



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2021 – 04:27 PM EDT

PDB ID : 4RFN
Title : Crystal structure of ADCC-potent Rhesus macaque ANTIBODY JR4 in complex with HIV-1 CLADE A/E GP120 and M48
Authors : Gohain, N.; Tolbert, W.D.; Pazgier, M.
Deposited on : 2014-09-26
Resolution : 3.21 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:

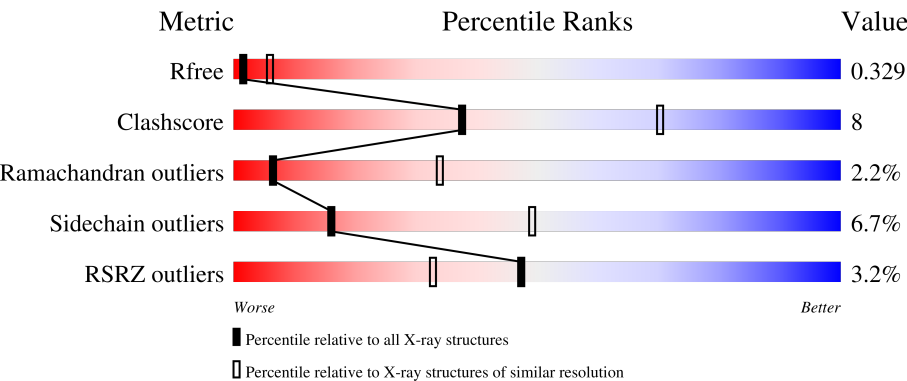
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

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 3.21 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.




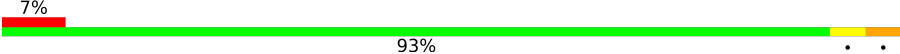

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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	353	<div><div>5%</div><div><div></div><div>75%</div><div>18%</div><div>• 5%</div></div></div>
1	G	353	<div><div>6%</div><div><div></div><div>77%</div><div>17%</div><div>• 5%</div></div></div>
2	B	233	<div><div>2%</div><div><div></div><div>67%</div><div>22%</div><div>• 7%</div></div></div>
2	H	233	<div><div>3%</div><div><div></div><div>63%</div><div>25%</div><div>• • 7%</div></div></div>
3	C	216	<div><div></div><div><div></div><div>81%</div><div>16%</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
3	L	216	
4	D	28	
4	M	28	

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
5	NAG	A	507	-	-	-	X
5	NAG	G	508	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12338 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 93TH057 (H375S) GP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	337	Total	C	N	O	S	0	0	0
			2648	1664	458	504	22			
1	A	337	Total	C	N	O	S	0	0	0
			2648	1664	458	504	22			

- Molecule 2 is a protein called FAB HEAVY CHAIN OF ADCC ANTI-HIV-1 ANTIBODY JR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1641	1043	273	321	4			
2	B	217	Total	C	N	O	S	0	0	0
			1641	1043	273	321	4			

- Molecule 3 is a protein called FAB LIGHT CHAIN OF ADCC ANTI-HIV-1 ANTIBODY JR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1553	972	261	316	4			
3	C	210	Total	C	N	O	S	0	0	0
			1553	972	261	316	4			

- Molecule 4 is a protein called T-CELL SURFACE GLYCOPROTEIN CD4 mimetic M48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	28	Total	C	N	O	S	0	0	1
			201	126	38	31	6			
4	D	28	Total	C	N	O	S	0	0	1
			201	126	38	31	6			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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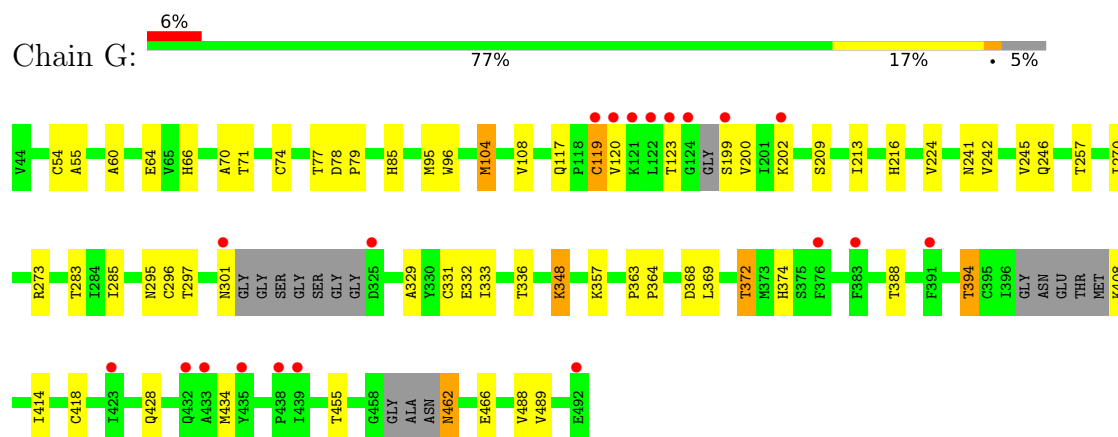
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

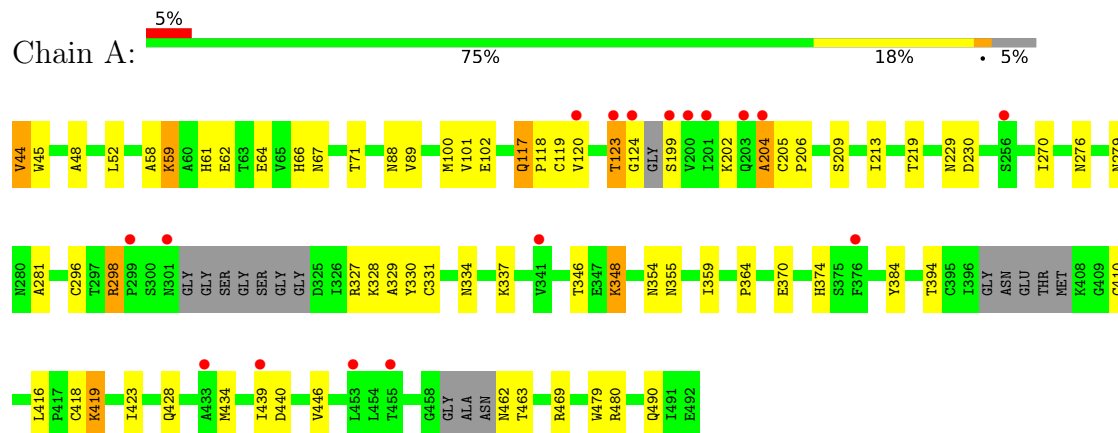
3 Residue-property plots [i](#)

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

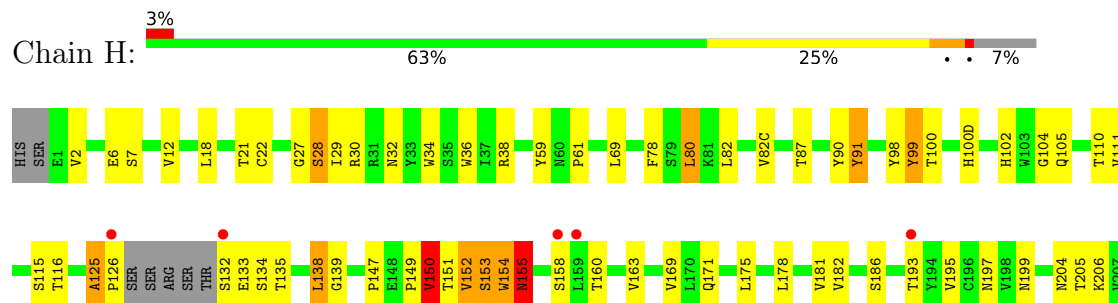
- Molecule 1: HIV-1 CLADE A/E 93TH057 (H375S) GP120

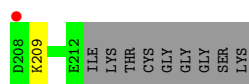


- Molecule 1: HIV-1 CLADE A/E 93TH057 (H375S) GP120



- Molecule 2: FAB HEAVY CHAIN OF ADCC ANTI-HIV-1 ANTIBODY JR4

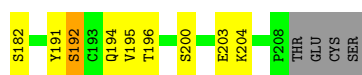
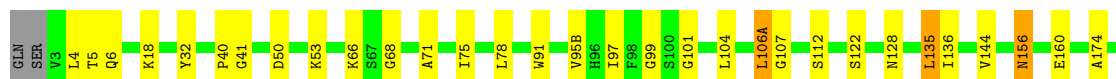
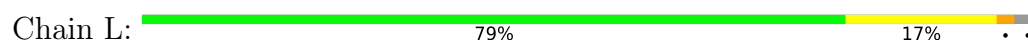




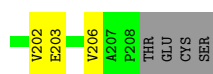
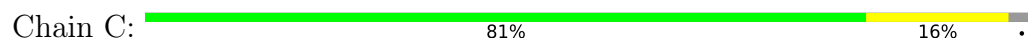
- Molecule 2: FAB HEAVY CHAIN OF ADCC ANTI-HIV-1 ANTIBODY JR4



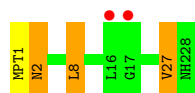
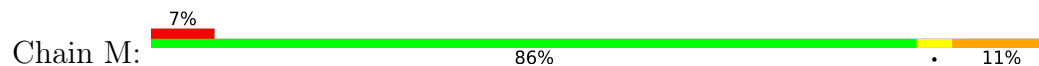
- Molecule 3: FAB LIGHT CHAIN OF ADCC ANTI-HIV-1 ANTIBODY JR4



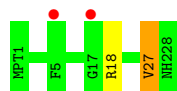
- Molecule 3: FAB LIGHT CHAIN OF ADCC ANTI-HIV-1 ANTIBODY JR4



- Molecule 4: T-CELL SURFACE GLYCOPROTEIN CD4 mimetic M48



- Molecule 4: T-CELL SURFACE GLYCOPROTEIN CD4 mimetic M48



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.25Å 77.83Å 127.59Å 90.00° 114.26° 90.00°	Depositor
Resolution (Å)	45.00 – 3.21 44.98 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.00-3.21) 93.3 (44.98-3.11)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.273 , 0.332 0.271 , 0.329	Depositor DCC
R_{free} test set	1790 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	69.8	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.126 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12338	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, DPR, MPT, 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	A	0.34	0/2701	0.50	0/3663
1	G	0.34	0/2701	0.52	0/3663
2	B	0.47	0/1686	0.67	0/2309
2	H	0.48	0/1686	0.67	1/2309 (0.0%)
3	C	0.37	0/1589	0.51	0/2167
3	L	0.38	0/1589	0.51	0/2167
4	D	0.38	0/189	0.61	0/250
4	M	0.47	0/189	0.68	0/250
All	All	0.39	0/12330	0.56	1/16778 (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
4	M	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	125	ALA	C-N-CD	-5.38	108.77	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	M	1	MPT	Mainchain

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Mol	Chain	Res	Type	Group
4	M	2	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2648	0	2582	33	0
1	G	2648	0	2581	30	0
2	B	1641	0	1602	39	0
2	H	1641	0	1602	49	0
3	C	1553	0	1517	22	0
3	L	1553	0	1517	25	0
4	D	201	0	201	1	0
4	M	201	0	201	2	0
5	A	126	0	117	4	0
5	G	126	0	117	0	0
All	All	12338	0	12037	187	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ALA:HB1	2:B:126:PRO:HD2	1.29	1.14
2:B:125:ALA:HB1	2:B:126:PRO:CD	1.88	1.04
2:H:135:THR:HA	2:H:186:SER:OG	1.85	0.75
2:H:126:PRO:HD3	2:H:138:LEU:HD23	1.69	0.74
2:H:125:ALA:HB1	2:H:126:PRO:HD2	1.70	0.73
1:G:64:GLU:OE1	1:G:66:HIS:HB2	1.88	0.72
3:L:32:TYR:HB3	3:L:50:ASP:HA	1.70	0.71
2:H:125:ALA:CB	2:H:126:PRO:HD2	2.18	0.69
3:L:128:ASN:HA	3:L:182:SER:HB3	1.74	0.69
2:H:2:VAL:HB	2:H:102:HIS:CE1	2.29	0.67
1:A:229:ASN:HB3	5:A:502:NAG:H5	1.79	0.64
2:B:155:ASN:OD1	2:B:194:TYR:HA	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:270:ILE:O	1:G:348:LYS:HD3	1.97	0.63
1:G:55:ALA:HB1	1:G:77:THR:HA	1.80	0.63
1:G:199:SER:HB2	1:G:200:VAL:HG23	1.81	0.62
2:H:2:VAL:HB	2:H:102:HIS:ND1	2.15	0.62
2:B:132:SER:HB2	3:C:116:THR:HG23	1.82	0.61
1:G:70:ALA:O	1:G:74:CYS:HB2	2.01	0.61
2:H:126:PRO:HD3	2:H:138:LEU:CD2	2.31	0.61
2:B:125:ALA:CB	2:B:126:PRO:CD	2.71	0.60
2:H:155:ASN:C	2:H:155:ASN:HD22	2.06	0.59
2:B:153:SER:O	2:B:197:ASN:N	2.34	0.59
1:G:55:ALA:HB3	1:G:216:HIS:HB2	1.83	0.59
1:G:257:THR:O	1:G:374:HIS:HD2	1.87	0.58
1:G:60:ALA:HA	1:G:71:THR:HG21	1.84	0.58
2:B:155:ASN:CG	2:B:194:TYR:HA	2.23	0.58
2:B:155:ASN:C	2:B:157:GLY:N	2.56	0.58
2:H:154:TRP:HA	2:H:195:VAL:O	2.04	0.57
1:G:66:HIS:HB3	1:G:213:ILE:HG12	1.84	0.57
3:L:50:ASP:HB2	3:L:53:LYS:HD2	1.86	0.57
1:G:295:ASN:HB3	1:G:332:GLU:HB2	1.87	0.57
2:B:124:LEU:O	2:B:125:ALA:O	2.23	0.57
3:L:196:THR:HA	3:L:200:SER:O	2.05	0.56
3:C:149:LYS:HB2	3:C:192:SER:HB2	1.88	0.56
1:G:364:PRO:HB2	1:G:372:THR:HG22	1.88	0.56
1:A:120:VAL:HB	1:A:434:MET:HB3	1.86	0.56
2:B:154:TRP:O	2:B:157:GLY:C	2.44	0.56
2:H:151:THR:OG1	2:H:199:ASN:HB2	2.05	0.56
2:H:154:TRP:CD1	2:H:154:TRP:N	2.73	0.55
2:B:36:TRP:HB3	2:B:48:ILE:HD12	1.88	0.55
2:B:100(C):THR:HG22	3:C:32:TYR:CD2	2.41	0.55
3:L:191:TYR:O	3:L:192:SER:CB	2.54	0.55
3:L:4:LEU:HB2	3:L:99:GLY:HA2	1.89	0.55
1:G:119:CYS:O	1:G:202:LYS:HA	2.08	0.54
3:L:192:SER:HA	3:L:204:LYS:O	2.06	0.54
1:A:44:VAL:HB	1:A:45:TRP:CE3	2.41	0.54
1:A:330:TYR:HA	1:A:416:LEU:O	2.07	0.54
2:H:181:VAL:HG21	3:L:135:LEU:HD11	1.88	0.54
2:H:150:VAL:HG21	2:H:178:LEU:HD21	1.88	0.54
3:L:194:GLN:HG2	3:L:203:GLU:HG3	1.88	0.54
1:G:296:CYS:HA	1:G:331:CYS:HA	1.89	0.54
3:L:191:TYR:O	3:L:192:SER:HB2	2.08	0.54
1:A:279:ASN:HB2	5:A:504:NAG:O5	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:THR:HG23	2:H:110:THR:HA	1.91	0.53
2:B:132:SER:OG	2:B:133:GLU:N	2.42	0.53
2:H:152:VAL:O	2:H:153:SER:HB2	2.09	0.52
1:G:295:ASN:O	1:G:332:GLU:N	2.39	0.52
1:A:124:GLY:C	1:A:199:SER:N	2.63	0.52
2:H:155:ASN:CG	2:H:193:THR:O	2.48	0.52
1:A:410:CYS:SG	5:A:509:NAG:H62	2.49	0.52
3:C:92:ASP:HB2	3:C:97:ILE:HD11	1.92	0.52
2:B:133:GLU:HG3	2:B:135:THR:H	1.74	0.51
2:B:154:TRP:O	2:B:158:SER:N	2.44	0.51
2:B:181:VAL:HG21	3:C:135:LEU:HD11	1.93	0.51
1:G:120:VAL:HB	1:G:434:MET:HB3	1.92	0.51
1:A:281:ALA:O	4:D:18:ARG:NH2	2.43	0.51
2:B:163:VAL:HG22	2:B:182:VAL:HG12	1.91	0.51
2:B:93:ALA:HA	2:B:102:HIS:O	2.11	0.50
3:L:6:GLN:HG3	3:L:101:GLY:H	1.77	0.50
1:G:394:THR:HG22	1:G:408:LYS:HE3	1.94	0.50
1:A:229:ASN:HB3	5:A:502:NAG:C5	2.42	0.50
2:B:154:TRP:HA	2:B:195:VAL:O	2.12	0.50
3:L:78:LEU:HD21	3:L:104:LEU:HD21	1.94	0.49
4:M:2:ASN:OD1	4:M:2:ASN:C	2.50	0.49
3:C:15:PRO:HD3	3:C:106(A):LEU:O	2.12	0.49
1:A:204:ALA:O	1:A:206:PRO:HD3	2.12	0.49
2:B:154:TRP:CD1	2:B:154:TRP:N	2.80	0.49
1:G:54:CYS:O	1:G:74:CYS:HB3	2.13	0.49
1:A:298:ARG:HB2	1:A:329:ALA:HB2	1.95	0.49
2:B:50:HIS:C	2:B:50:HIS:CD2	2.85	0.49
1:G:273:ARG:HB2	1:G:285:ILE:HB	1.95	0.48
2:H:36:TRP:CD1	2:H:69:LEU:HD22	2.48	0.48
1:G:363:PRO:HG3	1:G:388:THR:HG23	1.95	0.48
2:H:169:VAL:HG21	3:L:160:GLU:HB3	1.96	0.48
2:H:18:LEU:HB3	2:H:82:LEU:HB3	1.96	0.48
2:H:36:TRP:HD1	2:H:69:LEU:HD22	1.79	0.48
1:A:66:HIS:HB3	1:A:213:ILE:HG12	1.94	0.48
2:H:22:CYS:HB3	2:H:78:PHE:O	2.14	0.48
2:H:153:SER:HA	2:H:154:TRP:CD1	2.48	0.48
2:B:40:PRO:HB2	2:B:43:LYS:HB2	1.96	0.48
2:B:151:THR:O	2:B:152:VAL:HG13	2.14	0.48
2:H:36:TRP:CD2	2:H:80:LEU:HD23	2.49	0.48
2:H:139:GLY:HA2	2:H:154:TRP:CZ3	2.49	0.47
2:B:184:VAL:HG11	2:B:194:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:18:LYS:HA	3:L:75:ILE:O	2.14	0.47
2:B:152:VAL:HG11	2:B:180:SER:CB	2.44	0.47
1:G:85:HIS:NE2	1:G:241:ASN:OD1	2.45	0.47
2:H:27:GLY:O	2:H:29:ILE:N	2.48	0.47
2:H:155:ASN:C	2:H:158:SER:H	2.18	0.47
2:B:154:TRP:O	2:B:155:ASN:HB2	2.15	0.47
3:L:136:ILE:HB	3:L:174:ALA:HB3	1.96	0.46
1:A:117:GLN:HA	1:A:118:PRO:HD3	1.81	0.46
2:H:6:GLU:HG2	2:H:91:TYR:HA	1.97	0.46
1:A:334:ASN:HB3	1:A:337:LYS:HB2	1.98	0.46
2:B:33:TYR:CZ	2:B:97:TRP:HD1	2.33	0.46
3:L:4:LEU:HG	3:L:97:ILE:HG22	1.97	0.46
3:C:23:CYS:HB3	3:C:71:ALA:HB3	1.96	0.46
2:H:126:PRO:CD	2:H:138:LEU:HD23	2.43	0.46
3:L:66:LYS:HA	3:L:71:ALA:HA	1.98	0.46
2:H:163:VAL:HG22	2:H:182:VAL:HG12	1.97	0.46
2:H:7:SER:HB2	2:H:21:THR:HB	1.98	0.46
2:B:42:GLY:HA3	3:C:163:THR:HG21	1.98	0.46
1:A:346:THR:HG23	1:A:359:ILE:HB	1.98	0.45
2:B:155:ASN:C	2:B:157:GLY:H	2.17	0.45
1:G:462:ASN:HD22	1:G:462:ASN:N	2.13	0.45
3:L:40:PRO:HA	3:L:41:GLY:HA2	1.63	0.45
2:H:100(D):HIS:HB2	3:L:91:TRP:HB2	1.98	0.45
2:H:133:GLU:HG3	2:H:134:SER:N	2.32	0.45
2:H:195:VAL:HA	2:H:209:LYS:O	2.17	0.45
1:A:296:CYS:HA	1:A:331:CYS:HA	1.97	0.45
2:H:12:VAL:O	2:H:111:VAL:HA	2.17	0.45
1:A:52:LEU:HD11	1:A:100:MET:HG2	1.98	0.45
1:G:64:GLU:HA	1:G:209:SER:HB3	1.98	0.45
1:A:59:LYS:HB3	1:A:61:HIS:CD2	2.52	0.45
3:C:106(A):LEU:HA	3:C:107:GLY:HA3	1.72	0.45
1:A:329:ALA:N	1:A:418:CYS:O	2.49	0.45
2:H:169:VAL:HG13	2:H:169:VAL:O	2.17	0.44
2:B:84:ALA:HA	2:B:111:VAL:HB	1.99	0.44
2:B:100(C):THR:HA	3:C:32:TYR:HB2	1.98	0.44
2:B:100(D):HIS:HB3	3:C:91:TRP:HB2	1.99	0.44
2:H:38:ARG:HB3	2:H:90:TYR:CE1	2.53	0.44
2:H:59:TYR:HE1	2:H:69:LEU:HG	1.81	0.44
3:C:116:THR:HB	3:C:135:LEU:HB3	1.98	0.44
2:H:98:TYR:O	2:H:100:THR:N	2.51	0.44
1:A:327:ARG:O	1:A:419:LYS:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:PRO:HD2	2:B:113:SER:HB3	2.00	0.44
2:B:159:LEU:HD23	2:B:182:VAL:HG11	1.99	0.44
3:C:156:ASN:N	3:C:156:ASN:OD1	2.50	0.44
3:C:40:PRO:HA	3:C:41:GLY:HA2	1.75	0.44
2:H:150:VAL:CG2	2:H:178:LEU:HD21	2.47	0.44
1:G:104:MET:O	1:G:108:VAL:HG23	2.18	0.43
3:C:25:GLY:O	3:C:69:SER:HB3	2.18	0.43
3:C:106(A):LEU:HD23	3:C:140:TYR:HE2	1.82	0.43
2:H:61:PRO:HD2	3:L:95(B):VAL:CG1	2.48	0.43
2:H:6:GLU:OE1	2:H:104:GLY:HA3	2.18	0.43
2:H:155:ASN:N	2:H:195:VAL:H	2.16	0.43
2:H:126:PRO:HA	2:H:132:SER:N	2.34	0.43
1:A:423:ILE:HA	1:A:434:MET:HA	2.01	0.43
2:B:100(D):HIS:CD2	3:C:91:TRP:CE3	3.06	0.43
3:C:4:LEU:HB2	3:C:99:GLY:HA2	2.00	0.43
1:G:357:LYS:HD3	1:G:466:GLU:HG2	2.01	0.43
2:B:166:PHE:HE1	3:C:135:LEU:HD21	1.84	0.43
1:G:329:ALA:HB3	1:G:418:CYS:HB2	2.01	0.42
1:A:270:ILE:O	1:A:348:LYS:HD3	2.19	0.42
1:A:101:VAL:HG21	1:A:480:ARG:HG2	2.00	0.42
3:C:83:GLU:HB2	3:C:106:VAL:HG23	2.02	0.42
2:H:29:ILE:HA	2:H:34:TRP:CZ2	2.54	0.42
1:A:62:GLU:HG3	1:A:64:GLU:HB3	2.02	0.42
1:A:123:THR:OG1	1:A:124:GLY:N	2.49	0.42
2:B:133:GLU:HG3	2:B:134:SER:N	2.34	0.42
2:B:197:ASN:HA	2:B:207:VAL:O	2.19	0.42
4:M:8:LEU:C	4:M:8:LEU:HD23	2.40	0.42
3:L:128:ASN:CA	3:L:182:SER:HB3	2.46	0.42
1:A:45:TRP:HZ2	1:A:89:VAL:HG11	1.85	0.42
2:H:169:VAL:CG2	3:L:160:GLU:HB3	2.50	0.42
1:A:64:GLU:HA	1:A:209:SER:HB3	2.01	0.42
2:H:27:GLY:C	2:H:29:ILE:H	2.24	0.41
1:A:101:VAL:HG13	1:A:479:TRP:HB2	2.02	0.41
1:G:364:PRO:HG2	1:G:372:THR:HA	2.01	0.41
2:H:171:GLN:N	2:H:175:LEU:O	2.51	0.41
3:L:136:ILE:HG12	3:L:195:VAL:HG21	2.02	0.41
3:L:156:ASN:OD1	3:L:156:ASN:N	2.53	0.41
2:B:100(C):THR:OG1	2:B:100(D):HIS:N	2.50	0.41
3:C:80:THR:HA	3:C:106:VAL:HG11	2.02	0.41
1:G:54:CYS:HA	1:G:216:HIS:O	2.21	0.41
1:G:95:MET:HG3	1:G:96:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:194:GLN:HG2	3:C:203:GLU:HG3	2.02	0.41
1:A:370:GLU:HG3	1:A:384:TYR:CE1	2.55	0.41
1:G:78:ASP:OD2	1:G:79:PRO:HD2	2.21	0.41
1:G:257:THR:O	1:G:374:HIS:CD2	2.71	0.41
2:H:153:SER:H	2:H:197:ASN:H	1.69	0.41
1:A:119:CYS:O	1:A:202:LYS:HA	2.21	0.41
1:A:276:ASN:HB3	1:A:279:ASN:HB3	2.02	0.41
1:A:364:PRO:HA	1:A:469:ARG:HD2	2.03	0.41
2:H:28:SER:O	2:H:32:ASN:ND2	2.53	0.40
1:A:48:ALA:HB3	1:A:490:GLN:HB2	2.04	0.40
3:L:106(A):LEU:HA	3:L:107:GLY:HA3	1.78	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	327/353 (93%)	285 (87%)	35 (11%)	7 (2%)	7	35
1	G	327/353 (93%)	300 (92%)	27 (8%)	0	100	100
2	B	213/233 (91%)	182 (85%)	19 (9%)	12 (6%)	2	13
2	H	213/233 (91%)	187 (88%)	18 (8%)	8 (4%)	3	21
3	C	208/216 (96%)	180 (86%)	25 (12%)	3 (1%)	11	45
3	L	208/216 (96%)	186 (89%)	20 (10%)	2 (1%)	15	52
4	D	25/28 (89%)	23 (92%)	1 (4%)	1 (4%)	3	20
4	M	25/28 (89%)	23 (92%)	1 (4%)	1 (4%)	3	20
All	All	1546/1660 (93%)	1366 (88%)	146 (9%)	34 (2%)	6	34

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	28	SER
2	H	99	TYR
2	H	149	PRO
2	H	153	SER
2	H	155	ASN
3	L	192	SER
4	M	27	VAL
2	B	99	TYR
2	B	125	ALA
2	B	147	PRO
2	B	149	PRO
2	B	155	ASN
1	A	58	ALA
1	A	123	THR
2	B	158	SER
3	C	68	GLY
3	C	78	LEU
4	D	27	VAL
2	H	116	THR
1	A	88	ASN
1	A	374	HIS
3	C	52	ASN
3	L	68	GLY
1	A	354	ASN
2	B	28	SER
2	B	134	SER
2	B	153	SER
2	B	191	THR
1	A	204	ALA
1	A	355	ASN
2	B	204	ASN
2	B	2	VAL
2	H	150	VAL
2	H	147	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	A	304/311 (98%)	284 (93%)	20 (7%)	16	50
1	G	304/311 (98%)	280 (92%)	24 (8%)	12	42
2	B	188/201 (94%)	172 (92%)	16 (8%)	10	38
2	H	188/201 (94%)	172 (92%)	16 (8%)	10	38
3	C	176/182 (97%)	170 (97%)	6 (3%)	37	69
3	L	176/182 (97%)	169 (96%)	7 (4%)	31	65
4	D	21/21 (100%)	20 (95%)	1 (5%)	25	60
4	M	21/21 (100%)	19 (90%)	2 (10%)	8	31
All	All	1378/1430 (96%)	1286 (93%)	92 (7%)	16	49

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	104	MET
1	G	117	GLN
1	G	119	CYS
1	G	123	THR
1	G	224	VAL
1	G	242	VAL
1	G	245	VAL
1	G	246	GLN
1	G	283	THR
1	G	297	THR
1	G	301	ASN
1	G	333	ILE
1	G	336	THR
1	G	348	LYS
1	G	368	ASP
1	G	369	LEU
1	G	372	THR
1	G	394	THR
1	G	414	ILE
1	G	428	GLN
1	G	455	THR
1	G	462	ASN
1	G	488	VAL
1	G	489	VAL
2	H	30	ARG
2	H	80	LEU
2	H	82(C)	VAL

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Mol	Chain	Res	Type
2	H	91	TYR
2	H	99	TYR
2	H	105	GLN
2	H	115	SER
2	H	138	LEU
2	H	150	VAL
2	H	152	VAL
2	H	154	TRP
2	H	155	ASN
2	H	160	THR
2	H	204	ASN
2	H	205	THR
2	H	206	LYS
3	L	5	THR
3	L	106(A)	LEU
3	L	112	SER
3	L	122	SER
3	L	135	LEU
3	L	144	VAL
3	L	156	ASN
4	M	8	LEU
4	M	27	VAL
1	A	44	VAL
1	A	59	LYS
1	A	67	ASN
1	A	71	THR
1	A	102	GLU
1	A	117	GLN
1	A	205	CYS
1	A	219	THR
1	A	230	ASP
1	A	298	ARG
1	A	328	LYS
1	A	348	LYS
1	A	394	THR
1	A	419	LYS
1	A	428	GLN
1	A	439	ILE
1	A	440	ASP
1	A	446	VAL
1	A	462	ASN
1	A	463	THR

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Mol	Chain	Res	Type
2	B	30	ARG
2	B	31	ARG
2	B	50	HIS
2	B	82(A)	THR
2	B	107	VAL
2	B	110	THR
2	B	133	GLU
2	B	152	VAL
2	B	154	TRP
2	B	160	THR
2	B	169	VAL
2	B	196	CYS
2	B	201	LYS
2	B	206	LYS
2	B	208	ASP
2	B	210	ARG
3	C	20	THR
3	C	39	VAL
3	C	135	LEU
3	C	166	LYS
3	C	202	VAL
3	C	206	VAL
4	D	27	VAL

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

Mol	Chain	Res	Type
1	G	117	GLN
1	G	374	HIS
1	G	428	GLN
1	G	432	GLN
2	H	105	GLN
2	H	155	ASN
2	H	197	ASN
1	A	66	HIS
1	A	67	ASN
1	A	411	ASN
1	A	428	GLN
1	A	465	ASN
2	B	102	HIS
3	C	170	ASN
4	D	4	HIS

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.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

18 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	502	1	14,14,15	0.73	0	17,19,21	1.73	6 (35%)
5	NAG	A	503	1	14,14,15	0.57	0	17,19,21	1.21	2 (11%)
5	NAG	A	506	1	14,14,15	0.58	0	17,19,21	1.68	3 (17%)
5	NAG	G	503	1	14,14,15	0.55	0	17,19,21	1.14	1 (5%)
5	NAG	A	508	1	14,14,15	1.05	1 (7%)	17,19,21	1.48	3 (17%)
5	NAG	A	505	1	14,14,15	0.71	0	17,19,21	1.46	3 (17%)
5	NAG	A	509	1	14,14,15	1.89	3 (21%)	17,19,21	2.74	7 (41%)

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	0.49	0	17,19,21	1.80	4 (23%)
5	NAG	G	507	1	14,14,15	0.76	1 (7%)	17,19,21	1.36	2 (11%)
5	NAG	G	506	1	14,14,15	0.54	0	17,19,21	1.16	1 (5%)
5	NAG	G	508	1	14,14,15	0.70	0	17,19,21	1.85	3 (17%)
5	NAG	A	502	1	14,14,15	0.54	0	17,19,21	1.61	4 (23%)
5	NAG	G	505	1	14,14,15	0.51	0	17,19,21	1.44	2 (11%)
5	NAG	A	504	1	14,14,15	0.85	1 (7%)	17,19,21	1.47	1 (5%)
5	NAG	A	501	1	14,14,15	0.53	0	17,19,21	1.23	3 (17%)
5	NAG	A	507	1	14,14,15	0.76	1 (7%)	17,19,21	1.36	2 (11%)
5	NAG	G	509	1	14,14,15	1.67	2 (14%)	17,19,21	2.16	5 (29%)
5	NAG	G	504	1	14,14,15	0.72	0	17,19,21	1.26	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
5	NAG	G	502	1	-	1/6/23/26	0/1/1/1
5	NAG	A	503	1	-	2/6/23/26	0/1/1/1
5	NAG	A	506	1	-	2/6/23/26	0/1/1/1
5	NAG	G	503	1	-	2/6/23/26	0/1/1/1
5	NAG	A	508	1	-	0/6/23/26	0/1/1/1
5	NAG	A	505	1	-	2/6/23/26	0/1/1/1
5	NAG	A	509	1	-	0/6/23/26	0/1/1/1
5	NAG	G	501	1	-	1/6/23/26	0/1/1/1
5	NAG	G	507	1	-	2/6/23/26	0/1/1/1
5	NAG	G	506	1	-	2/6/23/26	0/1/1/1
5	NAG	G	508	1	-	0/6/23/26	0/1/1/1
5	NAG	A	502	1	-	0/6/23/26	0/1/1/1
5	NAG	G	505	1	-	1/6/23/26	0/1/1/1
5	NAG	A	504	1	-	0/6/23/26	0/1/1/1
5	NAG	A	501	1	-	0/6/23/26	0/1/1/1
5	NAG	A	507	1	-	2/6/23/26	0/1/1/1
5	NAG	G	509	1	-	0/6/23/26	0/1/1/1
5	NAG	G	504	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	509	NAG	C1-C2	6.02	1.61	1.52
5	G	509	NAG	C1-C2	5.33	1.60	1.52
5	A	508	NAG	C1-C2	3.16	1.57	1.52
5	A	504	NAG	C1-C2	2.28	1.55	1.52
5	A	507	NAG	C1-C2	2.27	1.55	1.52
5	G	507	NAG	C1-C2	2.17	1.55	1.52
5	A	509	NAG	O5-C1	2.06	1.47	1.43
5	G	509	NAG	C2-N2	2.04	1.49	1.46
5	A	509	NAG	C3-C2	2.04	1.56	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	508	NAG	C1-O5-C5	5.69	119.91	112.19
5	A	509	NAG	C1-O5-C5	5.57	119.74	112.19
5	A	509	NAG	O5-C1-C2	-5.22	103.05	111.29
5	G	509	NAG	C1-O5-C5	4.99	118.96	112.19
5	A	509	NAG	C1-C2-N2	4.77	118.64	110.49
5	G	509	NAG	C1-C2-N2	4.74	118.58	110.49
5	A	504	NAG	C1-O5-C5	4.72	118.59	112.19
5	A	506	NAG	C4-C3-C2	4.59	117.75	111.02
5	A	509	NAG	O5-C5-C6	4.17	113.75	107.20
5	A	505	NAG	C4-C3-C2	4.07	116.99	111.02
5	G	507	NAG	C4-C3-C2	4.02	116.91	111.02
5	A	503	NAG	C1-O5-C5	3.95	117.54	112.19
5	G	502	NAG	C1-O5-C5	3.94	117.53	112.19
5	G	501	NAG	C3-C4-C5	3.90	117.19	110.24
5	A	507	NAG	C1-O5-C5	3.81	117.36	112.19
5	G	505	NAG	C1-O5-C5	3.66	117.15	112.19
5	G	505	NAG	O5-C1-C2	-3.65	105.52	111.29
5	A	508	NAG	C1-O5-C5	3.55	117.00	112.19
5	G	501	NAG	C4-C3-C2	3.35	115.92	111.02
5	A	506	NAG	C3-C4-C5	3.33	116.18	110.24
5	G	503	NAG	C1-O5-C5	3.09	116.37	112.19
5	G	501	NAG	O5-C1-C2	-3.07	106.44	111.29
5	A	502	NAG	C3-C4-C5	3.02	115.63	110.24
5	G	501	NAG	C1-O5-C5	2.94	116.18	112.19
5	G	508	NAG	O5-C5-C4	-2.90	103.76	110.83
5	G	506	NAG	C1-O5-C5	2.82	116.01	112.19
5	G	502	NAG	C3-C4-C5	2.79	115.21	110.24
5	G	504	NAG	C4-C3-C2	2.69	114.97	111.02
5	A	501	NAG	O5-C1-C2	-2.67	107.06	111.29
5	A	505	NAG	C3-C4-C5	2.65	114.96	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	509	NAG	C2-N2-C7	2.64	126.66	122.90
5	A	508	NAG	C1-C2-N2	2.62	114.97	110.49
5	A	502	NAG	C1-O5-C5	-2.50	108.81	112.19
5	A	508	NAG	O3-C3-C2	-2.50	104.30	109.47
5	G	504	NAG	O5-C5-C6	2.49	111.11	107.20
5	A	509	NAG	C2-N2-C7	2.48	126.43	122.90
5	A	501	NAG	C1-O5-C5	2.38	115.42	112.19
5	G	508	NAG	O3-C3-C2	-2.37	104.57	109.47
5	A	506	NAG	C1-O5-C5	2.35	115.38	112.19
5	G	502	NAG	O5-C5-C6	2.35	110.88	107.20
5	A	502	NAG	O5-C1-C2	2.31	114.94	111.29
5	A	501	NAG	O5-C5-C6	2.29	110.80	107.20
5	G	504	NAG	O5-C5-C4	-2.28	105.28	110.83
5	A	509	NAG	O3-C3-C2	2.24	114.10	109.47
5	A	502	NAG	C2-N2-C7	2.21	126.04	122.90
5	G	507	NAG	O5-C5-C6	2.21	110.66	107.20
5	G	502	NAG	C4-C3-C2	2.17	114.20	111.02
5	A	507	NAG	C4-C3-C2	2.15	114.16	111.02
5	G	502	NAG	O4-C4-C3	-2.12	105.44	110.35
5	G	509	NAG	O5-C1-C2	-2.09	107.98	111.29
5	A	505	NAG	O5-C5-C6	2.05	110.42	107.20
5	A	509	NAG	O7-C7-C8	-2.05	118.25	122.06
5	G	502	NAG	O7-C7-C8	-2.03	118.28	122.06
5	A	503	NAG	O5-C1-C2	-2.03	108.08	111.29
5	G	509	NAG	O5-C5-C4	-2.00	105.96	110.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	506	NAG	O5-C5-C6-O6
5	G	507	NAG	O5-C5-C6-O6
5	A	506	NAG	C4-C5-C6-O6
5	A	507	NAG	C4-C5-C6-O6
5	G	506	NAG	O5-C5-C6-O6
5	A	507	NAG	O5-C5-C6-O6
5	G	507	NAG	C4-C5-C6-O6
5	G	506	NAG	C4-C5-C6-O6
5	A	505	NAG	O5-C5-C6-O6
5	A	505	NAG	C4-C5-C6-O6
5	A	503	NAG	C4-C5-C6-O6
5	G	503	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	G	503	NAG	O5-C5-C6-O6
5	A	503	NAG	O5-C5-C6-O6
5	G	502	NAG	C4-C5-C6-O6
5	G	505	NAG	C4-C5-C6-O6
5	G	501	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	509	NAG	1	0
5	A	502	NAG	2	0
5	A	504	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, 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	337/353 (95%)	0.26	17 (5%) 28 17	68, 104, 154, 178	0
1	G	337/353 (95%)	0.24	20 (5%) 22 13	69, 102, 160, 197	0
2	B	217/233 (93%)	-0.04	4 (1%) 68 56	57, 75, 108, 133	0
2	H	217/233 (93%)	-0.05	6 (2%) 53 39	60, 76, 113, 130	0
3	C	210/216 (97%)	-0.12	0 100 100	67, 83, 120, 137	0
3	L	210/216 (97%)	-0.20	0 100 100	62, 80, 113, 129	0
4	D	25/28 (89%)	0.54	2 (8%) 12 7	119, 125, 135, 140	0
4	M	25/28 (89%)	0.49	2 (8%) 12 7	118, 129, 143, 145	0
All	All	1578/1660 (95%)	0.07	51 (3%) 47 33	57, 87, 146, 197	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	122	LEU	9.4
1	A	200	VAL	6.0
1	G	123	THR	6.0
2	B	158	SER	5.5
1	A	124	GLY	5.4
1	G	199	SER	5.4
1	G	121	LYS	4.6
2	H	158	SER	4.0
1	G	433	ALA	3.8
1	A	199	SER	3.7
1	G	391	PHE	3.5
1	A	204	ALA	3.4
1	G	325	ASP	3.3
1	G	438	PRO	3.3
4	D	17	GLY	3.1
2	B	155	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
4	M	17	GLY	2.8
1	A	341	VAL	2.7
1	A	123	THR	2.7
1	G	119	CYS	2.6
1	G	435	TYR	2.6
1	G	383	PHE	2.6
1	A	439	ILE	2.6
4	D	5	PHE	2.5
1	A	376	PHE	2.5
1	G	120	VAL	2.5
1	A	203	GLN	2.4
1	G	202	LYS	2.4
2	B	157	GLY	2.4
1	A	201	ILE	2.4
1	A	256	SER	2.4
2	H	159	LEU	2.4
1	A	433	ALA	2.4
2	H	132	SER	2.3
1	A	455	THR	2.2
2	H	193	THR	2.2
4	M	16	LEU	2.2
2	H	126	PRO	2.2
2	H	208	ASP	2.2
1	A	299	PRO	2.2
1	G	376	PHE	2.2
1	A	301	ASN	2.2
1	A	120	VAL	2.2
1	G	124	GLY	2.2
1	A	453	LEU	2.1
1	G	439	ILE	2.1
1	G	492	GLU	2.1
1	G	432	GLN	2.1
1	G	301	ASN	2.0
1	G	423	ILE	2.0
2	B	194	TYR	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. 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(\AA^2)	Q<0.9
4	DPR	D	21	7/8	0.87	0.20	114,114,115,115	0
4	DPR	M	21	7/8	0.94	0.22	115,117,119,121	0

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, 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(\AA^2)	Q<0.9
5	NAG	G	505	14/15	0.78	0.38	100,113,120,121	0
5	NAG	G	508	14/15	0.79	0.41	121,139,141,142	0
5	NAG	G	502	14/15	0.80	0.30	95,104,110,110	0
5	NAG	A	504	14/15	0.80	0.32	97,115,126,127	0
5	NAG	A	507	14/15	0.80	0.47	101,110,112,112	0
5	NAG	A	505	14/15	0.81	0.28	75,99,107,108	0
5	NAG	A	508	14/15	0.83	0.25	114,126,130,133	0
5	NAG	A	506	14/15	0.85	0.28	72,79,86,88	0
5	NAG	A	502	14/15	0.87	0.26	91,99,106,107	0
5	NAG	G	507	14/15	0.87	0.46	95,109,113,113	0
5	NAG	A	509	14/15	0.87	0.27	110,129,136,141	0
5	NAG	G	509	14/15	0.88	0.29	102,112,119,123	0
5	NAG	G	506	14/15	0.88	0.16	70,76,80,82	0
5	NAG	G	504	14/15	0.90	0.15	82,96,100,100	0
5	NAG	G	501	14/15	0.93	0.16	67,74,78,78	0
5	NAG	A	501	14/15	0.94	0.20	61,69,72,75	0
5	NAG	G	503	14/15	0.94	0.22	53,61,70,74	0
5	NAG	A	503	14/15	0.95	0.17	56,63,71,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.