Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 11:09 PM EDT

PDB ID	:	7S1B
Title	:	Crystal structure of Epstein-Barr virus glycoproteins gH/gL/gp42-peptide in complex with human neutralizing antibodies 769C2 and 770F7
Authors	:	Chen, W.-H.; Cohen, J.I.; Kanekiyo, M.; Joyce, M.G.
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:

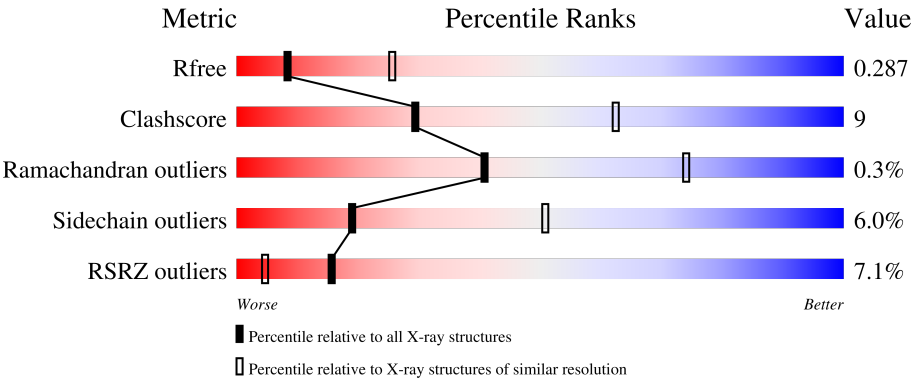
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (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 <=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	% 84% 16%
2	B	114	6% 61% 23% • 13%
3	H	230	80% 15% • •
4	L	215	91% 8%
5	X	225	22% 39% 27% 7% 27%

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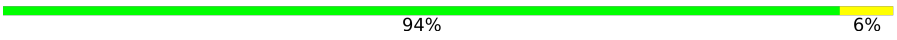
Mol	Chain	Length	Quality of chain
6	Y	215	
7	C	33	

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
8	NAG	B	202	-	-	-	X

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			

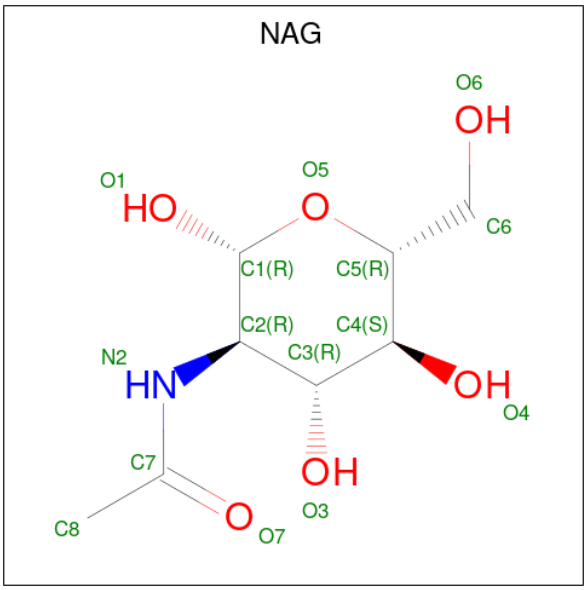
- Molecule 6 is a protein called 769C2 Fab light chain.

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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

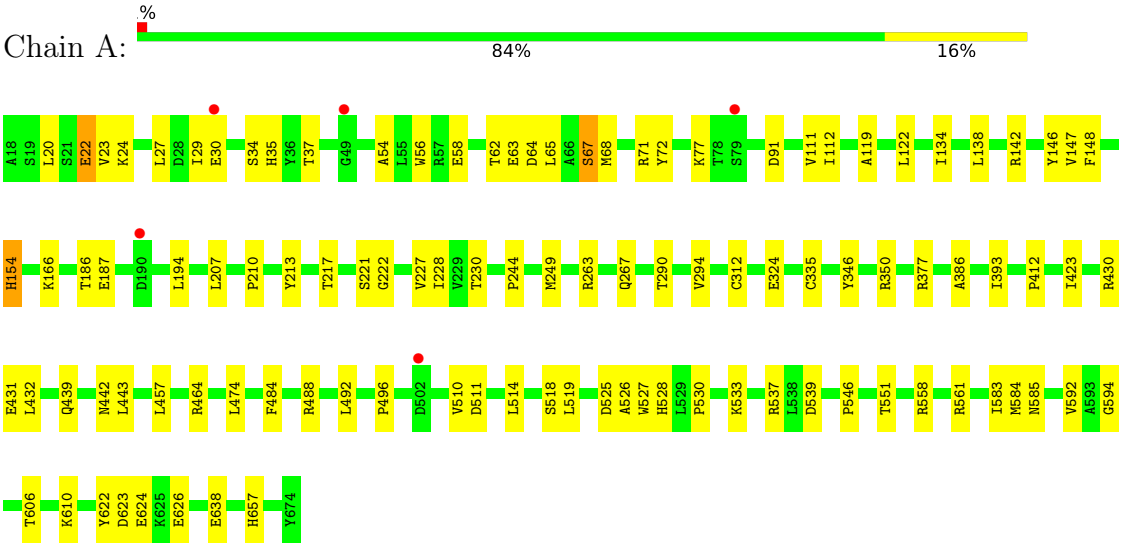


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

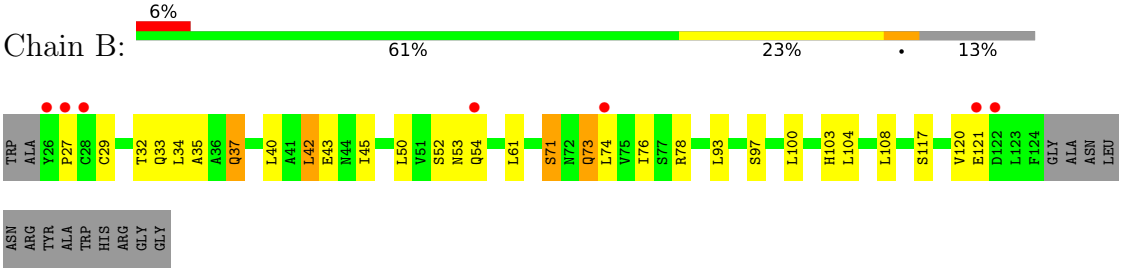
3 Residue-property plots (i)

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.

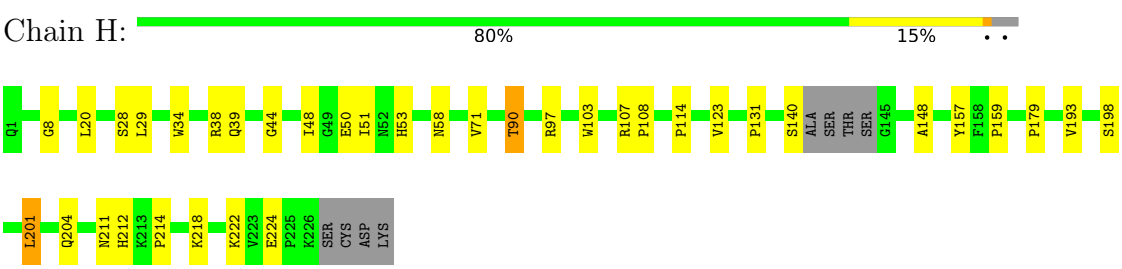
• Molecule 1: Envelope glycoprotein H



• Molecule 2: Envelope glycoprotein L

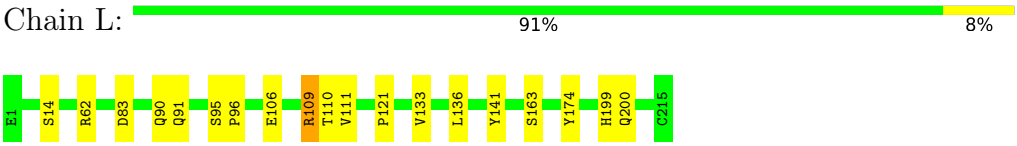


• Molecule 3: 770F7 Fab heavy chain



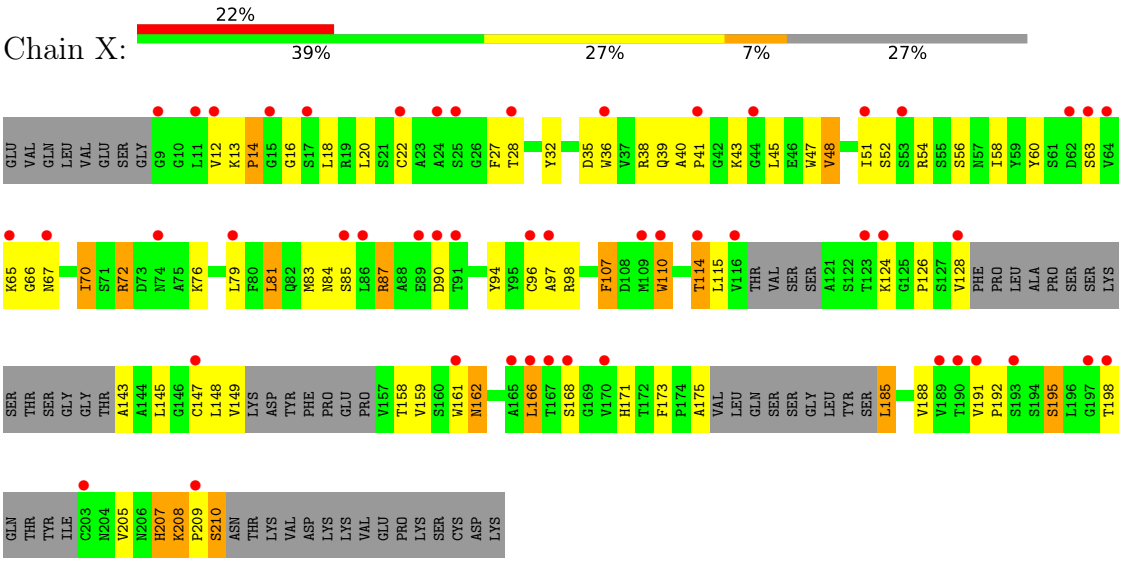
• Molecule 4: 770F7 Fab light chain

Chain L:



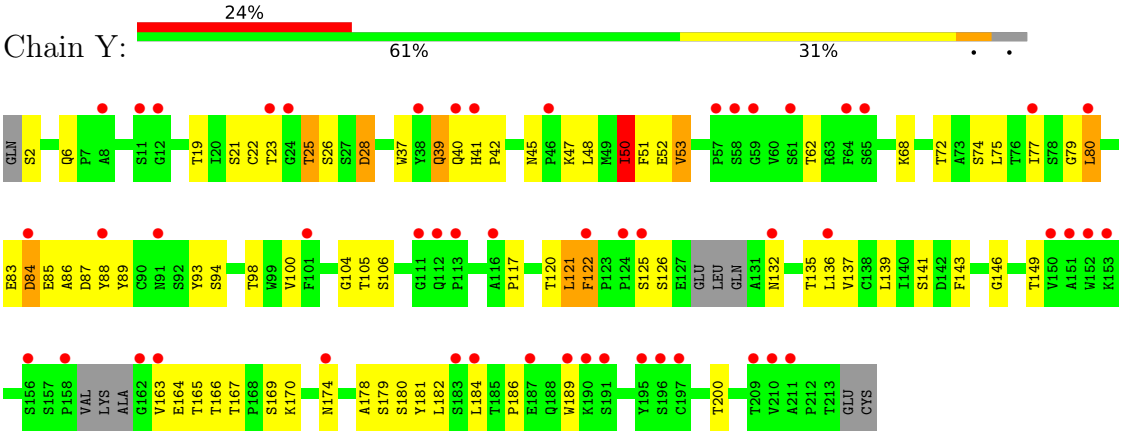
• Molecule 5: 769C2 Fab heavy chain

Chain X:



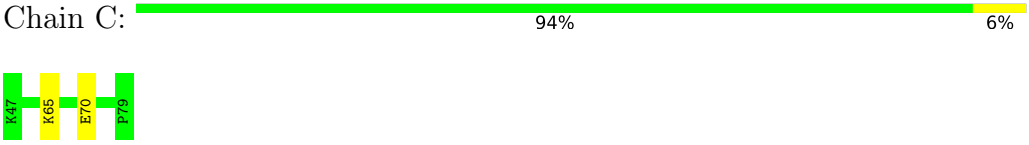
• Molecule 6: 769C2 Fab light chain

Chain Y:



• Molecule 7: Soluble gp42

Chain C:



4 Data and refinement statistics (i)

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 77.12 – 3.03	Depositor EDS
% Data completeness (in resolution range)	89.7 (71.32-3.03) 89.7 (77.12-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.241 , 0.288 0.241 , 0.287	Depositor DCC
R_{free} test set	2005 reflections (5.49%)	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)	0.30 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, HIP

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	0.28	0/5205	0.45	0/7063
2	B	0.29	0/768	0.49	0/1043
3	H	0.29	0/1727	0.48	0/2358
4	L	0.29	0/1680	0.48	0/2280
5	X	0.35	0/1237	0.67	0/1673
6	Y	0.28	0/1565	0.54	0/2137
7	C	0.26	0/276	0.43	0/380
All	All	0.29	0/12458	0.50	0/16934

There are no bond length outliers.

There are no bond angle outliers.

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	74	0
2	B	756	0	748	20	0
3	H	1680	0	1648	25	0
4	L	1645	0	1602	10	0
5	X	1213	0	1171	69	0
6	Y	1529	0	1458	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	230	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 9.

All (230) 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:HE3	1.46	1.12
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
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:67:ASN:OD1	5:X:83:MET:HE1	1.88	0.73
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:67:ASN:CG	5:X:83:MET:CE	2.63	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:67:ASN:CG	5:X:83:MET:HE3	2.24	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
1:A:22:GLU:OE2	1:A:24:LYS:NZ	2.38	0.51
5:X:51:ILE:HB	5:X:70:ILE:HD11	1.93	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
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
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
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
1:A:244:PRO:HB2	1:A:249:MET:HE1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:50:ILE:O	6:Y:50:ILE:HG22	2.13	0.48
5:X:67:ASN:CG	5:X:83:MET:HE1	2.30	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:195:SER:O	5:X:195:SER:OG	2.29	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
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
5:X:162:ASN:HD22	5:X:162:ASN:C	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:526:ALA:C	1:A:528:HIS:H	2.21	0.44
1:A:610:LYS:HE2	1:A:610:LYS:HB3	1.87	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:X:66:GLY:O	5:X:67:ASN:CG	2.57	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
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
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
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
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
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: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:393:ILE:CD1	1:A:431:GLU:HG3	2.51	0.40
2:B:71:SER:C	2:B:73:GLN:H	2.23	0.40
5:X:20:LEU:HB2	5:X:81:LEU:CD2	2.36	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	A	654/657 (100%)	627 (96%)	26 (4%)	1 (0%)	47 80
2	B	97/114 (85%)	88 (91%)	8 (8%)	1 (1%)	15 49
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%)	12 42
6	Y	200/215 (93%)	161 (80%)	38 (19%)	1 (0%)	29 65
7	C	31/33 (94%)	25 (81%)	6 (19%)	0	100 100
All	All	1565/1689 (93%)	1442 (92%)	118 (8%)	5 (0%)	41 74

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	561/561 (100%)	551 (98%)	10 (2%)	59 83
2	B	88/97 (91%)	80 (91%)	8 (9%)	9 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	H	188/195 (96%)	183 (97%)	5 (3%)	44 75
4	L	185/185 (100%)	183 (99%)	2 (1%)	73 90
5	X	133/189 (70%)	95 (71%)	38 (29%)	0 1
6	Y	175/183 (96%)	156 (89%)	19 (11%)	6 23
7	C	31/31 (100%)	31 (100%)	0	100 100
All	All	1361/1441 (94%)	1279 (94%)	82 (6%)	19 51

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	65	LEU
1	A	67	SER
1	A	91	ASP
1	A	186	THR
1	A	213	TYR
1	A	335	CYS
1	A	518	SER
1	A	592	VAL
1	A	606	THR
2	B	37	GLN
2	B	42	LEU
2	B	52	SER
2	B	54	GLN
2	B	71	SER
2	B	73	GLN
2	B	74	LEU
2	B	76	ILE
3	H	53	HIS
3	H	90	THR
3	H	140	SER
3	H	201	LEU
3	H	204	GLN
4	L	14	SER
4	L	109	ARG
5	X	18	LEU
5	X	22	CYS
5	X	27	PHE
5	X	28	THR
5	X	38	ARG

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Mol	Chain	Res	Type
5	X	48	VAL
5	X	63	SER
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	87	ARG
5	X	90	ASP
5	X	94	TYR
5	X	96	CYS
5	X	107	PHE
5	X	110	TRP
5	X	114	THR
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	168	SER
5	X	185	LEU
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	22	CYS
6	Y	25	THR
6	Y	28	ASP
6	Y	39	GLN
6	Y	41	HIS
6	Y	48	LEU
6	Y	50	ILE
6	Y	53	VAL
6	Y	80	LEU

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Mol	Chain	Res	Type
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	164	GLU
6	Y	166	THR
6	Y	169	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	GLN
1	A	442	ASN
2	B	30	HIS
2	B	33	GLN
2	B	103	HIS
5	X	39	GLN
6	Y	6	GLN
6	Y	45	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	3.57	3 (30%)	6,20,22	6.10	4 (66%)

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	CG-ND1	9.04	1.49	1.37
1	A	154	HIP	P-O2P	-4.44	1.45	1.54
1	A	154	HIP	P-O3P	-4.27	1.46	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	HIP	O3P-P-O1P	-9.96	91.91	113.44
1	A	154	HIP	O2P-P-O1P	-8.84	94.32	113.44
1	A	154	HIP	CB-CA-C	5.81	122.36	111.47
1	A	154	HIP	CG-CD2-NE2	-3.37	102.53	108.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	154	HIP	C-CA-CB-CG
1	A	154	HIP	N-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 monosaccharides 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	B	202	2	14,14,15	0.34	0	17,19,21	0.60	0
8	NAG	B	201	2	14,14,15	0.40	0	17,19,21	0.57	0
8	NAG	A	702	1	14,14,15	0.17	0	17,19,21	0.60	0
8	NAG	A	701	1	14,14,15	0.63	0	17,19,21	1.57	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
8	NAG	B	202	2	-	2/6/23/26	0/1/1/1
8	NAG	B	201	2	-	2/6/23/26	0/1/1/1
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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	701	NAG	C2-N2-C7	4.38	129.13	122.90
8	A	701	NAG	C1-O5-C5	3.56	117.01	112.19
8	A	701	NAG	O3-C3-C2	2.07	113.74	109.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	701	NAG	C3-C2-N2-C7
8	B	201	NAG	C1-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, 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	A	656/657 (99%)	-0.24	5 (0%) 86 65	6, 26, 62, 103	0
2	B	99/114 (86%)	0.28	7 (7%) 16 5	29, 47, 97, 107	0
3	H	222/230 (96%)	-0.22	0 100 100	10, 31, 64, 86	0
4	L	215/215 (100%)	-0.31	0 100 100	16, 27, 47, 70	0
5	X	164/225 (72%)	1.59	50 (30%) 0 0	52, 92, 122, 138	0
6	Y	206/215 (95%)	1.35	51 (24%) 0 0	50, 94, 145, 160	0
7	C	33/33 (100%)	-0.15	0 100 100	13, 36, 58, 71	0
All	All	1595/1689 (94%)	0.18	113 (7%) 16 5	6, 35, 116, 160	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	Y	11	SER	6.3
5	X	9	GLY	6.0
6	Y	210	VAL	5.9
6	Y	189	TRP	5.2
5	X	197	GLY	5.1
5	X	63	SER	4.9
5	X	170	VAL	4.8
5	X	64	VAL	4.6
6	Y	152	TRP	4.4
5	X	165	ALA	4.4
1	A	30	GLU	4.3
6	Y	124	PRO	4.3
5	X	116	VAL	4.3
6	Y	122	PHE	4.2
5	X	198	THR	4.2
6	Y	112	GLN	4.1
5	X	90	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
6	Y	158	PRO	3.9
6	Y	151	ALA	3.8
5	X	110	TRP	3.8
6	Y	58	SER	3.8
6	Y	88	TYR	3.7
5	X	25	SER	3.7
5	X	124	LYS	3.6
5	X	189	VAL	3.6
2	B	27	PRO	3.6
5	X	91	THR	3.6
6	Y	190	LYS	3.4
6	Y	111	GLY	3.4
6	Y	174	ASN	3.4
6	Y	61	SER	3.3
5	X	96	CYS	3.3
6	Y	59	GLY	3.3
2	B	28	CYS	3.3
2	B	122	ASP	3.2
6	Y	24	GLY	3.2
6	Y	184	LEU	3.2
5	X	74	ASN	3.2
5	X	128	VAL	3.2
5	X	203	CYS	3.2
1	A	502	ASP	3.2
5	X	89	GLU	3.1
6	Y	64	PHE	3.1
5	X	24	ALA	3.1
6	Y	191	SER	3.1
6	Y	40	GLN	3.1
5	X	17	SER	3.1
6	Y	150	VAL	3.0
6	Y	91	ASN	3.0
6	Y	209	THR	3.0
2	B	26	TYR	2.9
6	Y	8	ALA	2.9
5	X	22	CYS	2.9
5	X	28	THR	2.9
5	X	191	VAL	2.8
6	Y	163	VAL	2.8
2	B	54	GLN	2.8
5	X	147	CYS	2.8
5	X	67	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
6	Y	38	TYR	2.8
5	X	62	ASP	2.8
6	Y	195	TYR	2.8
5	X	168	SER	2.7
5	X	44	GLY	2.7
6	Y	132	ASN	2.7
2	B	121	GLU	2.7
2	B	74	LEU	2.6
5	X	11	LEU	2.6
6	Y	211	ALA	2.6
6	Y	153	LYS	2.6
6	Y	77	ILE	2.6
5	X	15	GLY	2.6
5	X	166	LEU	2.6
6	Y	84	ASP	2.5
5	X	85	SER	2.5
5	X	193	SER	2.5
6	Y	183	SER	2.5
6	Y	57	PRO	2.5
5	X	97	ALA	2.5
6	Y	162	GLY	2.5
6	Y	156	SER	2.5
6	Y	196	SER	2.4
6	Y	41	HIS	2.4
6	Y	12	GLY	2.4
5	X	36	TRP	2.4
5	X	65	LYS	2.4
5	X	53	SER	2.4
5	X	114	THR	2.3
6	Y	46	PRO	2.3
5	X	109	MET	2.3
5	X	190	THR	2.3
5	X	79	LEU	2.3
6	Y	125	SER	2.3
1	A	190	ASP	2.2
5	X	123	THR	2.2
5	X	161	TRP	2.2
1	A	49	GLY	2.2
6	Y	80	LEU	2.2
6	Y	197	CYS	2.2
5	X	41	PRO	2.2
6	Y	187	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
5	X	12	VAL	2.1
5	X	209	PRO	2.1
6	Y	136	LEU	2.1
1	A	79	SER	2.1
5	X	167	THR	2.1
6	Y	113	PRO	2.1
5	X	51	ILE	2.1
6	Y	65	SER	2.1
6	Y	116	ALA	2.0
5	X	86	LEU	2.0
6	Y	101	PHE	2.0
6	Y	23	THR	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	HIP	A	154	14/15	0.84	0.22	12,34,50,57	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	B	202	14/15	0.74	0.51	75,86,90,99	0
8	NAG	B	201	14/15	0.85	0.27	28,37,63,65	0
8	NAG	A	701	14/15	0.86	0.22	22,42,58,80	0
8	NAG	A	702	14/15	0.92	0.23	22,25,48,54	0

6.5 Other polymers (i)

There are no such residues in this entry.