



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:48 AM UTC

PDB ID : 7S1B / pdb_00007s1b
Title : Crystal structure of Epstein-Barr virus glycoproteins gH/gL/gp42-peptide in complex with human neutralizing antibodies 769C2 and 770F7
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Deposited on : 2021-09-02
Resolution : 3.03 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

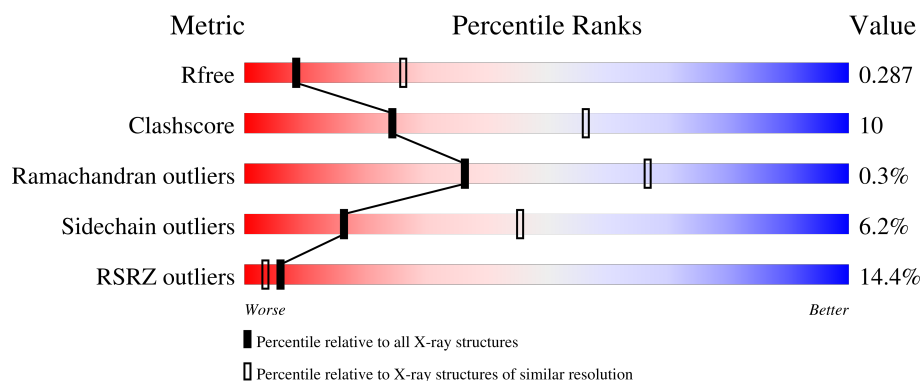
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	657	4% 81% 19%
2	B	114	11% 61% 22% 13%
3	H	230	% 81% 14% ..
4	L	215	92% 7% .
5	X	225	38% 38% 28% 8% 27%

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Mol	Chain	Length	Quality of chain
6	Y	215	48% 61% 31% ...
7	C	33	94% 6%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12257 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	657	Total	C	N	O	P	S	0	0	0
			5112	3274	844	962	1	31			

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			756	478	127	147	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	35	ALA	ARG	conflict	UNP P03212

- Molecule 3 is a protein called 770F7 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	222	Total	C	N	O	S	0	0	0
			1680	1069	282	323	6			

- Molecule 4 is a protein called 770F7 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	215	Total	C	N	O	S	0	0	0
			1645	1028	280	332	5			

- Molecule 5 is a protein called 769C2 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	164	Total	C	N	O	S	0	0	0
			1213	762	211	233	7			

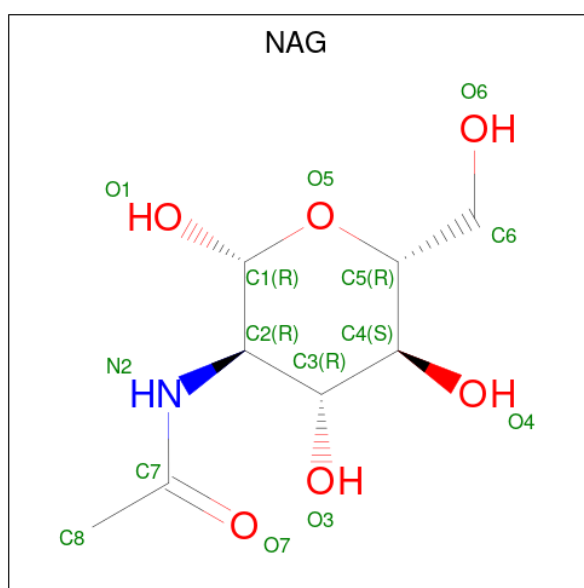
- Molecule 6 is a protein called 769C2 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	Y	206	Total	C	N	O	S	0	0	0
			1529	953	252	319	5			

- Molecule 7 is a protein called Soluble gp42.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	C	33	Total	C	N	O	0	0	0
			266	173	42	51			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

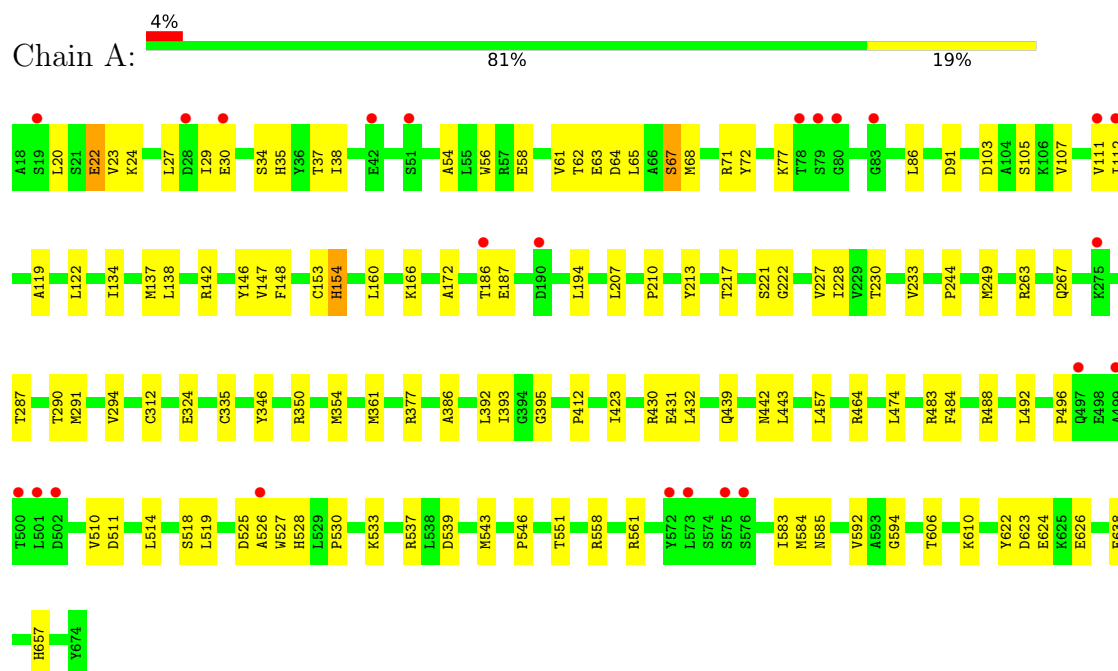


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

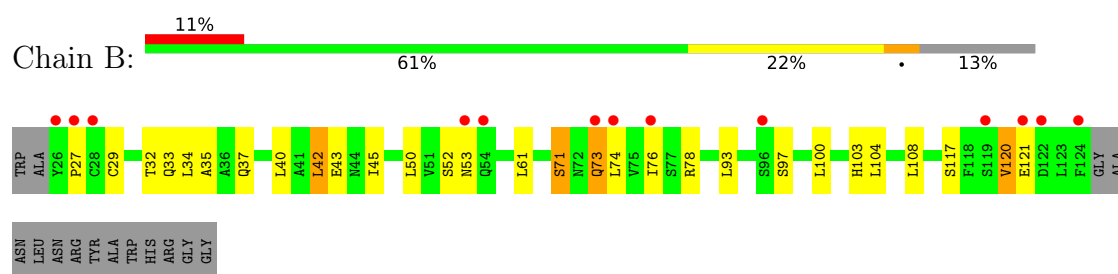
3 Residue-property plots [i](#)

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

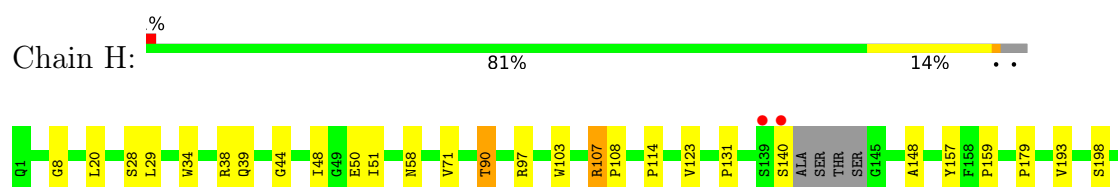
• Molecule 1: Envelope glycoprotein H



• Molecule 2: Envelope glycoprotein L



• Molecule 3: 770F7 Fab heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.33Å 107.70Å 110.65Å 90.00° 93.11° 90.00°	Depositor
Resolution (Å)	71.32 – 3.03 71.32 – 3.03	Depositor EDS
% Data completeness (in resolution range)	89.7 (71.32-3.03) 89.7 (71.32-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.241 , 0.288 0.243 , 0.287	Depositor DCC
R_{free} test set	2005 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12257	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: HIP, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/5205	0.34	0/7063
2	B	0.22	0/768	0.51	0/1043
3	H	0.17	0/1727	0.36	0/2358
4	L	0.17	0/1680	0.39	0/2280
5	X	0.39	1/1237 (0.1%)	0.76	5/1673 (0.3%)
6	Y	0.23	0/1565	0.52	2/2137 (0.1%)
7	C	0.16	0/276	0.37	0/380
All	All	0.22	1/12458 (0.0%)	0.44	7/16934 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	191	VAL	C-N	5.66	1.40	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	69	THR	N-CA-C	6.25	119.55	110.42
6	Y	39	GLN	CA-C-N	5.90	132.81	121.54
6	Y	39	GLN	C-N-CA	5.90	132.81	121.54
5	X	84	ASN	CA-C-N	-5.84	115.00	122.77
5	X	84	ASN	C-N-CA	-5.84	115.00	122.77
5	X	68	PHE	CA-C-N	5.26	129.76	121.56
5	X	68	PHE	C-N-CA	5.26	129.76	121.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5112	0	5123	83	0
2	B	756	0	748	21	0
3	H	1680	0	1648	25	0
4	L	1645	0	1602	10	0
5	X	1213	0	1171	68	0
6	Y	1529	0	1458	55	0
7	C	266	0	257	2	0
8	A	28	0	26	2	0
8	B	28	0	26	0	0
All	All	12257	0	12059	240	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (240) 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)
5:X:67:ASN:OD1	5:X:83:MET:HE1	1.13	1.25
5:X:67:ASN:CG	5:X:83:MET:HE1	1.71	1.14
5:X:191:VAL:CG1	5:X:192:PRO:CD	2.31	1.08
5:X:67:ASN:OD1	5:X:83:MET:CE	2.03	1.05
5:X:48:VAL:CG2	5:X:67:ASN:ND2	2.20	1.03
5:X:191:VAL:HG12	5:X:192:PRO:CD	1.89	1.03
5:X:191:VAL:CG1	5:X:192:PRO:HD2	1.90	1.02
5:X:48:VAL:HG22	5:X:67:ASN:ND2	1.76	1.01
5:X:191:VAL:HG12	5:X:192:PRO:HD2	1.44	0.94
5:X:191:VAL:HG13	5:X:192:PRO:CD	1.98	0.92
5:X:20:LEU:HB2	5:X:81:LEU:HD23	1.51	0.90
5:X:185:LEU:N	6:Y:181:TYR:HH	1.68	0.90
5:X:48:VAL:CG2	5:X:67:ASN:HD21	1.85	0.88
1:A:484:PHE:HE2	1:A:519:LEU:HD21	1.36	0.87
5:X:13:LYS:HG2	5:X:14:PRO:HD2	1.56	0.87
5:X:48:VAL:HG21	5:X:67:ASN:HD21	1.44	0.82
5:X:191:VAL:HG13	5:X:192:PRO:HD3	1.62	0.82
1:A:484:PHE:CE2	1:A:519:LEU:HD21	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:32:TYR:O	5:X:72:ARG:NH2	2.12	0.82
5:X:48:VAL:HG21	5:X:67:ASN:ND2	1.95	0.79
5:X:66:GLY:O	5:X:67:ASN:OD1	2.02	0.76
3:H:198:SER:HA	3:H:201:LEU:HD12	1.68	0.75
5:X:191:VAL:HG12	5:X:192:PRO:N	1.99	0.75
1:A:217:THR:HG22	1:A:227:VAL:HG22	1.70	0.74
5:X:48:VAL:CG2	5:X:67:ASN:HD22	2.01	0.72
6:Y:21:SER:HA	6:Y:74:SER:HA	1.71	0.71
5:X:48:VAL:CG1	5:X:67:ASN:HD22	2.03	0.70
5:X:36:TRP:CZ2	5:X:81:LEU:HB3	2.27	0.69
1:A:62:THR:O	2:B:33:GLN:NE2	2.25	0.69
5:X:39:GLN:HE22	6:Y:45:ASN:HB2	1.60	0.67
2:B:29:CYS:SG	2:B:61:LEU:HD23	2.36	0.66
1:A:386:ALA:HB2	1:A:430:ARG:HB3	1.78	0.65
5:X:48:VAL:HG13	5:X:67:ASN:HD22	1.61	0.64
5:X:210:SER:O	5:X:210:SER:OG	2.11	0.64
8:A:701:NAG:O7	8:A:701:NAG:O3	2.09	0.63
5:X:35:ASP:OD2	5:X:47:TRP:NE1	2.30	0.63
5:X:48:VAL:HG22	5:X:67:ASN:HD22	1.61	0.63
5:X:39:GLN:OE1	6:Y:45:ASN:ND2	2.31	0.63
1:A:137:MET:HE2	1:A:172:ALA:HB1	1.80	0.62
5:X:191:VAL:HG13	5:X:192:PRO:HD2	1.71	0.62
1:A:558:ARG:NH2	1:A:594:GLY:O	2.32	0.62
5:X:51:ILE:HG13	5:X:58:ILE:HG12	1.81	0.62
8:A:701:NAG:H62	2:B:33:GLN:NE2	2.14	0.62
3:H:8:GLY:HA3	3:H:20:LEU:HD23	1.82	0.62
6:Y:80:LEU:HD11	6:Y:85:GLU:HG3	1.81	0.61
3:H:211:ASN:HD21	3:H:218:LYS:HE2	1.66	0.60
6:Y:186:PRO:HA	6:Y:189:TRP:HB3	1.82	0.60
5:X:20:LEU:HD12	5:X:81:LEU:HD21	1.84	0.59
3:H:39:GLN:HG3	3:H:44:GLY:HA3	1.83	0.59
1:A:484:PHE:HE2	1:A:519:LEU:CD2	2.11	0.59
2:B:32:THR:O	2:B:78:ARG:NH2	2.35	0.59
1:A:244:PRO:HB2	1:A:249:MET:HE1	1.85	0.58
5:X:67:ASN:CG	5:X:83:MET:CE	2.63	0.58
5:X:147:CYS:HB2	5:X:161:TRP:CZ2	2.39	0.57
5:X:162:ASN:O	5:X:162:ASN:ND2	2.30	0.57
6:Y:19:THR:HA	6:Y:75:LEU:O	2.04	0.57
1:A:134:ILE:HB	1:A:154:HIP:HE1	1.87	0.57
4:L:121:PRO:HD3	4:L:133:VAL:HG22	1.86	0.56
1:A:439:GLN:OE1	1:A:442:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:HH22	7:C:65:LYS:HB3	1.69	0.56
6:Y:135:THR:HG22	6:Y:181:TYR:HB3	1.87	0.56
6:Y:62:THR:HB	6:Y:79:GLY:HA3	1.88	0.56
1:A:22:GLU:OE2	1:A:24:LYS:NZ	2.38	0.56
1:A:111:VAL:HG22	1:A:112:ILE:HD12	1.88	0.56
3:H:90:THR:HB	3:H:123:VAL:H	1.71	0.55
6:Y:165:THR:OG1	6:Y:180:SER:HA	2.05	0.55
1:A:525:ASP:OD1	3:H:107:ARG:NH1	2.39	0.55
1:A:112:ILE:HG12	1:A:119:ALA:HB2	1.87	0.55
2:B:40:LEU:HD11	2:B:45:ILE:HD11	1.88	0.55
1:A:64:ASP:OD1	1:A:64:ASP:N	2.40	0.55
5:X:148:LEU:HD13	6:Y:137:VAL:HG21	1.88	0.54
1:A:464:ARG:HB2	1:A:496:PRO:HG2	1.90	0.54
3:H:212:HIS:CD2	3:H:214:PRO:HD2	2.43	0.54
1:A:530:PRO:HD2	1:A:585:ASN:HD22	1.73	0.54
6:Y:87:ASP:HA	6:Y:106:SER:HA	1.88	0.54
6:Y:50:ILE:HG23	6:Y:52:GLU:O	2.08	0.53
1:A:142:ARG:NH1	1:A:146:TYR:OH	2.41	0.53
6:Y:75:LEU:HD21	6:Y:77:ILE:HD11	1.89	0.53
6:Y:39:GLN:HG2	6:Y:86:ALA:HB3	1.90	0.53
1:A:166:LYS:NZ	1:A:187:GLU:OE1	2.31	0.53
3:H:97:ARG:HH11	3:H:114:PRO:HD3	1.72	0.53
5:X:171:HIS:HB3	5:X:188:VAL:O	2.09	0.52
6:Y:163:VAL:HG13	6:Y:182:LEU:HG	1.90	0.52
1:A:638:GLU:OE1	1:A:638:GLU:N	2.42	0.52
3:H:51:ILE:HD13	3:H:71:VAL:HG13	1.92	0.52
3:H:159:PRO:HD2	3:H:214:PRO:HG2	1.90	0.52
6:Y:25:THR:N	6:Y:28:ASP:OD1	2.42	0.52
5:X:143:ALA:HA	5:X:191:VAL:H	1.74	0.52
1:A:37:THR:H	2:B:103:HIS:HE1	1.56	0.51
1:A:412:PRO:HG3	1:A:457:LEU:HB3	1.92	0.51
6:Y:88:TYR:HB2	6:Y:105:THR:OG1	2.10	0.51
1:A:63:GLU:HA	2:B:33:GLN:HE22	1.76	0.51
6:Y:132:ASN:HA	6:Y:186:PRO:HD2	1.92	0.51
1:A:63:GLU:HA	2:B:33:GLN:NE2	2.25	0.51
5:X:51:ILE:HB	5:X:70:ILE:HD11	1.93	0.51
5:X:61:SER:OG	5:X:65:LYS:O	2.19	0.51
5:X:54:ARG:O	5:X:56:SER:N	2.44	0.50
1:A:537:ARG:HG2	3:H:28:SER:HB2	1.92	0.50
3:H:131:PRO:HB3	3:H:157:TYR:HB3	1.93	0.50
1:A:346:TYR:O	1:A:350:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:VAL:HG12	2:B:121:GLU:H	1.75	0.50
5:X:35:ASP:HB2	5:X:97:ALA:HB3	1.94	0.50
6:Y:6:GLN:HE21	6:Y:104:GLY:H	1.60	0.50
6:Y:23:THR:HG22	6:Y:72:THR:HG23	1.94	0.50
3:H:148:ALA:HB3	3:H:201:LEU:HD11	1.93	0.50
5:X:162:ASN:HD22	5:X:162:ASN:C	2.18	0.50
1:A:138:LEU:HD13	1:A:148:PHE:HB3	1.94	0.50
1:A:439:GLN:HG3	1:A:442:ASN:HB2	1.94	0.49
6:Y:83:GLU:OE2	6:Y:174:ASN:ND2	2.45	0.49
3:H:34:TRP:CE3	3:H:97:ARG:HB2	2.48	0.49
1:A:623:ASP:OD1	1:A:624:GLU:N	2.46	0.49
5:X:173:PHE:CZ	6:Y:141:SER:HB3	2.48	0.49
1:A:361:MET:HE3	1:A:395:GLY:HA3	1.93	0.49
1:A:526:ALA:C	1:A:528:HIS:H	2.21	0.49
5:X:114:THR:HG22	5:X:115:LEU:H	1.78	0.48
6:Y:122:PHE:HE1	6:Y:136:LEU:HA	1.77	0.48
6:Y:50:ILE:O	6:Y:50:ILE:HG22	2.13	0.48
5:X:126:PRO:HG3	5:X:210:SER:OG	2.14	0.48
1:A:37:THR:H	2:B:103:HIS:CE1	2.31	0.48
1:A:533:LYS:O	1:A:561:ARG:NH2	2.38	0.48
2:B:100:LEU:HG	2:B:104:LEU:HB2	1.95	0.48
4:L:111:VAL:O	4:L:141:TYR:O	2.31	0.48
1:A:546:PRO:HA	1:A:551:THR:HG22	1.96	0.48
6:Y:51:PHE:CD2	6:Y:52:GLU:HG2	2.48	0.48
1:A:488:ARG:NH1	1:A:511:ASP:OD1	2.46	0.47
5:X:12:VAL:HG11	5:X:16:GLY:HA3	1.94	0.47
6:Y:137:VAL:HG22	6:Y:181:TYR:HD1	1.77	0.47
6:Y:2:SER:N	6:Y:100:VAL:HG23	2.29	0.47
6:Y:37:TRP:HA	6:Y:89:TYR:O	2.14	0.47
1:A:488:ARG:HG3	1:A:514:LEU:HD22	1.97	0.47
2:B:97:SER:HA	2:B:100:LEU:HD13	1.95	0.47
1:A:56:TRP:CD2	2:B:42:LEU:HG	2.50	0.47
1:A:68:MET:HG3	1:A:210:PRO:HG3	1.96	0.47
1:A:267:GLN:HG2	1:A:474:LEU:HD13	1.95	0.47
6:Y:25:THR:HG22	6:Y:26:SER:H	1.79	0.47
3:H:34:TRP:CZ3	3:H:97:ARG:HB2	2.49	0.47
1:A:377:ARG:HE	1:A:423:ILE:HD13	1.78	0.47
5:X:66:GLY:O	5:X:67:ASN:CG	2.57	0.47
1:A:20:LEU:N	2:B:43:GLU:OE1	2.48	0.47
1:A:290:THR:O	1:A:294:VAL:HG23	2.14	0.47
6:Y:122:PHE:CE1	6:Y:136:LEU:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:MET:HE2	1:A:392:LEU:HA	1.97	0.46
1:A:22:GLU:HG2	1:A:23:VAL:N	2.30	0.46
4:L:95:SER:HB2	4:L:96:PRO:HD3	1.97	0.46
5:X:32:TYR:CD2	5:X:98:ARG:HD3	2.50	0.46
1:A:530:PRO:HB2	1:A:585:ASN:HB3	1.97	0.46
1:A:623:ASP:HB3	1:A:626:GLU:HB3	1.98	0.46
2:B:35:ALA:O	2:B:37:GLN:N	2.49	0.46
6:Y:53:VAL:HG21	6:Y:68:LYS:HE3	1.98	0.45
6:Y:117:PRO:HB3	6:Y:143:PHE:HB3	1.98	0.45
5:X:126:PRO:HG3	5:X:210:SER:CB	2.46	0.45
1:A:27:LEU:HD23	2:B:50:LEU:HB2	1.97	0.45
1:A:72:TYR:CZ	1:A:77:LYS:HE2	2.52	0.45
6:Y:37:TRP:HD1	6:Y:50:ILE:CG2	2.30	0.45
1:A:111:VAL:HG22	1:A:112:ILE:H	1.81	0.45
5:X:114:THR:HG22	5:X:115:LEU:HD22	1.97	0.45
6:Y:167:THR:HG23	6:Y:178:ALA:HA	1.99	0.45
5:X:32:TYR:HD2	5:X:98:ARG:HD3	1.82	0.45
2:B:93:LEU:HB2	2:B:108:LEU:HD13	1.99	0.45
3:H:97:ARG:NH1	3:H:114:PRO:HD3	2.32	0.44
4:L:109:ARG:HG2	4:L:110:THR:H	1.81	0.44
1:A:287:THR:HG22	1:A:291:MET:HE3	1.99	0.44
1:A:610:LYS:HE2	1:A:610:LYS:HB3	1.87	0.44
2:B:71:SER:C	2:B:73:GLN:H	2.23	0.44
1:A:539:ASP:OD1	1:A:539:ASP:N	2.50	0.44
1:A:27:LEU:HB2	1:A:34:SER:HB2	1.99	0.44
1:A:525:ASP:HB3	3:H:103:TRP:HB2	1.99	0.44
5:X:45:LEU:HD23	5:X:45:LEU:HA	1.87	0.44
1:A:528:HIS:O	1:A:530:PRO:HD3	2.17	0.43
6:Y:40:GLN:HB2	6:Y:47:LYS:CB	2.47	0.43
6:Y:40:GLN:HB2	6:Y:47:LYS:HB2	1.99	0.43
6:Y:84:ASP:HB2	6:Y:170:LYS:HD3	1.99	0.43
1:A:432:LEU:HD23	1:A:443:LEU:HD13	2.00	0.43
5:X:208:LYS:HA	5:X:208:LYS:HD3	1.54	0.43
1:A:583:ILE:HG22	1:A:584:MET:HG2	2.00	0.43
5:X:166:LEU:HD13	5:X:166:LEU:HA	1.80	0.43
1:A:147:VAL:HG12	1:A:207:LEU:HD22	2.00	0.43
6:Y:42:PRO:HD3	6:Y:85:GLU:O	2.17	0.43
1:A:263:ARG:NH2	1:A:324:GLU:OE2	2.47	0.43
3:H:50:GLU:HG2	3:H:58:ASN:HB2	2.00	0.43
4:L:90:GLN:HG2	4:L:91:GLN:N	2.33	0.43
5:X:107:PHE:HB2	5:X:110:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:106:GLU:OE2	4:L:174:TYR:OH	2.36	0.43
5:X:60:TYR:CE1	5:X:70:ILE:HG23	2.53	0.43
1:A:72:TYR:CE2	1:A:77:LYS:HE2	2.54	0.43
5:X:40:ALA:HB1	5:X:41:PRO:HD2	2.01	0.43
5:X:207:HIS:ND1	5:X:209:PRO:HD2	2.34	0.43
1:A:112:ILE:HD12	1:A:112:ILE:H	1.82	0.43
1:A:194:LEU:HD12	1:A:230:THR:HB	2.00	0.43
1:A:483:ARG:HG2	1:A:543:MET:HE2	2.01	0.43
4:L:62:ARG:NH1	4:L:83:ASP:OD2	2.49	0.43
5:X:43:LYS:HE2	5:X:43:LYS:HB3	1.75	0.43
5:X:107:PHE:HB2	5:X:110:TRP:HZ3	1.84	0.43
2:B:53:ASN:ND2	2:B:117:SER:HB2	2.34	0.42
3:H:179:PRO:HG2	4:L:163:SER:HB2	2.01	0.42
6:Y:37:TRP:HD1	6:Y:50:ILE:HG21	1.85	0.42
6:Y:149:THR:OG1	6:Y:200:THR:HB	2.19	0.42
3:H:29:LEU:HA	3:H:34:TRP:CZ2	2.54	0.42
1:A:63:GLU:OE2	1:A:71:ARG:NH2	2.44	0.42
1:A:194:LEU:HD11	1:A:228:ILE:HD11	2.01	0.42
2:B:34:LEU:HD11	2:B:40:LEU:HB2	2.01	0.42
1:A:64:ASP:OD1	1:A:67:SER:HB2	2.18	0.42
1:A:134:ILE:HB	1:A:154:HIP:CE1	2.50	0.42
3:H:193:VAL:HG21	4:L:136:LEU:HD22	2.02	0.42
5:X:36:TRP:CE2	5:X:81:LEU:HB3	2.54	0.42
6:Y:6:GLN:HB3	6:Y:105:THR:CG2	2.49	0.42
1:A:346:TYR:HB3	7:C:70:GLU:HG2	2.01	0.42
6:Y:37:TRP:CD1	6:Y:50:ILE:HG21	2.55	0.42
6:Y:39:GLN:HB2	6:Y:88:TYR:CD2	2.54	0.42
1:A:35:HIS:HB2	6:Y:93:TYR:CE2	2.55	0.41
4:L:199:HIS:CD2	4:L:200:GLN:H	2.37	0.41
5:X:173:PHE:CE2	6:Y:139:LEU:HB3	2.54	0.41
6:Y:122:PHE:CD1	6:Y:122:PHE:C	2.98	0.41
1:A:492:LEU:HD23	1:A:510:VAL:HG21	2.02	0.41
6:Y:68:LYS:HE3	6:Y:68:LYS:HB3	1.84	0.41
3:H:107:ARG:HG3	3:H:108:PRO:HD2	2.01	0.41
6:Y:121:LEU:HD23	6:Y:122:PHE:H	1.85	0.41
5:X:43:LYS:HD2	6:Y:87:ASP:OD2	2.19	0.41
6:Y:184:LEU:HD23	6:Y:184:LEU:HA	1.83	0.41
3:H:222:LYS:HE2	3:H:224:GLU:HG2	2.02	0.41
1:A:103:ASP:OD1	1:A:105:SER:OG	2.38	0.41
5:X:175:ALA:HA	5:X:185:LEU:HA	2.02	0.41
6:Y:165:THR:OG1	6:Y:179:SER:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:SER:OG	1:A:222:GLY:N	2.53	0.41
6:Y:143:PHE:HE2	6:Y:146:GLY:HA2	1.85	0.41
5:X:39:GLN:CD	6:Y:45:ASN:HD22	2.26	0.41
1:A:29:ILE:O	1:A:29:ILE:HG13	2.21	0.41
1:A:122:LEU:HD23	1:A:312:CYS:HB3	2.03	0.41
1:A:137:MET:HE3	1:A:137:MET:HB2	1.88	0.41
3:H:34:TRP:CH2	3:H:97:ARG:HD2	2.56	0.41
6:Y:28:ASP:HB3	6:Y:94:SER:HB2	2.02	0.41
1:A:30:GLU:HB3	5:X:52:SER:OG	2.21	0.41
1:A:354:MET:HE2	1:A:354:MET:HB3	1.99	0.41
1:A:622:TYR:CE1	1:A:657:HIS:HB2	2.56	0.41
1:A:54:ALA:O	1:A:58:GLU:HG3	2.22	0.40
3:H:38:ARG:HB3	3:H:48:ILE:HD11	2.03	0.40
1:A:134:ILE:HG13	1:A:153:CYS:C	2.46	0.40
1:A:393:ILE:CD1	1:A:431:GLU:HG3	2.51	0.40
5:X:20:LEU:HB2	5:X:81:LEU:CD2	2.36	0.40
2:B:35:ALA:C	2:B:37:GLN:H	2.30	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	654/657 (100%)	627 (96%)	26 (4%)	1 (0%)	43	73
2	B	97/114 (85%)	88 (91%)	8 (8%)	1 (1%)	12	41
3	H	218/230 (95%)	206 (94%)	12 (6%)	0	100	100
4	L	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
5	X	152/225 (68%)	130 (86%)	20 (13%)	2 (1%)	9	35
6	Y	200/215 (93%)	161 (80%)	38 (19%)	1 (0%)	24	57
7	C	31/33 (94%)	25 (81%)	6 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1565/1689 (93%)	1442 (92%)	118 (8%)	5 (0%)	36 67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	TRP
2	B	27	PRO
5	X	87	ARG
5	X	14	PRO
6	Y	50	ILE

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	561/561 (100%)	545 (97%)	16 (3%)	37 67
2	B	88/97 (91%)	81 (92%)	7 (8%)	11 36
3	H	188/195 (96%)	183 (97%)	5 (3%)	39 68
4	L	185/185 (100%)	183 (99%)	2 (1%)	65 80
5	X	133/189 (70%)	96 (72%)	37 (28%)	0 2
6	Y	175/183 (96%)	158 (90%)	17 (10%)	8 28
7	C	31/31 (100%)	31 (100%)	0	100 100
All	All	1361/1441 (94%)	1277 (94%)	84 (6%)	16 45

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	38	ILE
1	A	61	VAL
1	A	65	LEU
1	A	67	SER
1	A	86	LEU

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Mol	Chain	Res	Type
1	A	91	ASP
1	A	107	VAL
1	A	160	LEU
1	A	186	THR
1	A	213	TYR
1	A	233	VAL
1	A	335	CYS
1	A	518	SER
1	A	592	VAL
1	A	606	THR
2	B	42	LEU
2	B	52	SER
2	B	71	SER
2	B	73	GLN
2	B	74	LEU
2	B	76	ILE
2	B	120	VAL
3	H	90	THR
3	H	107	ARG
3	H	140	SER
3	H	201	LEU
3	H	204	GLN
4	L	109	ARG
4	L	111	VAL
5	X	18	LEU
5	X	22	CYS
5	X	27	PHE
5	X	28	THR
5	X	37	VAL
5	X	48	VAL
5	X	63	SER
5	X	64	VAL
5	X	65	LYS
5	X	70	ILE
5	X	72	ARG
5	X	76	LYS
5	X	79	LEU
5	X	81	LEU
5	X	84	ASN
5	X	85	SER
5	X	90	ASP
5	X	96	CYS

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Mol	Chain	Res	Type
5	X	114	THR
5	X	115	LEU
5	X	124	LYS
5	X	128	VAL
5	X	145	LEU
5	X	149	VAL
5	X	158	THR
5	X	159	VAL
5	X	162	ASN
5	X	166	LEU
5	X	170	VAL
5	X	185	LEU
5	X	188	VAL
5	X	195	SER
5	X	198	THR
5	X	205	VAL
5	X	207	HIS
5	X	208	LYS
5	X	210	SER
6	Y	25	THR
6	Y	39	GLN
6	Y	41	HIS
6	Y	48	LEU
6	Y	50	ILE
6	Y	53	VAL
6	Y	80	LEU
6	Y	84	ASP
6	Y	98	THR
6	Y	120	THR
6	Y	121	LEU
6	Y	122	PHE
6	Y	125	SER
6	Y	126	SER
6	Y	133	LYS
6	Y	166	THR
6	Y	169	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	GLN
1	A	442	ASN

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Mol	Chain	Res	Type
1	A	528	HIS
2	B	30	HIS
2	B	33	GLN
2	B	103	HIS
3	H	5	GLN
3	H	176	HIS
3	H	183	GLN
3	H	211	ASN
4	L	139	ASN
4	L	167	GLN
4	L	199	HIS
5	X	39	GLN
5	X	67	ASN
5	X	84	ASN
5	X	204	ASN
6	Y	6	GLN
6	Y	45	ASN
6	Y	174	ASN
6	Y	201	HIS
7	C	62	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	HIP	A	154	1	10,14,15	2.17	3 (30%)	4,20,22	5.97	3 (75%)

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
1	HIP	A	154	1	-	2/5/12/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	HIP	P-O2P	-4.19	1.45	1.56
1	A	154	HIP	P-O3P	-4.06	1.46	1.56
1	A	154	HIP	CD2-CG	-2.57	1.33	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	HIP	O3P-P-O1P	-8.55	91.91	112.95
1	A	154	HIP	O2P-P-O1P	-7.57	94.32	112.95
1	A	154	HIP	CG-CD2-NE2	-3.43	102.53	109.79

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	154	HIP	N-CA-CB-CG
1	A	154	HIP	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	154	HIP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	A	702	1	14,14,15	0.17	0	17,19,21	0.61	1 (5%)
8	NAG	A	701	1	14,14,15	0.62	0	17,19,21	1.63	3 (17%)
8	NAG	B	201	2	14,14,15	0.42	0	17,19,21	0.57	0
8	NAG	B	202	2	14,14,15	0.36	0	17,19,21	0.63	0

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
8	NAG	A	702	1	-	0/6/23/26	0/1/1/1
8	NAG	A	701	1	-	1/6/23/26	0/1/1/1
8	NAG	B	201	2	-	1/6/23/26	0/1/1/1
8	NAG	B	202	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	701	NAG	C2-N2-C7	4.65	129.13	122.90
8	A	701	NAG	C1-O5-C5	3.60	117.01	112.19
8	A	701	NAG	O3-C3-C2	2.09	113.74	109.40
8	A	702	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	701	NAG	C3-C2-N2-C7
8	B	202	NAG	C1-C2-N2-C7
8	B	201	NAG	C3-C2-N2-C7
8	B	202	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	701	NAG	2	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	656/657 (99%)	0.20	24 (3%) 45 25	6, 26, 62, 103	0
2	B	99/114 (86%)	0.88	13 (13%) 7 4	29, 47, 97, 107	0
3	H	222/230 (96%)	0.21	3 (1%) 73 50	10, 31, 64, 86	0
4	L	215/215 (100%)	0.11	1 (0%) 87 72	16, 27, 47, 70	0
5	X	164/225 (72%)	2.24	86 (52%) 0 0	52, 92, 122, 138	0
6	Y	206/215 (95%)	2.16	103 (50%) 0 0	50, 94, 145, 160	0
7	C	33/33 (100%)	0.45	0 100 100	13, 36, 58, 71	0
All	All	1595/1689 (94%)	0.70	230 (14%) 6 3	6, 35, 116, 160	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	Y	131	ALA	6.2
5	X	128	VAL	6.0
5	X	64	VAL	5.6
6	Y	8	ALA	5.2
6	Y	111	GLY	5.1
5	X	198	THR	4.8
6	Y	122	PHE	4.8
5	X	185	LEU	4.8
5	X	170	VAL	4.8
1	A	502	ASP	4.7
5	X	166	LEU	4.7
5	X	67	ASN	4.5
5	X	165	ALA	4.5
6	Y	195	TYR	4.5
6	Y	210	VAL	4.3
5	X	86	LEU	4.2
5	X	124	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
6	Y	124	PRO	4.1
6	Y	158	PRO	4.1
6	Y	152	TRP	4.0
6	Y	213	THR	4.0
2	B	74	LEU	4.0
6	Y	166	THR	4.0
6	Y	11	SER	3.9
5	X	116	VAL	3.9
5	X	9	GLY	3.9
6	Y	82	ALA	3.9
6	Y	123	PRO	3.8
5	X	28	THR	3.8
5	X	209	PRO	3.8
6	Y	146	GLY	3.8
6	Y	196	SER	3.8
5	X	191	VAL	3.8
2	B	122	ASP	3.7
6	Y	110	LEU	3.7
5	X	194	SER	3.7
1	A	30	GLU	3.7
5	X	22	CYS	3.7
1	A	501	LEU	3.7
6	Y	59	GLY	3.7
2	B	121	GLU	3.6
6	Y	162	GLY	3.6
6	Y	84	ASP	3.6
6	Y	190	LYS	3.6
5	X	157	VAL	3.6
2	B	28	CYS	3.6
5	X	89	GLU	3.6
6	Y	108	THR	3.6
5	X	63	SER	3.5
6	Y	58	SER	3.5
6	Y	132	ASN	3.5
1	A	576	SER	3.5
5	X	193	SER	3.5
6	Y	104	GLY	3.5
6	Y	85	GLU	3.5
6	Y	189	TRP	3.5
2	B	26	TYR	3.5
5	X	148	LEU	3.5
6	Y	121	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
6	Y	23	THR	3.4
5	X	210	SER	3.4
6	Y	174	ASN	3.4
1	A	112	ILE	3.4
5	X	25	SER	3.4
6	Y	112	GLN	3.4
6	Y	80	LEU	3.3
6	Y	186	PRO	3.3
6	Y	150	VAL	3.3
5	X	92	ALA	3.3
6	Y	178	ALA	3.3
6	Y	197	CYS	3.3
6	Y	156	SER	3.3
5	X	149	VAL	3.3
6	Y	12	GLY	3.3
5	X	11	LEU	3.2
5	X	115	LEU	3.2
6	Y	7	PRO	3.2
6	Y	65	SER	3.2
6	Y	199	VAL	3.2
6	Y	184	LEU	3.1
5	X	34	MET	3.1
6	Y	203	GLY	3.1
5	X	203	CYS	3.1
5	X	27	PHE	3.1
5	X	143	ALA	3.1
6	Y	81	GLN	3.1
5	X	164	GLY	3.1
6	Y	157	SER	3.1
6	Y	10	VAL	3.1
6	Y	206	VAL	3.1
6	Y	42	PRO	3.1
5	X	196	LEU	3.0
6	Y	14	LEU	3.0
6	Y	125	SER	3.0
5	X	114	THR	3.0
5	X	190	THR	3.0
5	X	29	PHE	3.0
5	X	20	LEU	3.0
6	Y	116	ALA	3.0
6	Y	179	SER	3.0
1	A	83	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
6	Y	167	THR	3.0
5	X	110	TRP	2.9
6	Y	192	HIS	2.9
5	X	144	ALA	2.9
5	X	189	VAL	2.9
6	Y	136	LEU	2.9
5	X	96	CYS	2.9
5	X	186	SER	2.9
6	Y	182	LEU	2.9
6	Y	24	GLY	2.9
5	X	65	LYS	2.9
5	X	90	ASP	2.9
6	Y	149	THR	2.9
6	Y	163	VAL	2.9
5	X	197	GLY	2.9
5	X	126	PRO	2.8
6	Y	151	ALA	2.8
6	Y	148	VAL	2.8
6	Y	153	LYS	2.8
1	A	190	ASP	2.8
5	X	147	CYS	2.8
4	L	95	SER	2.8
5	X	14	PRO	2.8
1	A	111	VAL	2.7
6	Y	38	TYR	2.7
6	Y	3	VAL	2.7
6	Y	40	GLN	2.7
6	Y	41	HIS	2.7
5	X	17	SER	2.7
6	Y	183	SER	2.7
5	X	121	ALA	2.7
2	B	27	PRO	2.6
6	Y	64	PHE	2.6
1	A	275	LYS	2.6
5	X	10	GLY	2.6
1	A	499	ALA	2.6
3	H	140	SER	2.6
6	Y	191	SER	2.6
2	B	73	GLN	2.6
1	A	186	THR	2.6
5	X	24	ALA	2.6
5	X	69	THR	2.6

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Mol	Chain	Res	Type	RSRZ
5	X	123	THR	2.6
6	Y	107	LEU	2.6
5	X	30	SER	2.6
6	Y	77	ILE	2.6
1	A	573	LEU	2.6
6	Y	13	SER	2.6
6	Y	113	PRO	2.6
5	X	66	GLY	2.6
5	X	12	VAL	2.6
1	A	500	THR	2.6
5	X	158	THR	2.6
2	B	96	SER	2.5
6	Y	61	SER	2.5
6	Y	194	SER	2.5
6	Y	200	THR	2.5
1	A	78	THR	2.5
6	Y	193	ARG	2.5
1	A	575	SER	2.5
5	X	68	PHE	2.5
6	Y	43	GLY	2.5
5	X	84	ASN	2.4
5	X	206	ASN	2.4
1	A	80	GLY	2.4
3	H	139	SER	2.4
6	Y	201	HIS	2.4
6	Y	211	ALA	2.4
2	B	53	ASN	2.4
5	X	169	GLY	2.4
6	Y	164	GLU	2.4
2	B	119	SER	2.4
6	Y	109	VAL	2.4
5	X	163	SER	2.4
5	X	42	GLY	2.3
6	Y	208	LYS	2.3
5	X	43	LYS	2.3
5	X	161	TRP	2.3
6	Y	138	CYS	2.3
2	B	76	ILE	2.3
5	X	74	ASN	2.3
5	X	162	ASN	2.3
1	A	28	ASP	2.3
5	X	159	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	497	GLN	2.3
5	X	36	TRP	2.3
6	Y	62	THR	2.3
2	B	124	PHE	2.3
6	Y	144	TYR	2.3
5	X	205	VAL	2.3
1	A	79	SER	2.2
2	B	54	GLN	2.2
6	Y	137	VAL	2.2
6	Y	145	PRO	2.2
5	X	31	THR	2.2
6	Y	185	THR	2.2
5	X	91	THR	2.2
1	A	572	TYR	2.2
5	X	195	SER	2.2
6	Y	91	ASN	2.2
6	Y	168	PRO	2.2
1	A	19	SER	2.1
6	Y	127	GLU	2.1
5	X	23	ALA	2.1
6	Y	180	SER	2.1
5	X	207	HIS	2.1
3	H	204	GLN	2.1
1	A	42	GLU	2.1
5	X	102	GLY	2.1
6	Y	204	SER	2.1
5	X	145	LEU	2.1
6	Y	155	ASP	2.1
5	X	101	GLY	2.1
5	X	192	PRO	2.1
6	Y	212	PRO	2.1
5	X	111	GLY	2.1
1	A	51	SER	2.0
6	Y	2	SER	2.0
6	Y	176	TYR	2.0
6	Y	209	THR	2.0
5	X	41	PRO	2.0
5	X	13	LYS	2.0
5	X	105	SER	2.0
6	Y	45	ASN	2.0
6	Y	49	MET	2.0
1	A	526	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
5	X	113	GLY	2.0
6	Y	44	LYS	2.0
6	Y	83	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	HIP	A	154	14/15	0.83	0.15	12,34,50,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NAG	B	202	14/15	0.51	0.23	75,86,90,99	0
8	NAG	A	701	14/15	0.81	0.15	22,42,58,80	0
8	NAG	B	201	14/15	0.88	0.17	28,37,63,65	0
8	NAG	A	702	14/15	0.91	0.14	22,25,48,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.