
2:H:81:MET:HE1	2:H:83:LEU:CG	2.43	0.47
2:H:62:ARG:CZ	2:H:65:GLN:NE2	2.77	0.47
1:L:104:VAL:O	1:L:105:PHE:CD1	2.67	0.47
1:L:56:VAL:HA	4:L:245:HOH:O	2.00	0.47
2:A:191:PRO:O	2:A:193:SER:O	2.32	0.47
2:A:30:SER:O	2:A:54:LYS:HE2	2.15	0.47
1:L:65:TRP:HB3	3:L:1000:NAG:H83	1.95	0.47
1:L:114:LEU:N	1:L:114:LEU:HD12	2.29	0.47
1:L:32:TYR:CE1	1:L:48:ASP:HB2	2.49	0.47
2:A:74:ALA:HB2	2:A:78:TYR:CE1	2.50	0.47
1:B:38(A):ARG:HH22	1:B:92:ARG:HB3	1.80	0.47
1:L:140:ASP:HA	1:L:180:VAL:HG13	1.96	0.47
2:A:62:ARG:CZ	2:A:65:GLN:NE2	2.78	0.46
2:H:191:PRO:O	2:H:193:SER:O	2.32	0.46
1:L:90(C):VAL:CG1	4:L:236:HOH:O	2.64	0.46
1:L:113:GLN:HG3	2:H:128:PHE:CE2	2.51	0.46
2:A:125:PRO:CA	2:A:151:TYR:HB3	2.46	0.46
2:H:29:ILE:HG21	2:H:78:TYR:CD2	2.51	0.46
1:B:114:LEU:HD12	1:B:114:LEU:N	2.28	0.46
1:B:92:ARG:NH1	1:B:131:ARG:CZ	2.79	0.46
1:B:183:CYS:O	1:B:195:THR:HG23	2.16	0.46
2:A:213:VAL:HG23	2:A:214:ASP:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:40:ALA:HB1	2:A:41:PRO:HD2	1.98	0.45
1:B:92:ARG:HH12	1:B:131:ARG:HD2	1.81	0.45
1:B:178:HIS:N	1:B:178:HIS:CD2	2.84	0.45
1:B:32:TYR:CE1	1:B:48:ASP:HB2	2.51	0.45
2:H:62:ARG:NH1	2:H:65:GLN:HE22	2.14	0.45
1:B:90(C):VAL:HG13	1:B:90(D):PRO:CD	2.33	0.45
2:H:152:PHE:CD1	2:H:153:PRO:CA	2.99	0.45
2:H:184:LEU:C	2:H:184:LEU:HD12	2.36	0.45
1:L:178:HIS:CD2	1:L:178:HIS:N	2.84	0.45
1:L:200:ARG:HD3	1:L:200:ARG:HA	1.59	0.45
1:L:90(C):VAL:HG12	4:L:236:HOH:O	2.16	0.45
2:H:176:LEU:HD13	2:H:182:TYR:CE1	2.51	0.45
1:L:147:ASN:C	1:L:147:ASN:OD1	2.55	0.45
1:L:175:TYR:O	1:L:181:TYR:OH	2.35	0.45
1:L:90(C):VAL:CG1	1:L:90(D):PRO:CD	2.94	0.45
1:L:112:GLU:OE1	2:H:215:LYS:NZ	2.49	0.45
1:B:50:SER:OG	4:B:239:HOH:O	2.21	0.45
1:B:90(C):VAL:HG12	1:B:90(E):GLY:H	1.81	0.45
2:A:152:PHE:CD1	2:A:153:PRO:CA	3.00	0.45
2:A:81:MET:CE	2:A:83:LEU:HG	2.47	0.44
2:H:129:PRO:HD3	2:H:215:LYS:HZ2	1.81	0.44
2:H:125:PRO:CA	2:H:151:TYR:HB3	2.47	0.44
2:H:213:VAL:HG23	2:H:214:ASP:H	1.82	0.44
1:L:123:CYS:HB2	1:L:137:TRP:CZ2	2.52	0.44
1:L:38:ARG:O	1:L:38(A):ARG:C	2.56	0.44
2:A:131:ALA:HA	2:A:132:PRO:HD3	1.80	0.44
1:L:170:LEU:CD1	1:L:175:TYR:HB2	2.48	0.44
1:L:3:GLN:HG2	4:L:227:HOH:O	2.16	0.44
2:A:128:PHE:CD1	1:B:113:GLN:HB2	2.52	0.44
2:A:52:ASN:HA	2:A:53:PRO:HD3	1.90	0.44
1:B:174:ASP:O	1:B:178:HIS:NE2	2.50	0.44
2:H:74(B):TRP:O	2:H:75:PHE:CD2	2.69	0.44
2:A:152:PHE:HA	2:A:153:PRO:HA	1.69	0.44
2:H:43:GLN:HE21	2:H:43:GLN:HB2	1.46	0.44
1:L:183:CYS:O	1:L:195:THR:HG23	2.17	0.44
1:B:38:ARG:O	1:B:38(A):ARG:C	2.55	0.44
2:A:154:GLU:HG2	2:A:182:TYR:CD2	2.53	0.44
1:B:192:SER:O	1:B:193:PRO:C	2.54	0.44
2:A:195:LEU:HA	2:A:195:LEU:HD12	1.84	0.44
1:B:38:ARG:O	1:B:40:LYS:N	2.52	0.43
1:B:92:ARG:HH22	1:B:131:ARG:HH11	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:30:SER:O	2:H:54:LYS:HE2	2.18	0.43
2:A:62:ARG:NH1	2:A:65:GLN:HE22	2.16	0.43
1:B:92:ARG:HH12	1:B:131:ARG:CZ	2.30	0.43
1:B:170:LEU:CD1	1:B:175:TYR:HB2	2.49	0.43
1:L:146:GLY:O	1:L:147:ASN:OD1	2.36	0.43
1:L:135:VAL:HG23	1:L:185:VAL:CG1	2.48	0.43
2:H:61:PRO:O	2:H:62:ARG:C	2.56	0.43
1:L:38:ARG:O	1:L:40:LYS:N	2.51	0.43
1:B:79:GLU:H	1:B:79:GLU:HG3	1.33	0.43
1:L:192:SER:O	1:L:193:PRO:C	2.54	0.43
1:B:4:MET:HE1	1:B:90(A):PHE:HB3	2.01	0.42
1:L:59:ARG:NH1	1:L:80:ASP:OD2	2.36	0.42
1:B:108:PRO:HB3	1:B:198:PHE:CE1	2.54	0.42
1:L:174:ASP:O	1:L:178:HIS:NE2	2.52	0.42
1:L:38(A):ARG:HG2	1:L:38(A):ARG:H	1.54	0.42
1:L:3:GLN:NE2	4:L:227:HOH:O	2.39	0.42
1:B:146:GLY:O	1:B:147:ASN:OD1	2.36	0.42
2:A:39:GLN:HB2	2:A:45:LEU:HD23	2.02	0.42
2:A:61:PRO:O	2:A:62:ARG:C	2.57	0.42
1:L:110:SER:O	1:L:114:LEU:CD1	2.68	0.42
1:B:92:ARG:NH2	1:B:131:ARG:NH1	2.68	0.42
2:H:74(C):ASP:O	2:H:75:PHE:HB2	2.20	0.42
2:H:91:THR:HA	2:H:115:VAL:O	2.19	0.42
1:B:147:ASN:OD1	1:B:168:LEU:CD1	2.67	0.42
2:H:35:HIS:HE1	2:H:104:TRP:CZ2	2.38	0.42
1:B:177:LYS:HB2	1:B:178:HIS:CD2	2.55	0.42
2:H:191:PRO:O	2:H:193:SER:N	2.53	0.42
2:H:74(C):ASP:OD2	2:H:76:ASP:OD1	2.37	0.42
1:L:107:PHE:HA	1:L:108:PRO:HD2	1.75	0.42
1:L:33:LEU:HD11	1:L:86:CYS:HB2	2.01	0.42
2:H:217:VAL:HA	4:H:230:HOH:O	2.20	0.41
2:A:91:THR:HA	2:A:115:VAL:O	2.19	0.41
1:B:135:VAL:HG23	1:B:185:VAL:CG1	2.50	0.41
1:L:109:PRO:HB2	1:L:114:LEU:HD11	2.03	0.41
1:B:6:GLN:N	4:B:240:HOH:O	1.80	0.41
1:B:65:TRP:HB3	3:B:1000:NAG:H83	2.02	0.41
1:B:109:PRO:HD3	1:B:121:VAL:HG22	2.02	0.41
1:B:21:ILE:HG21	1:B:21:ILE:HD13	1.77	0.41
2:A:53:PRO:O	2:A:72:ARG:HD2	2.21	0.41
2:H:195:LEU:HA	2:H:195:LEU:HD12	1.85	0.41
1:L:201:GLY:O	1:L:202:GLU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:GLN:HB2	1:B:184:GLU:O	2.21	0.41
1:L:90(C):VAL:HG12	1:L:90(E):GLY:H	1.85	0.41
2:A:191:PRO:O	2:A:193:SER:N	2.53	0.41
2:A:35:HIS:HE1	2:A:104:TRP:CZ2	2.38	0.41
1:L:90(B):ILE:HG22	1:L:90(C):VAL:O	2.21	0.41
1:B:147:ASN:C	1:B:147:ASN:OD1	2.60	0.40
1:L:149:GLN:OE1	1:L:149:GLN:CA	2.68	0.40
2:A:28:LYS:HG2	2:A:31:ASP:CG	2.41	0.40
2:A:81:MET:HE1	2:A:83:LEU:CG	2.51	0.40
2:A:129:PRO:HD3	2:A:215:LYS:HZ2	1.86	0.40
1:B:109:PRO:HB2	1:B:114:LEU:HD11	2.04	0.40
1:B:123:CYS:HB2	1:B:137:TRP:CZ2	2.55	0.40
1:B:52:LEU:HD11	1:B:56:VAL:HB	2.04	0.40
2:H:169:VAL:HA	2:H:187:VAL:O	2.22	0.40
1:B:201:GLY:O	1:B:202:GLU:C	2.59	0.40
2:H:207:LYS:N	2:H:208:PRO:HD2	2.37	0.40
2:H:28:LYS:HG2	2:H:31:ASP:CG	2.42	0.40
2:H:52:ASN:OD1	2:H:52:ASN:C	2.60	0.40
1:L:136:GLN:HB2	1:L:184:GLU:O	2.21	0.40
1:B:110:SER:O	1:B:114:LEU:CD1	2.68	0.40
1:B:73:ILE:HD13	1:B:73:ILE:HG21	1.73	0.40
2:H:62:ARG:NH1	2:H:65:GLN:NE2	2.69	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	B	201/206 (98%)	184 (92%)	15 (8%)	2 (1%)	15	22
1	L	201/206 (98%)	183 (91%)	16 (8%)	2 (1%)	15	22
2	A	208/229 (91%)	188 (90%)	16 (8%)	4 (2%)	8	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	208/229 (91%)	187 (90%)	17 (8%)	4 (2%)	8 10
All	All	818/870 (94%)	742 (91%)	64 (8%)	12 (2%)	10 14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	38(A)	ARG
1	B	38(A)	ARG
2	H	195	LEU
2	H	210	ASN
2	A	195	LEU
2	A	210	ASN
2	H	192	SER
2	A	192	SER
1	L	201	GLY
1	B	201	GLY
2	H	208	PRO
2	A	208	PRO

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	B	179/182 (98%)	157 (88%)	22 (12%)	4 6
1	L	179/182 (98%)	157 (88%)	22 (12%)	4 6
2	A	181/196 (92%)	160 (88%)	21 (12%)	5 7
2	H	181/196 (92%)	157 (87%)	24 (13%)	4 4
All	All	720/756 (95%)	631 (88%)	89 (12%)	4 5

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	7	SER

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Mol	Chain	Res	Type
1	L	14	ARG
1	L	38(A)	ARG
1	L	63	ARG
1	L	68	GLU
1	L	79	GLU
1	L	90(A)	PHE
1	L	103	SER
1	L	134	LYS
1	L	139	VAL
1	L	143	LEU
1	L	148	SER
1	L	151	SER
1	L	171	SER
1	L	174	ASP
1	L	176	GLU
1	L	178	HIS
1	L	180	VAL
1	L	190	LEU
1	L	194	VAL
1	L	197	SER
2	H	2	VAL
2	H	13	LYS
2	H	30	SER
2	H	38	ARG
2	H	43	GLN
2	H	54	LYS
2	H	69	SER
2	H	72	ARG
2	H	74(C)	ASP
2	H	87	ARG
2	H	119	SER
2	H	126	SER
2	H	130	LEU
2	H	141	THR
2	H	156	VAL
2	H	159	SER
2	H	179	SER
2	H	184	LEU
2	H	188	VAL
2	H	194	SER
2	H	195	LEU
2	H	203	ASN

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Mol	Chain	Res	Type
2	H	207	LYS
2	H	213	VAL
2	A	13	LYS
2	A	30	SER
2	A	38	ARG
2	A	43	GLN
2	A	54	LYS
2	A	69	SER
2	A	72	ARG
2	A	87	ARG
2	A	119	SER
2	A	126	SER
2	A	130	LEU
2	A	156	VAL
2	A	159	SER
2	A	179	SER
2	A	184	LEU
2	A	188	VAL
2	A	194	SER
2	A	195	LEU
2	A	203	ASN
2	A	207	LYS
2	A	213	VAL
1	B	5	THR
1	B	7	SER
1	B	14	ARG
1	B	38(A)	ARG
1	B	63	ARG
1	B	68	GLU
1	B	79	GLU
1	B	90(A)	PHE
1	B	92	ARG
1	B	103	SER
1	B	134	LYS
1	B	139	VAL
1	B	143	LEU
1	B	148	SER
1	B	171	SER
1	B	174	ASP
1	B	176	GLU
1	B	178	HIS
1	B	180	VAL

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Mol	Chain	Res	Type
1	B	190	LEU
1	B	194	VAL
1	B	197	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	178	HIS
1	L	187	HIS
2	H	43	GLN
2	H	65	GLN
2	A	65	GLN
1	B	178	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

There are no monosaccharides 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	L	1000	1	14,14,15	2.22	5 (35%)	17,19,21	1.50	3 (17%)
3	NAG	B	1000	1	14,14,15	1.91	5 (35%)	17,19,21	1.68	5 (29%)

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	L	1000	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1000	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	1000	NAG	C1-C2	4.31	1.58	1.52
3	B	1000	NAG	C1-C2	4.16	1.58	1.52
3	L	1000	NAG	O5-C5	-3.69	1.36	1.43
3	L	1000	NAG	O5-C1	-3.62	1.37	1.43
3	B	1000	NAG	O5-C5	-3.00	1.37	1.43
3	B	1000	NAG	C7-N2	2.89	1.44	1.34
3	L	1000	NAG	C3-C2	2.78	1.58	1.52
3	L	1000	NAG	C7-N2	2.59	1.43	1.34
3	B	1000	NAG	C3-C2	2.32	1.57	1.52
3	B	1000	NAG	O5-C1	-2.12	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	1000	NAG	C1-C2-N2	-3.04	105.29	110.49
3	B	1000	NAG	C2-N2-C7	-2.80	118.92	122.90
3	L	1000	NAG	O3-C3-C2	-2.36	104.59	109.47
3	L	1000	NAG	O5-C1-C2	-2.29	107.68	111.29
3	B	1000	NAG	O5-C1-C2	-2.28	107.68	111.29
3	B	1000	NAG	O5-C5-C6	-2.20	103.76	107.20
3	B	1000	NAG	C1-O5-C5	2.18	115.15	112.19
3	B	1000	NAG	O6-C6-C5	-2.00	104.41	111.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	1000	NAG	O5-C5-C6-O6
3	L	1000	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1000	NAG	1	0
3	B	1000	NAG	1	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, 95^{th} 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	B	203/206 (98%)	0.43	22 (10%) 5 4	23, 58, 125, 157	0
1	L	203/206 (98%)	0.49	24 (11%) 4 3	22, 59, 125, 157	0
2	A	212/229 (92%)	0.15	5 (2%) 59 55	27, 60, 107, 131	0
2	H	212/229 (92%)	0.33	11 (5%) 27 24	25, 62, 114, 145	0
All	All	830/870 (95%)	0.35	62 (7%) 14 11	22, 60, 122, 157	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	182	ALA	4.9
2	H	64	PHE	4.6
1	L	186	THR	4.5
1	L	190	LEU	4.4
1	L	138	LYS	4.2
2	H	196	GLY	4.0
2	A	196	GLY	3.9
1	B	141	ASN	3.8
1	L	192	SER	3.8
1	B	198	PHE	3.7
2	H	197	THR	3.6
1	B	180	VAL	3.6
1	B	199	ASN	3.6
2	H	74(B)	TRP	3.6
1	B	196	LYS	3.6
1	L	141	ASN	3.5
1	L	191	SER	3.5
1	L	140	ASP	3.4
1	B	200	ARG	3.4
2	A	197	THR	3.3
1	B	192	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	105	PHE	3.3
1	B	185	VAL	3.2
1	L	4	MET	3.2
1	B	140	ASP	3.1
1	L	106	ILE	3.1
1	B	195	THR	3.1
1	L	198	PHE	3.1
2	A	62	ARG	3.1
1	B	4	MET	3.1
1	B	138	LYS	3.0
1	L	194	VAL	3.0
1	B	182	ALA	2.9
1	L	201	GLY	2.9
1	L	143	LEU	2.8
1	B	65	TRP	2.8
1	B	194	VAL	2.8
2	H	217	VAL	2.7
1	B	142	ALA	2.7
1	B	190	LEU	2.7
2	H	199	THR	2.7
2	H	75	PHE	2.6
1	L	139	VAL	2.6
1	L	180	VAL	2.6
2	A	208	PRO	2.5
1	L	185	VAL	2.5
1	L	179	LYS	2.5
2	A	201	ILE	2.5
1	L	5	THR	2.4
1	L	199	ASN	2.4
2	H	214	ASP	2.4
1	L	105	PHE	2.4
1	B	179	LYS	2.4
1	B	107	PHE	2.3
1	L	181	TYR	2.3
2	H	74	ALA	2.2
1	B	197	SER	2.1
1	L	187	HIS	2.1
1	B	106	ILE	2.1
2	H	191	PRO	2.1
2	H	195	LEU	2.1
1	L	200	ARG	2.1

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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
3	NAG	B	1000	14/15	0.89	0.20	38,55,71,73	0
3	NAG	L	1000	14/15	0.90	0.22	36,59,77,83	0

6.5 Other polymers (i)

There are no such residues in this entry.