Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:12 PM GMT

PDB ID	:	4RFO
Title	:	Crystal structure of the ADCC-Potent Antibody N60-I3 Fab in complex with HIV-1 Clade A/E gp120 and M48u1
Authors	:	Tolbert, W.D.; Gohain, N.; Pazgier, M.
Deposited on	:	2014-09-26
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

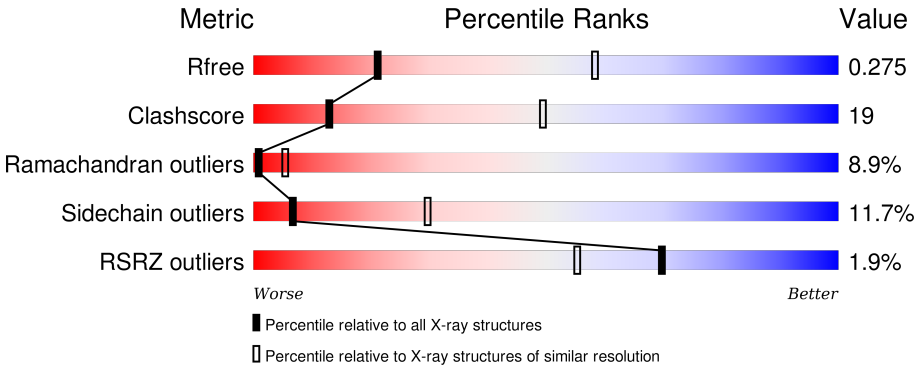
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	G	353	% 57% 31% 6% • 5%
2	N	28	71% 21% • •
3	H	229	3% 50% 30% 10% • 7%
4	L	221	3% 59% 30% 6% • •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	G	507	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6169 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 HIV-1 clade A/E gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	336	Total	C	N	O	S	0	0	0
			2640	1657	458	503	22			

- Molecule 2 is a protein called m48u1 CD4 mimetic peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			

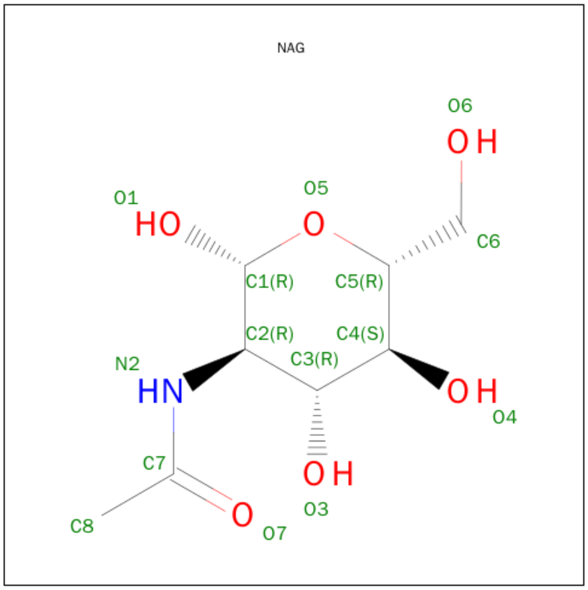
- Molecule 3 is a protein called N60-i3 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	214	Total	C	N	O	S	0	0	0
			1614	1027	269	314	4			

- Molecule 4 is a protein called N60-i3 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	212	Total	C	N	O	S	0	0	0
			1579	986	261	327	5			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

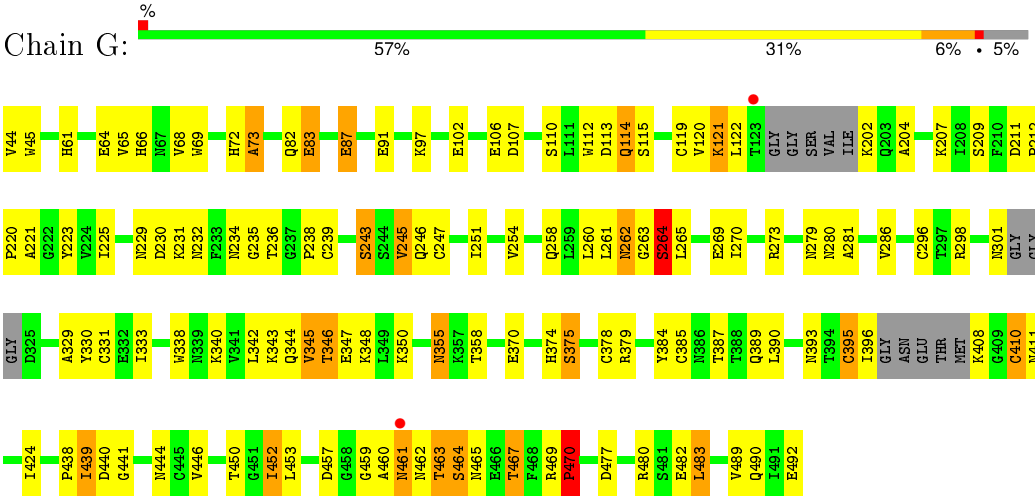
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

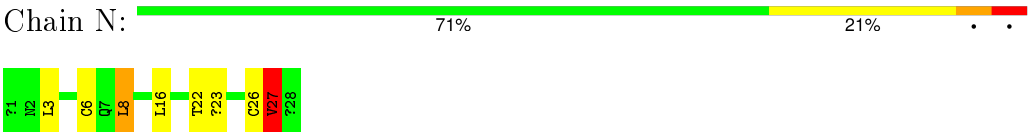
- Molecule 1: HIV-1 clade A/E gp120

Chain G:



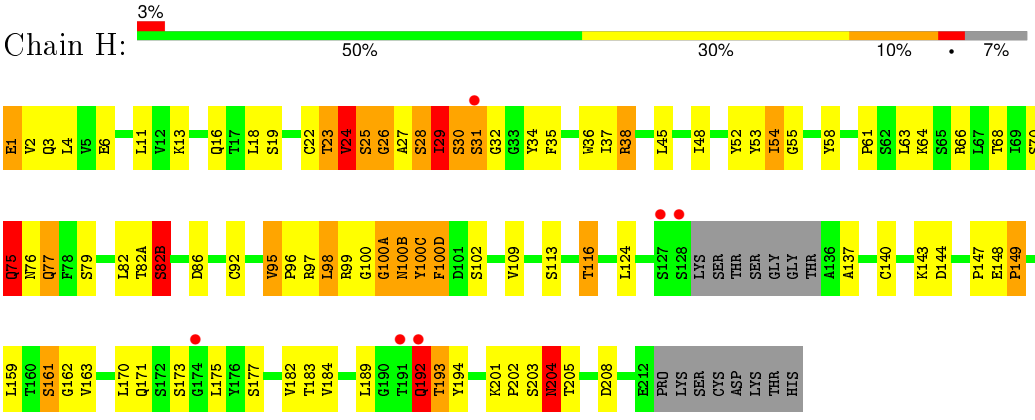
- Molecule 2: m48u1 CD4 mimetic peptide

Chain N:



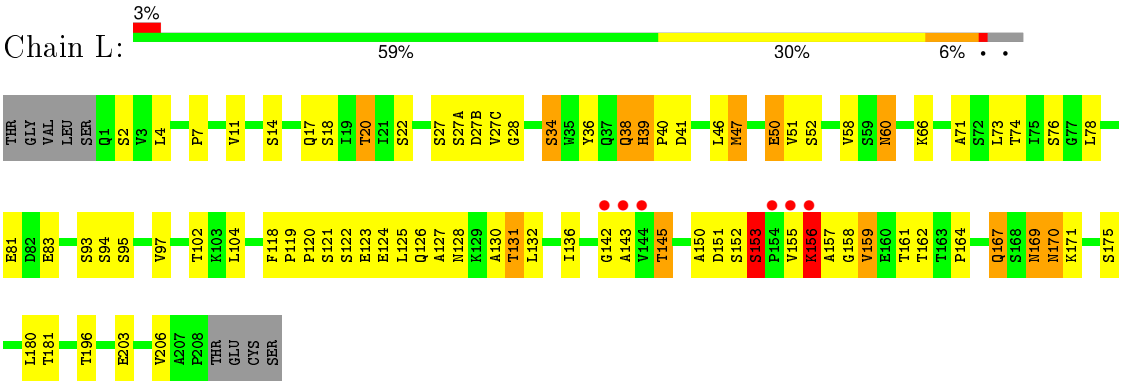
- Molecule 3: N60-i3 Fab heavy chain

Chain H:



- Molecule 4: N60-i3 Fab light chain

Chain L:


3%
59%
30%
6%
THR GLY VAL LEU SER Q1 S2 V3 L4 P7 V11 S14 Q17 S18 I19 T20 I21 S22 S27 S27A D27B V27C G28 S34 W35 Y36 Q37 Q38 H39 P40 D41 L46 M47 E50 V51 S52 V58 S59 N60 K66 A71 S72 L73 T74 I75 S76 G77 L78
E81 D82 E83 S93 S94 S95 V97 T102 K103 L104 F118 P119 P120 S121 S122 E123 E124 L125 Q126 A127 N128 K129 A130 T131 L132 I136 G142 A143 V144 T145 A150 D151 S152 S153 P154 V155 K156 A157 G158 V159 E160 T161 T162 T163 P164 Q167 S168 N169 N170 K171 S175
L180 T181 T196 E203 V206 A207 P208 THR GLU CYS SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.31Å 102.58Å 108.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.01 – 3.20 36.01 – 3.19	Depositor EDS
% Data completeness (in resolution range)	93.8 (36.01-3.20) 93.7 (36.01-3.19)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.220 , 0.277 0.221 , 0.275	Depositor DCC
R_{free} test set	876 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	102.1	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 43.9	EDS
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 17508 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6169	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MPT, U2X, DPR, NH2

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	G	0.41	1/2694 (0.0%)	0.62	0/3655
2	N	0.43	0/176	0.58	0/231
3	H	0.47	0/1655	0.81	4/2263 (0.2%)
4	L	0.41	0/1618	0.64	0/2208
All	All	0.43	1/6143 (0.0%)	0.68	4/8357 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
2	N	0	2
3	H	0	4
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	355	ASN	C-N	7.22	1.50	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	100	GLY	C-N-CA	7.95	139.00	122.30
3	H	100(C)	TYR	O-C-N	-7.57	110.59	122.70
3	H	100(C)	TYR	CA-C-N	5.93	130.25	117.20
3	H	100	GLY	O-C-N	-5.33	114.13	123.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	217	TYR	Peptide
3	H	100(B)	ASN	Peptide
3	H	23	THR	Peptide
3	H	29	ILE	Peptide
3	H	75	GLN	Peptide
2	N	22	THR	Mainchain
2	N	23	U2X	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2640	0	2568	92	0
2	N	209	0	212	4	0
3	H	1614	0	1590	91	0
4	L	1579	0	1524	53	0
5	G	126	0	117	2	0
6	H	1	0	0	0	0
All	All	6169	0	6011	233	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 19.

All (233) 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)
4:L:167:GLN:HG3	4:L:171:LYS:O	1.59	1.01
3:H:34:TYR:CD1	3:H:96:PRO:HB3	1.98	0.98
3:H:171:GLN:NE2	3:H:177:SER:OG	1.96	0.98
3:H:72:ASP:O	3:H:75:GLN:N	2.00	0.94
3:H:72:ASP:O	3:H:75:GLN:CA	2.19	0.91
3:H:95:VAL:HB	3:H:96:PRO:HA	1.54	0.89
1:G:460:ALA:HA	1:G:461:ASN:CB	2.03	0.88
1:G:345:VAL:O	1:G:347:GLU:N	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:158:GLY:HA3	4:L:159:VAL:HG23	1.58	0.84
3:H:189:LEU:HA	3:H:192:GLN:HE21	1.40	0.83
3:H:72:ASP:O	3:H:75:GLN:C	2.19	0.80
1:G:410:CYS:SG	1:G:411:ASN:N	2.55	0.80
1:G:338:TRP:CZ2	1:G:342:LEU:HD11	2.16	0.79
1:G:338:TRP:CE2	1:G:342:LEU:HD11	2.17	0.79
1:G:258:GLN:HG2	1:G:470:PRO:HB3	1.65	0.79
1:G:460:ALA:HA	1:G:461:ASN:HB2	1.66	0.78
3:H:29:ILE:HB	3:H:30:SER:HB2	1.64	0.77
3:H:75:GLN:OE1	3:H:75:GLN:N	2.17	0.77
4:L:150:ALA:O	4:L:153:SER:HB2	1.86	0.75
3:H:29:ILE:HG22	3:H:30:SER:HA	1.69	0.73
1:G:110:SER:O	1:G:114:GLN:NE2	2.19	0.72
3:H:28:SER:O	3:H:29:ILE:HG13	1.89	0.72
1:G:346:THR:O	1:G:350:LYS:N	2.16	0.72
3:H:4:LEU:HD12	3:H:102:SER:O	1.89	0.72
3:H:3:GLN:O	3:H:24:VAL:O	2.08	0.72
4:L:20:THR:HG22	4:L:74:THR:HG23	1.72	0.70
3:H:73:THR:O	3:H:74:THR:OG1	2.07	0.70
3:H:30:SER:N	3:H:32:GLY:O	2.25	0.69
3:H:35:PHE:HB2	3:H:95:VAL:HG21	1.73	0.69
4:L:159:VAL:HG12	4:L:159:VAL:O	1.92	0.69
3:H:148:GLU:CG	3:H:149:PRO:HA	2.22	0.69
4:L:27(A):SER:HB3	4:L:93:SER:OG	1.93	0.69
1:G:64:GLU:OE2	1:G:211:ASP:N	2.24	0.69
3:H:30:SER:OG	3:H:31:SER:HB2	1.92	0.69
1:G:69:TRP:O	1:G:72:HIS:O	2.11	0.69
3:H:192:GLN:OE1	3:H:193:THR:N	2.26	0.68
1:G:329:ALA:O	1:G:417:PRO:O	2.11	0.67
4:L:27(C):VAL:O	4:L:66:LYS:HE3	1.95	0.67
1:G:72:HIS:O	1:G:73:ALA:HB3	1.96	0.66
4:L:167:GLN:CG	4:L:171:LYS:O	2.40	0.66
3:H:124:LEU:HD13	4:L:118:PHE:CD2	2.31	0.66
1:G:298:ARG:NH2	1:G:441:GLY:O	2.28	0.66
3:H:159:LEU:O	3:H:163:VAL:HG21	1.96	0.65
4:L:150:ALA:O	4:L:153:SER:CB	2.45	0.65
3:H:97:ARG:NH2	3:H:100(B):ASN:OD1	2.29	0.65
3:H:29:ILE:HG22	3:H:30:SER:CA	2.27	0.65
1:G:258:GLN:CG	1:G:470:PRO:HB3	2.26	0.64
1:G:296:CYS:O	1:G:444:ASN:ND2	2.31	0.64
4:L:14:SER:O	4:L:17:GLN:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:460:ALA:HA	1:G:461:ASN:HB3	1.79	0.63
3:H:72:ASP:N	3:H:75:GLN:O	2.32	0.63
1:G:246:GLN:N	1:G:246:GLN:OE1	2.31	0.63
3:H:54:ILE:HG22	3:H:55:GLY:H	1.64	0.63
4:L:156:LYS:HD3	4:L:156:LYS:N	2.15	0.62
1:G:83:GLU:OE2	1:G:243:SER:OG	2.07	0.62
3:H:34:TYR:CD1	3:H:96:PRO:CB	2.78	0.62
4:L:152:SER:N	4:L:153:SER:HB2	2.15	0.62
1:G:384:TYR:O	1:G:418:CYS:HA	1.99	0.62
4:L:180:LEU:HD12	4:L:181:THR:O	2.00	0.61
1:G:234:ASN:O	1:G:236:THR:N	2.32	0.61
3:H:66:ARG:NH2	3:H:86:ASP:OD1	2.32	0.61
3:H:124:LEU:HD13	4:L:118:PHE:CG	2.36	0.61
1:G:439:ILE:O	1:G:441:GLY:N	2.33	0.61
3:H:1:GLU:OE2	3:H:26:GLY:HA2	2.00	0.60
3:H:31:SER:N	3:H:32:GLY:HA2	2.16	0.60
2:N:16:LEU:N	2:N:27:VAL:O	2.25	0.60
3:H:148:GLU:HG2	3:H:149:PRO:HA	1.83	0.60
1:G:263:GLY:N	1:G:450:THR:HG21	2.17	0.59
4:L:7:PRO:O	4:L:102:THR:OG1	2.12	0.59
1:G:286:VAL:HG22	1:G:452:ILE:HG12	1.84	0.59
3:H:203:SER:O	3:H:205:THR:N	2.36	0.59
4:L:124:GLU:CD	4:L:130:ALA:O	2.40	0.59
3:H:137:ALA:HB2	3:H:183:THR:HG22	1.84	0.59
1:G:338:TRP:CE2	1:G:342:LEU:CD1	2.85	0.59
1:G:230:ASP:O	1:G:232:ASN:N	2.36	0.59
1:G:64:GLU:OE2	1:G:211:ASP:O	2.21	0.58
3:H:38:ARG:HB3	3:H:48:ILE:HD11	1.85	0.58
4:L:50:GLU:O	4:L:52:SER:N	2.31	0.58
3:H:66:ARG:O	3:H:82:LEU:HD12	2.04	0.58
3:H:35:PHE:HB2	3:H:95:VAL:CG2	2.34	0.57
4:L:94:SER:HA	4:L:95:SER:HB2	1.85	0.57
3:H:96:PRO:HD2	3:H:100(C):TYR:CZ	2.39	0.57
3:H:72:ASP:OD2	3:H:77:GLN:O	2.22	0.56
3:H:95:VAL:CB	3:H:96:PRO:HA	2.30	0.56
3:H:189:LEU:HA	3:H:192:GLN:NE2	2.17	0.56
1:G:260:LEU:HD21	1:G:453:LEU:HD11	1.87	0.55
3:H:72:ASP:O	3:H:73:THR:C	2.45	0.55
3:H:29:ILE:CB	3:H:30:SER:HB2	2.36	0.55
3:H:52:TYR:O	3:H:54:ILE:O	2.24	0.55
3:H:29:ILE:HG22	3:H:30:SER:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:13:LYS:O	3:H:16:GLN:HB2	2.07	0.55
1:G:64:GLU:OE1	1:G:66:HIS:N	2.40	0.54
4:L:38:GLN:O	4:L:39:HIS:HB2	2.07	0.54
1:G:102:GLU:O	1:G:106:GLU:HG3	2.08	0.54
4:L:60:ASN:HD22	4:L:60:ASN:N	2.06	0.54
1:G:102:GLU:OE1	1:G:102:GLU:N	2.41	0.54
1:G:254:VAL:HG11	1:G:261:LEU:HB2	1.89	0.54
1:G:396:ILE:O	1:G:408:LYS:N	2.41	0.54
3:H:28:SER:O	3:H:29:ILE:CG1	2.55	0.53
4:L:47:MET:HE2	4:L:58:VAL:HG13	1.91	0.53
1:G:439:ILE:HD12	1:G:439:ILE:N	2.22	0.53
3:H:97:ARG:O	3:H:97:ARG:HG2	2.08	0.53
3:H:155:ASN:O	3:H:157:GLY:N	2.42	0.53
1:G:44:VAL:HG23	1:G:45:TRP:CE3	2.43	0.52
1:G:112:TRP:O	1:G:114:GLN:N	2.41	0.52
4:L:158:GLY:HA3	4:L:159:VAL:CG2	2.37	0.52
1:G:384:TYR:OH	1:G:424:ILE:HG22	2.10	0.52
1:G:342:LEU:O	1:G:346:THR:HG23	2.10	0.52
1:G:457:ASP:OD1	1:G:467:THR:HB	2.09	0.52
1:G:346:THR:OG1	1:G:347:GLU:N	2.44	0.52
1:G:298:ARG:NH2	1:G:439:ILE:O	2.38	0.52
4:L:14:SER:O	4:L:17:GLN:CB	2.58	0.52
1:G:343:LYS:O	1:G:347:GLU:HG3	2.11	0.51
1:G:264:SER:OG	1:G:482:GLU:CD	2.49	0.51
1:G:72:HIS:O	1:G:73:ALA:CB	2.58	0.51
1:G:370:GLU:O	1:G:375:SER:OG	2.28	0.51
1:G:279:ASN:O	1:G:281:ALA:N	2.43	0.51
1:G:65:VAL:HB	1:G:115:SER:HB3	1.93	0.51
3:H:22:CYS:O	3:H:77:GLN:HB2	2.11	0.51
3:H:11:LEU:HD13	3:H:147:PRO:HG3	1.93	0.51
4:L:157:ALA:HB1	4:L:158:GLY:C	2.32	0.50
1:G:298:ARG:HG2	1:G:329:ALA:HB2	1.94	0.50
1:G:330:TYR:HA	1:G:417:PRO:O	2.12	0.49
1:G:263:GLY:H	1:G:450:THR:HG21	1.75	0.49
3:H:100(A):GLY:HA2	4:L:50:GLU:HG3	1.93	0.49
4:L:119:PRO:HB3	4:L:206:VAL:HG11	1.94	0.49
4:L:145:THR:HG22	4:L:196:THR:OG1	2.12	0.49
3:H:18:LEU:CD1	3:H:109:VAL:HG11	2.43	0.49
4:L:155:VAL:O	4:L:156:LYS:HB3	2.12	0.49
3:H:162:GLY:O	3:H:182:VAL:HG13	2.13	0.48
1:G:221:ALA:HB2	3:H:31:SER:OG	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:GLU:O	1:G:238:PRO:HA	2.14	0.48
3:H:72:ASP:O	3:H:75:GLN:O	2.30	0.48
3:H:30:SER:HB3	3:H:31:SER:CB	2.43	0.48
4:L:11:VAL:HG23	4:L:104:LEU:HD12	1.96	0.48
1:G:461:ASN:N	1:G:462:ASN:HA	2.28	0.48
1:G:230:ASP:OD2	1:G:239:CYS:O	2.31	0.48
3:H:18:LEU:C	3:H:18:LEU:HD23	2.34	0.48
3:H:95:VAL:CB	3:H:96:PRO:CA	2.92	0.48
1:G:270:ILE:O	1:G:348:LYS:HE2	2.13	0.48
3:H:6:GLU:N	3:H:6:GLU:OE2	2.46	0.47
1:G:45:TRP:HB2	1:G:490:GLN:O	2.14	0.47
4:L:120:PRO:HD3	4:L:132:LEU:HG	1.97	0.47
4:L:152:SER:HB3	4:L:153:SER:CA	2.45	0.47
1:G:261:LEU:HD12	5:G:503:NAG:H82	1.97	0.47
4:L:125:LEU:C	4:L:127:ALA:H	2.19	0.46
1:G:350:LYS:CG	1:G:355:ASN:HA	2.45	0.46
1:G:350:LYS:HG2	1:G:355:ASN:HA	1.98	0.46
1:G:463:THR:O	1:G:464:SER:CB	2.63	0.46
3:H:61:PRO:HA	3:H:64:LYS:HD2	1.97	0.46
3:H:58:TYR:N	3:H:58:TYR:CD2	2.83	0.46
1:G:110:SER:O	1:G:114:GLN:HB3	2.15	0.46
1:G:460:ALA:HB1	1:G:462:ASN:HA	1.98	0.45
3:H:38:ARG:CD	3:H:48:ILE:HD11	2.46	0.45
1:G:223:TYR:N	1:G:223:TYR:CD1	2.85	0.45
2:N:8:LEU:HD23	2:N:8:LEU:C	2.36	0.45
4:L:121:SER:O	4:L:123:GLU:N	2.49	0.45
4:L:40:PRO:HA	4:L:41:ASP:HA	1.78	0.45
1:G:333:ILE:HD12	1:G:390:LEU:HD11	1.97	0.45
4:L:20:THR:HA	4:L:73:LEU:O	2.16	0.45
1:G:286:VAL:CG2	1:G:452:ILE:HG12	2.46	0.45
4:L:27:SER:HA	4:L:28:GLY:HA3	1.99	0.45
3:H:30:SER:CB	3:H:31:SER:CB	2.95	0.45
1:G:460:ALA:CA	1:G:461:ASN:CB	2.86	0.45
4:L:152:SER:HB3	4:L:153:SER:CB	2.48	0.44
3:H:30:SER:HB3	3:H:31:SER:HB3	2.00	0.44
3:H:37:ILE:HD11	3:H:100(D):PHE:CD1	2.53	0.44
4:L:152:SER:HB3	4:L:153:SER:HA	2.00	0.44
1:G:264:SER:OG	1:G:482:GLU:OE1	2.35	0.43
4:L:169:ASN:O	4:L:171:LYS:N	2.51	0.43
1:G:258:GLN:NE2	1:G:387:THR:HG21	2.33	0.43
4:L:130:ALA:O	4:L:131:THR:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:490:GLN:HE21	1:G:492:GLU:HG3	1.83	0.43
2:N:3:LEU:O	2:N:6:CYS:N	2.51	0.43
3:H:53:TYR:C	3:H:53:TYR:CD1	2.91	0.43
4:L:27(C):VAL:O	4:L:66:LYS:CE	2.64	0.43
4:L:159:VAL:CG1	4:L:159:VAL:O	2.61	0.43
1:G:83:GLU:HG3	1:G:245:VAL:HG13	2.00	0.43
1:G:463:THR:O	1:G:464:SER:HB2	2.19	0.43
1:G:82:GLN:O	1:G:246:GLN:NE2	2.51	0.43
1:G:340:LYS:O	1:G:344:GLN:HB2	2.18	0.43
3:H:73:THR:O	3:H:76:ASN:N	2.52	0.43
1:G:207:LYS:HE2	1:G:439:ILE:HD11	2.00	0.43
3:H:54:ILE:HG22	3:H:55:GLY:N	2.30	0.43
3:H:38:ARG:HD2	3:H:48:ILE:HD11	2.01	0.43
1:G:107:ASP:OD1	3:H:99:ARG:NH1	2.51	0.43
4:L:34:SER:HB2	4:L:36:TYR:CE1	2.53	0.43
1:G:121:LYS:O	1:G:122:LEU:HD23	2.19	0.43
1:G:262:ASN:OD1	5:G:503:NAG:C5	2.65	0.42
3:H:73:THR:C	3:H:74:THR:HG1	2.09	0.42
3:H:116:THR:HG22	3:H:147:PRO:HD3	2.01	0.42
3:H:24:VAL:O	3:H:25:SER:CB	2.67	0.42
4:L:94:SER:HA	4:L:95:SER:CB	2.47	0.42
1:G:211:ASP:OD1	1:G:212:PRO:HD2	2.19	0.42
3:H:82(A):THR:O	3:H:82(B):SER:O	2.36	0.42
1:G:219:THR:HG23	1:G:225:ILE:CG1	2.49	0.42
4:L:83:GLU:OE1	4:L:170:ASN:ND2	2.52	0.42
3:H:3:GLN:N	3:H:3:GLN:OE1	2.52	0.42
1:G:331:CYS:SG	1:G:385:CYS:SG	3.17	0.42
4:L:66:LYS:HA	4:L:71:ALA:HA	2.00	0.42
3:H:184:VAL:HG11	3:H:194:TYR:CZ	2.55	0.42
3:H:72:ASP:C	3:H:75:GLN:O	2.58	0.42
3:H:201:LYS:N	3:H:202:PRO:CD	2.83	0.42
1:G:229:ASN:OD1	1:G:243:SER:HB2	2.19	0.42
1:G:264:SER:O	1:G:450:THR:HB	2.19	0.42
4:L:60:ASN:ND2	4:L:60:ASN:N	2.67	0.42
4:L:136:ILE:HD12	4:L:136:ILE:H	1.85	0.42
3:H:73:THR:OG1	3:H:73:THR:O	2.24	0.41
3:H:36:TRP:C	3:H:37:ILE:HG13	2.40	0.41
2:N:26:CYS:O	2:N:27:VAL:HG13	2.19	0.41
4:L:124:GLU:OE1	4:L:130:ALA:O	2.38	0.41
1:G:107:ASP:OD2	3:H:99:ARG:HD2	2.19	0.41
1:G:66:HIS:CG	1:G:212:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:ILE:CD1	1:G:483:LEU:CD1	2.99	0.41
1:G:345:VAL:HG12	1:G:346:THR:H	1.85	0.41
4:L:46:LEU:C	4:L:47:MET:HG2	2.41	0.41
3:H:159:LEU:C	3:H:161:SER:OG	2.59	0.41
3:H:203:SER:O	3:H:204:ASN:C	2.60	0.41
1:G:107:ASP:CG	3:H:99:ARG:HH11	2.24	0.41
1:G:477:ASP:OD1	1:G:480:ARG:NH1	2.53	0.41
3:H:95:VAL:HG12	3:H:96:PRO:C	2.40	0.41
1:G:384:TYR:OH	1:G:424:ILE:CG2	2.68	0.41
4:L:143:ALA:HB2	4:L:164:PRO:HG2	2.03	0.41
3:H:148:GLU:HG2	3:H:149:PRO:CA	2.49	0.40
1:G:64:GLU:OE1	1:G:66:HIS:HB2	2.21	0.40
3:H:203:SER:O	3:H:205:THR:OG1	2.33	0.40
3:H:18:LEU:HD11	3:H:109:VAL:HG11	2.01	0.40
1:G:64:GLU:O	1:G:68:VAL:HG23	2.20	0.40
3:H:98:LEU:HA	3:H:98:LEU:HD23	1.98	0.40
3:H:148:GLU:HG3	3:H:149:PRO:HA	2.00	0.40
1:G:390:LEU:CD1	1:G:416:LEU:HD11	2.52	0.40
4:L:142:GLY:HA2	4:L:143:ALA:HA	1.91	0.40
3:H:24:VAL:O	3:H:25:SER:HB2	2.21	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	G	328/353 (93%)	271 (83%)	29 (9%)	28 (8%)	1 6
2	N	24/28 (86%)	20 (83%)	3 (12%)	1 (4%)	3 26
3	H	210/229 (92%)	160 (76%)	25 (12%)	25 (12%)	0 3
4	L	210/221 (95%)	164 (78%)	31 (15%)	15 (7%)	1 10
All	All	772/831 (93%)	615 (80%)	88 (11%)	69 (9%)	1 5

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	87	GLU
1	G	114	GLN
1	G	121	LYS
1	G	235	GLY
1	G	345	VAL
1	G	346	THR
1	G	438	PRO
1	G	440	ASP
1	G	459	GLY
1	G	464	SER
2	N	27	VAL
3	H	27	ALA
3	H	28	SER
3	H	29	ILE
3	H	30	SER
3	H	82(B)	SER
3	H	100(A)	GLY
3	H	100(D)	PHE
3	H	156	SER
3	H	204	ASN
4	L	51	VAL
4	L	128	ASN
4	L	170	ASN
1	G	120	VAL
1	G	280	ASN
1	G	393	ASN
1	G	417	PRO
1	G	461	ASN
3	H	24	VAL
3	H	25	SER
3	H	73	THR
3	H	77	GLN
3	H	98	LEU
3	H	193	THR
4	L	4	LEU
4	L	81	GLU
4	L	122	SER
4	L	126	GLN
4	L	151	ASP
4	L	156	LYS
1	G	231	LYS
1	G	264	SER

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Mol	Chain	Res	Type
1	G	269	GLU
1	G	395	CYS
3	H	26	GLY
3	H	95	VAL
3	H	192	GLN
1	G	113	ASP
1	G	410	CYS
1	G	470	PRO
3	H	155	ASN
3	H	161	SER
3	H	173	SER
4	L	2	SER
4	L	39	HIS
4	L	50	GLU
4	L	131	THR
1	G	73	ALA
1	G	418	CYS
1	G	463	THR
3	H	144	ASP
4	L	169	ASN
1	G	204	ALA
1	G	374	HIS
3	H	2	VAL
3	H	54	ILE
4	L	153	SER
1	G	220	PRO
3	H	149	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	G	302/311 (97%)	270 (89%)	32 (11%)	8 34
2	N	20/20 (100%)	18 (90%)	2 (10%)	9 37
3	H	184/197 (93%)	158 (86%)	26 (14%)	4 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	L	180/188 (96%)	160 (89%)	20 (11%)	8 32
All	All	686/716 (96%)	606 (88%)	80 (12%)	7 30

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	61	HIS
1	G	83	GLU
1	G	87	GLU
1	G	97	LYS
1	G	119	CYS
1	G	202	LYS
1	G	209	SER
1	G	218	CYS
1	G	243	SER
1	G	245	VAL
1	G	247	CYS
1	G	262	ASN
1	G	264	SER
1	G	265	LEU
1	G	273	ARG
1	G	301	ASN
1	G	358	THR
1	G	375	SER
1	G	378	CYS
1	G	379	ARG
1	G	389	GLN
1	G	395	CYS
1	G	418	CYS
1	G	439	ILE
1	G	446	VAL
1	G	452	ILE
1	G	465	ASN
1	G	467	THR
1	G	469	ARG
1	G	470	PRO
1	G	483	LEU
1	G	489	VAL
2	N	8	LEU
2	N	27	VAL
3	H	1	GLU
3	H	19	SER

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Mol	Chain	Res	Type
3	H	23	THR
3	H	24	VAL
3	H	31	SER
3	H	38	ARG
3	H	45	LEU
3	H	63	LEU
3	H	68	THR
3	H	70	SER
3	H	71	VAL
3	H	72	ASP
3	H	75	GLN
3	H	79	SER
3	H	82(B)	SER
3	H	92	CYS
3	H	113	SER
3	H	116	THR
3	H	140	CYS
3	H	143	LYS
3	H	156	SER
3	H	170	LEU
3	H	175	LEU
3	H	192	GLN
3	H	204	ASN
3	H	208	ASP
4	L	18	SER
4	L	20	THR
4	L	22	SER
4	L	27(B)	ASP
4	L	34	SER
4	L	38	GLN
4	L	47	MET
4	L	60	ASN
4	L	76	SER
4	L	78	LEU
4	L	97	VAL
4	L	145	THR
4	L	153	SER
4	L	156	LYS
4	L	159	VAL
4	L	161	THR
4	L	162	THR
4	L	167	GLN

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Mol	Chain	Res	Type
4	L	175	SER
4	L	203	GLU

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

Mol	Chain	Res	Type
1	G	258	GLN
1	G	280	ASN
1	G	465	ASN
1	G	490	GLN
3	H	171	GLN
4	L	60	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	DPR	N	21	2	5,7,8	0.58	0	7,8,10	1.66	2 (28%)
2	U2X	N	23	2	18,20,21	0.32	0	23,25,27	0.96	1 (4%)

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
2	DPR	N	21	2	-	0/0/9/11	0/1/1/1
2	U2X	N	23	2	-	0/9/19/21	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	23	U2X	O-C-CA	-2.93	117.86	125.72
2	N	21	DPR	O-C-CA	-2.24	119.57	125.69
2	N	21	DPR	CD-N-CA	2.88	114.27	107.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
5	NAG	G	501	1	14,14,15	0.48	0	15,19,21	1.13	0
5	NAG	G	502	1	14,14,15	0.55	0	15,19,21	1.08	1 (6%)
5	NAG	G	503	1	14,14,15	0.98	1 (7%)	15,19,21	2.56	2 (13%)
5	NAG	G	504	1	14,14,15	0.58	0	15,19,21	1.43	2 (13%)
5	NAG	G	505	1	14,14,15	0.49	0	15,19,21	2.22	4 (26%)
5	NAG	G	506	1	14,14,15	0.58	0	15,19,21	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	G	507	1	14,14,15	0.55	0	15,19,21	0.83	0
5	NAG	G	508	1	14,14,15	0.60	0	15,19,21	0.70	0
5	NAG	G	509	1	14,14,15	0.77	1 (7%)	15,19,21	1.31	3 (20%)

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
5	NAG	G	501	1	-	0/6/23/26	0/1/1/1
5	NAG	G	502	1	-	0/6/23/26	0/1/1/1
5	NAG	G	503	1	-	0/6/23/26	0/1/1/1
5	NAG	G	504	1	-	0/6/23/26	0/1/1/1
5	NAG	G	505	1	-	0/6/23/26	0/1/1/1
5	NAG	G	506	1	-	0/6/23/26	0/1/1/1
5	NAG	G	507	1	-	0/6/23/26	0/1/1/1
5	NAG	G	508	1	-	0/6/23/26	0/1/1/1
5	NAG	G	509	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	509	NAG	C1-C2	2.37	1.55	1.52
5	G	503	NAG	C1-C2	2.79	1.56	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	503	NAG	C3-C4-C5	-2.96	104.96	110.23
5	G	505	NAG	C4-C3-C2	-2.22	107.89	111.34
5	G	502	NAG	O7-C7-C8	-2.21	118.00	122.07
5	G	509	NAG	C3-C4-C5	2.14	114.05	110.23
5	G	505	NAG	C1-O5-C5	2.17	115.33	112.14
5	G	509	NAG	C4-C3-C2	2.25	114.83	111.34
5	G	504	NAG	C1-O5-C5	2.27	115.48	112.14
5	G	509	NAG	C1-O5-C5	2.76	116.20	112.14
5	G	505	NAG	C8-C7-N2	3.62	123.03	116.10
5	G	504	NAG	C4-C3-C2	4.25	117.93	111.34
5	G	505	NAG	C2-N2-C7	6.16	131.12	123.11
5	G	503	NAG	C1-O5-C5	9.01	125.39	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	503	NAG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	G	336/353 (95%)	-0.48	2 (0%) 90 84	61, 105, 180, 200	0
2	N	24/28 (85%)	-0.66	0 100 100	84, 97, 102, 119	0
3	H	214/229 (93%)	-0.35	7 (3%) 50 35	66, 116, 171, 210	0
4	L	212/221 (95%)	-0.30	6 (2%) 56 42	76, 136, 179, 210	0
All	All	786/831 (94%)	-0.40	15 (1%) 70 55	61, 113, 179, 210	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	31	SER	4.2
1	G	123	THR	3.6
4	L	144	VAL	3.5
4	L	142	GLY	3.4
3	H	127	SER	3.3
3	H	158	ALA	2.8
3	H	192	GLN	2.7
3	H	191	THR	2.7
4	L	154	PRO	2.5
1	G	461	ASN	2.3
3	H	128	SER	2.1
3	H	174	GLY	2.1
4	L	155	VAL	2.1
4	L	156	LYS	2.1
4	L	143	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
2	DPR	N	21	7/8	0.93	0.23	-	87,89,93,95	0
2	U2X	N	23	19/20	0.98	0.21	-	78,79,86,86	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	G	507	14/15	0.93	0.32	3.37	114,121,127,131	0
5	NAG	G	503	14/15	0.91	0.21	0.13	76,94,101,104	0
5	NAG	G	506	14/15	0.93	0.16	-0.24	100,115,122,126	0
5	NAG	G	501	14/15	0.94	0.11	-1.01	99,109,124,125	0
5	NAG	G	505	14/15	0.93	0.14	-1.38	100,112,121,122	0
5	NAG	G	502	14/15	0.91	0.26	-	116,120,129,143	0
5	NAG	G	508	14/15	0.92	0.16	-	113,118,126,134	0
5	NAG	G	504	14/15	0.91	0.14	-	113,125,129,130	0
5	NAG	G	509	14/15	0.89	0.27	-	145,157,162,167	0

6.5 Other polymers (i)

There are no such residues in this entry.