Full wwPDB X-ray Structure Validation Report (i)

Dec 11, 2016 – 04:36 PM EST

PDB ID	:	5K9K
Title	:	Crystal structure of multidonor HV6-1-class broadly neutralizing Influenza A antibody 56.a.09 in complex with Hemagglutinin Hong Kong 1968.
Authors	:	Joyce, M.G.; Thomas, P.V.; Wheatley, A.K.; McDermott, A.B.; Mascola, J.R.; Kwong, P.D.
Deposited on	:	2016-05-31
Resolution	:	2.97 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

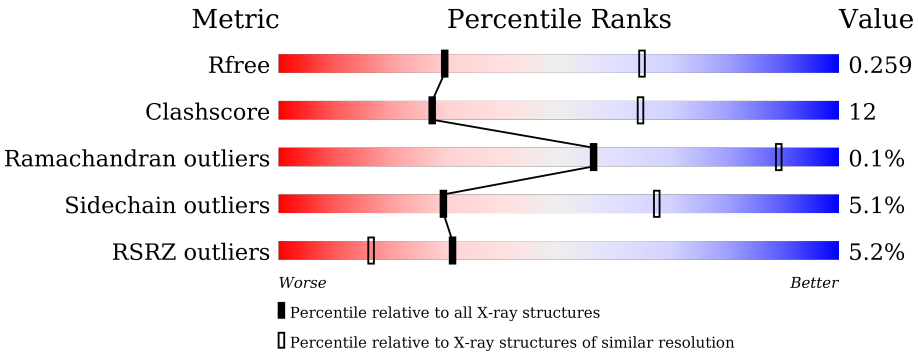
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.97 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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

Mol	Chain	Length	Quality of chain
1	A	229	3% 79% 18%
1	H	229	% 79% 17%
2	B	215	2% 76% 21%
2	L	215	4% 79% 20%
3	F	503	9% 73% 23%
3	I	503	6% 77% 18%

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
4	NAG	I	611	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15108 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 56.a.09 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1710	1082	288	333	7			
1	H	224	Total	C	N	O	S	0	0	0
			1695	1073	285	330	7			

- Molecule 2 is a protein called 56.a.09 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1652	1032	279	336	5			
2	L	215	Total	C	N	O	S	0	0	0
			1652	1032	279	336	5			

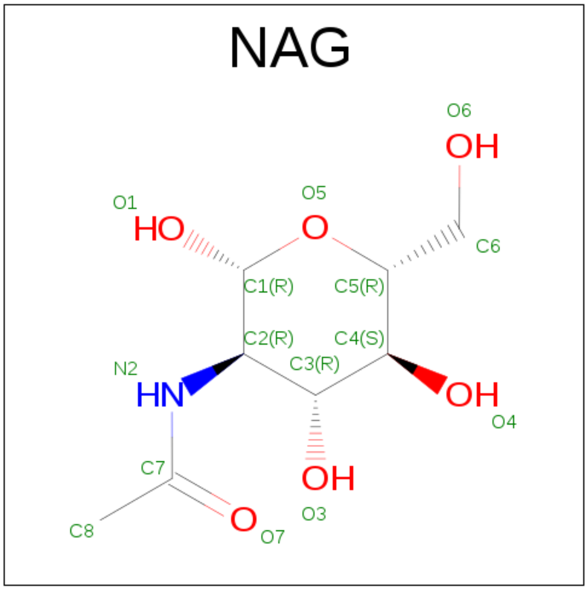
- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	490	Total	C	N	O	S	0	1	0
			3876	2416	681	760	19			
3	F	497	Total	C	N	O	S	0	1	0
			3923	2447	691	766	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	218	GLU	GLY	conflict	UNP Q91MA7
F	218	GLU	GLY	conflict	UNP Q91MA7

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total C N O 14 8 1 5	0	0
4	I	1	Total C N O 14 8 1 5	0	0
4	I	1	Total C N O 14 8 1 5	0	0
4	I	1	Total C N O 14 8 1 5	0	0
4	I	1	Total C N O 14 8 1 5	0	0
4	I	1	Total C N O 14 8 1 5	0	0
4	I	1	Total C N O 14 8 1 5	0	0
4	I	1	Total C N O 14 8 1 5	0	0
4	I	1	Total C N O 14 8 1 5	0	0
4	I	1	Total C N O 14 8 1 5	0	0
4	I	1	Total C N O 14 8 1 5	0	0
4	I	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0

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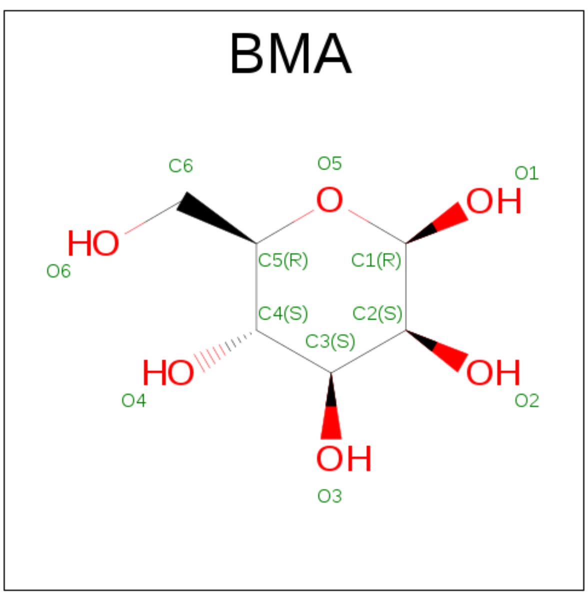
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total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

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total C O 11 6 5	0	0

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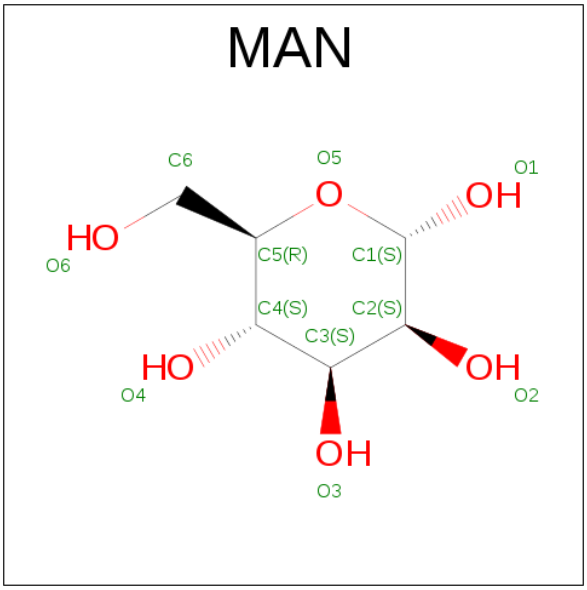
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total C O 11 6 5	0	0
5	I	1	Total C O 11 6 5	0	0
5	I	1	Total C O 11 6 5	0	0
5	F	1	Total C O 11 6 5	0	0
5	F	1	Total C O 11 6 5	0	0
5	F	1	Total C O 11 6 5	0	0
5	F	1	Total C O 11 6 5	0	0
5	F	1	Total C O 11 6 5	0	0

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total C O 11 6 5	0	0
6	I	1	Total C O 11 6 5	0	0
6	I	1	Total C O 11 6 5	0	0

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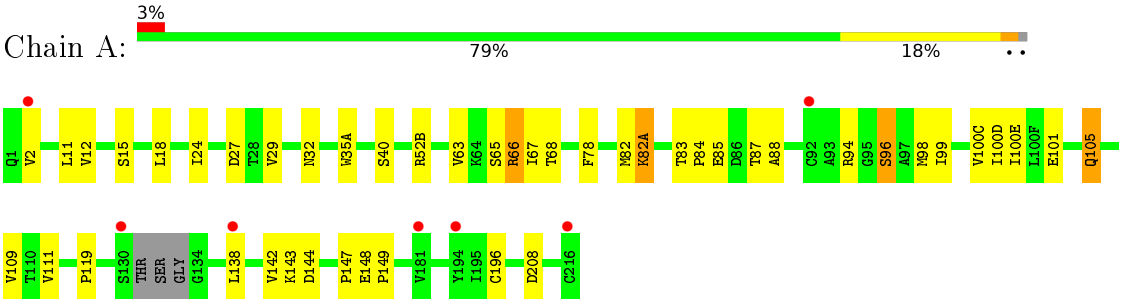
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total C O 11 6 5	0	0
6	I	1	Total C O 11 6 5	0	0
6	I	1	Total C O 11 6 5	0	0
6	F	1	Total C O 11 6 5	0	0
6	F	1	Total C O 11 6 5	0	0
6	F	1	Total C O 11 6 5	0	0
6	F	1	Total C O 11 6 5	0	0
6	F	1	Total C O 11 6 5	0	0
6	F	1	Total C O 11 6 5	0	0
6	F	1	Total C O 11 6 5	0	0
6	F	1	Total C O 11 6 5	0	0
6	F	1	Total C O 11 6 5	0	0

3 Residue-property plots (i)

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

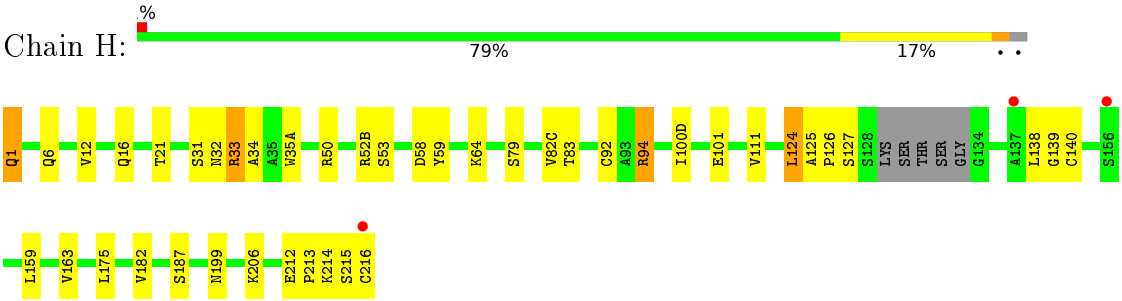
- Molecule 1: 56.a.09 Heavy chain

Chain A:



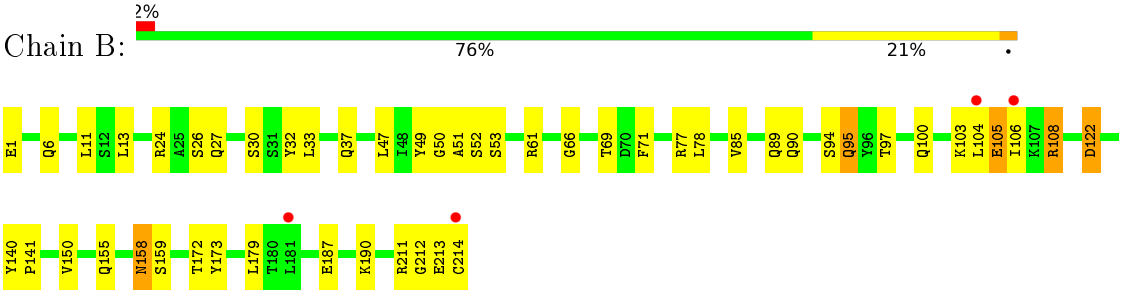
- Molecule 1: 56.a.09 Heavy chain

Chain H:



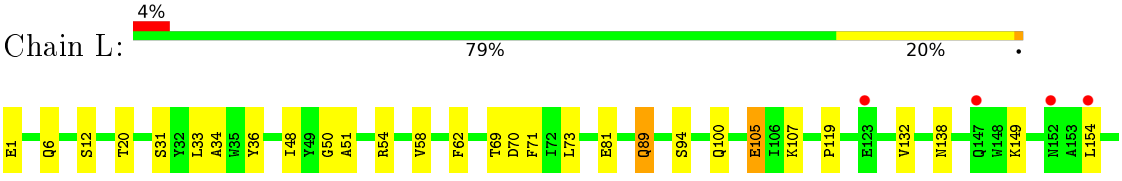
- Molecule 2: 56.a.09 Light chain

Chain B:

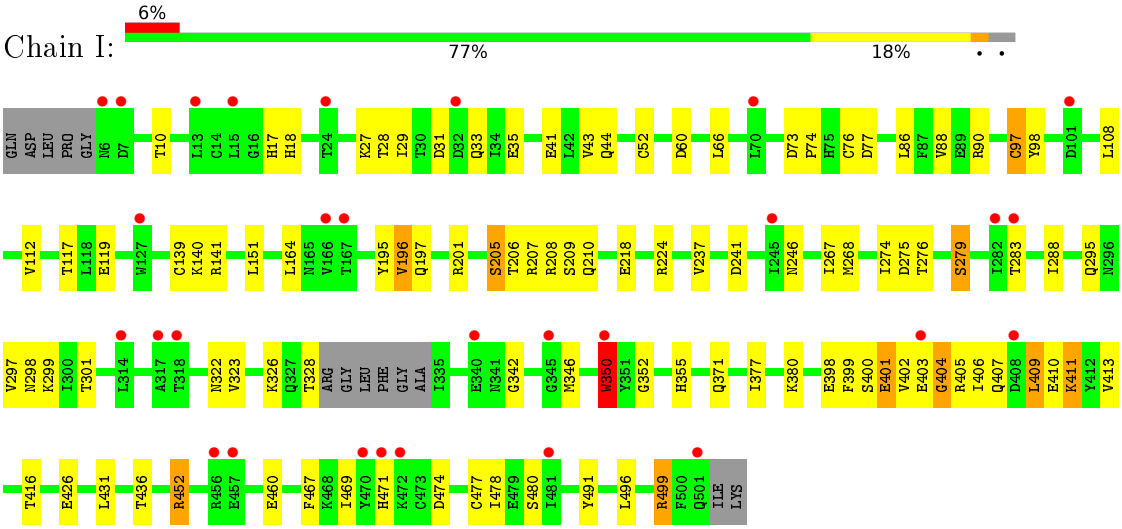


- Molecule 2: 56.a.09 Light chain

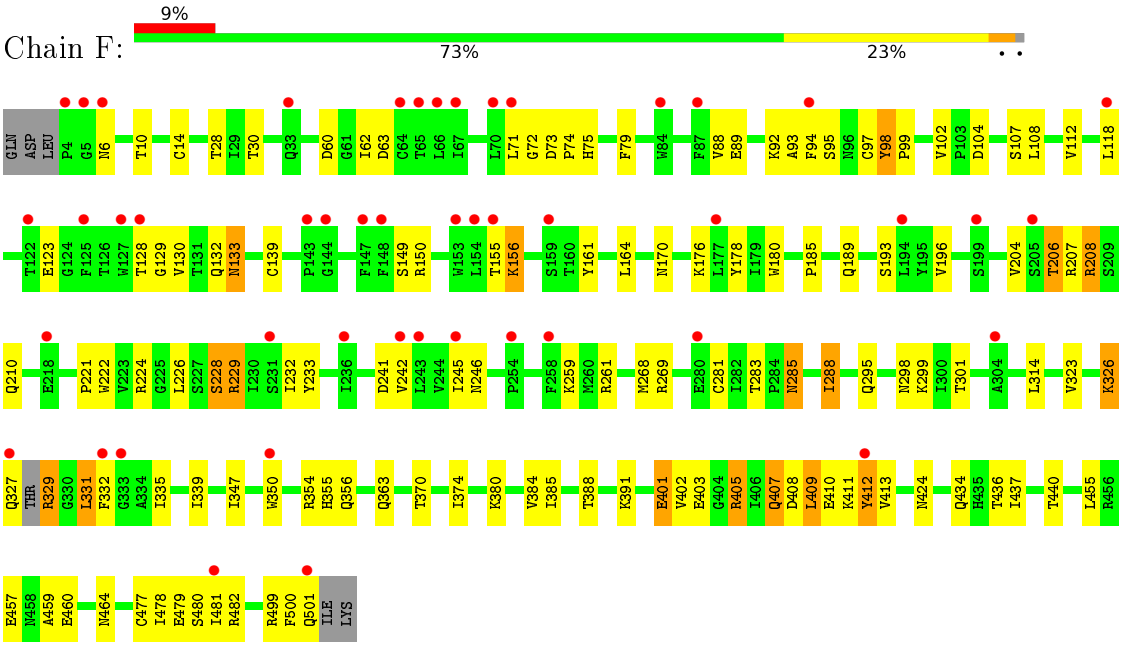
Chain L:



• Molecule 3: Hemagglutinin



• Molecule 3: Hemagglutinin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	123.90Å 136.56Å 311.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.01 – 2.97 46.01 – 2.97	Depositor EDS
% Data completeness (in resolution range)	75.0 (46.01-2.97) 71.6 (46.01-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.225 , 0.265 0.229 , 0.259	Depositor DCC
R_{free} test set	1968 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	59.8	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 20.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	15108	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: BMA, NAG, MAN

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	0.38	0/1750	0.55	1/2386 (0.0%)
1	H	0.36	0/1735	0.52	0/2367
2	B	0.41	0/1687	0.49	0/2288
2	L	0.42	0/1687	0.49	0/2288
3	F	0.34	0/4009	0.52	0/5436
3	I	0.38	0/3960	0.53	3/5372 (0.1%)
All	All	0.38	0/14828	0.52	4/20137 (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
3	I	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	148	GLU	C-N-CD	-9.57	99.55	120.60
3	I	350[A]	TRP	CB-CA-C	-5.78	98.84	110.40
3	I	350[B]	TRP	CB-CA-C	-5.78	98.84	110.40
3	I	404	GLY	N-CA-C	-5.36	99.70	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	350[A]	TRP	Mainchain
3	I	350[B]	TRP	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1710	0	1709	36	0
1	H	1695	0	1691	36	0
2	B	1652	0	1599	47	0
2	L	1652	0	1599	27	0
3	F	3923	0	3776	133	0
3	I	3876	0	3729	84	0
4	F	168	0	146	0	0
4	I	168	0	147	3	0
5	F	55	0	43	0	0
5	I	44	0	35	0	0
6	F	99	0	88	1	0
6	I	66	0	59	0	0
All	All	15108	0	14621	354	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 12.

All (354) 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)
3:F:402:VAL:CG1	3:F:409:LEU:HD11	1.52	1.39
3:F:402:VAL:CG1	3:F:409:LEU:CD1	2.06	1.31
3:F:402:VAL:HG13	3:F:409:LEU:CD1	1.64	1.24
3:F:156:LYS:HE2	3:F:193:SER:O	1.40	1.21
2:B:27:GLN:OE1	4:I:618:NAG:H81	1.43	1.17
3:F:75:HIS:CE1	3:F:94:PHE:CZ	2.35	1.14
3:I:206:THR:HG21	3:I:237:VAL:HG12	1.24	1.10
3:F:75:HIS:HE1	3:F:94:PHE:CZ	1.67	1.10
1:H:215:SER:O	1:H:216:CYS:O	1.78	1.02
2:B:27:GLN:OE1	4:I:618:NAG:C8	2.09	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:401:GLU:O	3:I:402:VAL:HG12	1.58	0.99
3:F:402:VAL:CG1	3:F:409:LEU:HD13	1.88	0.99
3:F:132:GLN:HG3	3:F:133:ASN:H	1.23	0.98
3:I:283:THR:HG22	3:I:301:THR:HG22	1.42	0.97
2:B:105:GLU:OE1	2:B:173:TYR:OH	1.83	0.97
3:F:402:VAL:HG12	3:F:409:LEU:CD1	1.96	0.94
3:I:499:ARG:HG2	3:I:499:ARG:HH21	1.32	0.93
3:F:75:HIS:CE1	3:F:94:PHE:CE2	2.59	0.89
3:I:206:THR:CG2	3:I:237:VAL:HG12	2.02	0.89
3:F:329:ARG:HH11	3:F:329:ARG:HG2	1.39	0.88
3:I:346:MET:SD	3:I:352:GLY:HA3	2.16	0.86
3:F:75:HIS:HE1	3:F:94:PHE:CE2	1.93	0.86
3:I:117:THR:OG1	3:I:119:GLU:HG3	1.76	0.86
2:B:212:GLY:O	2:B:213:GLU:HG3	1.77	0.84
3:F:326:LYS:HG3	3:F:327:GLN:N	1.91	0.84
3:F:281:CYS:SG	3:F:288:ILE:HD11	2.17	0.84
3:I:298:ASN:OD1	3:I:299:LYS:N	2.11	0.83
3:I:409:LEU:HD13	3:I:411:LYS:HD3	1.61	0.81
3:F:207:ARG:HG3	3:F:208:ARG:HD2	1.64	0.79
3:F:62:ILE:HD12	3:F:62:ILE:H	1.47	0.79
3:F:329:ARG:HH22	3:F:464:ASN:HD22	1.27	0.79
2:B:24:ARG:NH1	2:B:69:THR:O	2.16	0.78
1:A:32:ASN:O	1:A:52(B):ARG:NH1	2.15	0.78
3:F:156:LYS:CE	3:F:193:SER:O	2.27	0.78
1:H:35(A):TRP:CZ3	1:H:94:ARG:HG3	2.18	0.77
2:B:108:ARG:HD3	2:B:140:TYR:HB3	1.66	0.77
3:I:406:ILE:O	3:I:410:GLU:HG2	1.84	0.77
3:I:201:ARG:HB3	3:I:201:ARG:CZ	2.14	0.77
3:F:479:GLU:OE1	3:F:482:ARG:NH2	2.17	0.77
3:F:75:HIS:HE1	3:F:94:PHE:CE1	2.02	0.77
3:I:206:THR:HG21	3:I:237:VAL:CG1	2.11	0.76
2:B:150:VAL:CG1	2:B:155:GLN:OE1	2.33	0.76
3:F:73:ASP:OD1	3:F:74:PRO:HD2	1.86	0.75
1:H:1:GLN:NE2	6:F:610:MAN:O3	2.18	0.75
1:A:66:ARG:O	1:A:82(A):LYS:HG3	1.85	0.75
3:F:221:PRO:O	3:F:229:ARG:NH1	2.19	0.75
3:I:380:LYS:NZ	3:I:436:THR:OG1	2.18	0.75
1:A:24:ILE:HD12	1:A:29:VAL:HG22	1.68	0.74
3:I:452:ARG:HG3	3:I:467:PHE:CE1	2.22	0.74
3:F:402:VAL:HG13	3:F:409:LEU:HD11	0.76	0.74
2:B:108:ARG:HD3	2:B:140:TYR:CB	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:401:GLU:N	3:F:401:GLU:OE1	2.21	0.74
3:I:18:HIS:HD1	3:I:350[B]:TRP:HZ3	1.35	0.73
3:F:410:GLU:HA	3:F:410:GLU:OE1	1.89	0.72
3:I:460:GLU:OE1	3:I:499:ARG:NH1	2.19	0.72
3:F:460:GLU:OE2	3:F:499:ARG:NE	2.23	0.71
3:F:97:CYS:O	3:F:224:ARG:NH1	2.23	0.71
1:H:6:GLN:OE1	1:H:92:CYS:N	2.18	0.71
2:B:158:ASN:HD22	2:B:158:ASN:H	1.39	0.70
3:F:402:VAL:HG12	3:F:409:LEU:HD13	1.60	0.70
3:F:62:ILE:HD12	3:F:62:ILE:N	2.06	0.70
3:F:132:GLN:HG3	3:F:133:ASN:N	2.02	0.70
3:F:207:ARG:HG2	3:F:241:ASP:OD1	1.91	0.70
3:I:346:MET:CE	3:I:352:GLY:HA3	2.22	0.69
3:F:133:ASN:O	3:F:133:ASN:ND2	2.25	0.69
1:A:63:VAL:O	1:A:67:ILE:HG22	1.92	0.69
3:I:195:TYR:O	3:I:196:VAL:HG12	1.92	0.69
3:F:405:ARG:HD3	3:F:405:ARG:H	1.58	0.69
3:F:385:ILE:HA	3:F:388:THR:HG22	1.74	0.69
3:F:28:THR:OG1	3:F:434:GLN:HB2	1.94	0.68
3:I:97:CYS:O	3:I:224:ARG:NH2	2.28	0.67
2:B:30:SER:OG	3:I:371:GLN:NE2	2.26	0.67
3:F:409:LEU:C	3:F:409:LEU:HD23	2.15	0.67
3:I:409:LEU:HD12	3:I:409:LEU:C	2.16	0.66
3:I:27:LYS:NZ	3:I:426:GLU:OE2	2.23	0.66
1:A:2:VAL:HG11	1:A:94:ARG:NH2	2.10	0.66
3:F:62:ILE:H	3:F:62:ILE:CD1	2.09	0.66
2:L:54:ARG:HG2	2:L:58:VAL:HG23	1.76	0.66
2:L:81:GLU:HG2	2:L:81:GLU:O	1.94	0.66
3:I:401:GLU:O	3:I:402:VAL:CG1	2.41	0.65
3:F:98:TYR:HD1	3:F:99:PRO:HD2	1.62	0.65
3:F:6:ASN:ND2	3:F:10:THR:O	2.30	0.65
3:F:326:LYS:HG3	3:F:327:GLN:H	1.61	0.65
3:F:75:HIS:CE1	3:F:94:PHE:CE1	2.82	0.65
1:H:100(D):ILE:HD11	3:F:347:ILE:HD12	1.79	0.65
1:H:82(C):VAL:HG11	1:H:111:VAL:HG11	1.79	0.65
3:F:156:LYS:HB2	3:F:196:VAL:CG2	2.26	0.65
3:F:405:ARG:O	3:F:408:ASP:N	2.30	0.64
1:A:143:LYS:NZ	1:A:144:ASP:OD1	2.31	0.64
3:F:412:TYR:HD1	3:F:413:VAL:N	1.95	0.64
1:A:100(D):ILE:HD12	1:A:100(D):ILE:N	2.12	0.64
3:I:399:PHE:HZ	3:I:416:THR:HG23	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:410:GLU:O	3:I:413:VAL:HG22	1.98	0.63
2:B:150:VAL:HG12	2:B:155:GLN:OE1	1.98	0.63
3:F:380:LYS:NZ	3:F:436:THR:OG1	2.27	0.62
3:F:331:LEU:HG	3:F:332:PHE:N	2.13	0.62
3:F:281:CYS:SG	3:F:288:ILE:CD1	2.87	0.62
3:I:201:ARG:NH2	3:I:246:ASN:OD1	2.32	0.62
3:F:329:ARG:NH1	3:F:329:ARG:HG2	2.12	0.62
2:L:105:GLU:OE1	2:L:173:TYR:OH	2.17	0.62
3:I:201:ARG:HB3	3:I:201:ARG:NH1	2.15	0.62
3:I:196:VAL:HG12	3:I:197:GLN:OE1	2.00	0.62
3:I:288:ILE:HD13	3:I:297:VAL:HG11	1.82	0.61
3:I:77:ASP:OD2	3:I:141:ARG:NH2	2.34	0.61
1:H:33:ARG:H	1:H:52(B):ARG:NH1	1.98	0.61
3:F:98:TYR:N	3:F:139:CYS:SG	2.73	0.61
1:A:18:LEU:HD11	1:A:109:VAL:HG21	1.83	0.61
3:I:402:VAL:HG22	3:I:402:VAL:O	2.01	0.61
3:F:329:ARG:NH2	3:F:464:ASN:HD22	1.98	0.61
1:H:159:LEU:HD21	1:H:182:VAL:HG11	1.83	0.60
3:I:409:LEU:O	3:I:409:LEU:HD12	2.00	0.60
1:A:63:VAL:HG12	1:A:63:VAL:O	2.00	0.60
2:B:158:ASN:H	2:B:158:ASN:ND2	1.98	0.60
2:B:90:GLN:HE21	2:B:97:THR:HB	1.67	0.60
3:I:406:ILE:HD11	3:I:409:LEU:HB3	1.83	0.59
1:H:32:ASN:O	1:H:33:ARG:HG2	2.03	0.59
1:H:216:CYS:HA	2:L:214:CYS:HB2	1.85	0.59
2:B:6:GLN:O	2:B:100:GLN:NE2	2.36	0.58
3:F:14:CYS:SG	3:F:335:ILE:HG22	2.44	0.58
2:B:27:GLN:OE1	4:I:618:NAG:H83	2.03	0.58
3:I:410:GLU:OE1	3:I:410:GLU:HA	2.04	0.58
3:F:354:ARG:NE	3:F:363:GLN:OE1	2.27	0.58
2:B:108:ARG:CG	2:B:140:TYR:CG	2.86	0.57
3:I:452:ARG:HG3	3:I:467:PHE:CZ	2.39	0.57
3:F:73:ASP:OD1	3:F:74:PRO:CD	2.51	0.57
3:F:185:PRO:HA	3:F:228:SER:HB3	1.86	0.57
3:F:412:TYR:CE1	3:F:413:VAL:CG2	2.87	0.57
1:A:208:ASP:OD1	1:A:208:ASP:O	2.22	0.57
2:B:106:ILE:HD13	2:B:106:ILE:N	2.19	0.57
2:B:108:ARG:HG3	2:B:140:TYR:CD2	2.40	0.56
3:F:149:SER:OG	3:F:150:ARG:HD3	2.05	0.56
2:B:190:LYS:O	2:B:211:ARG:N	2.23	0.56
3:F:412:TYR:CE1	3:F:413:VAL:HG23	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ARG:HH21	2:B:172:THR:HG22	1.70	0.56
3:F:95:SER:O	3:F:224:ARG:NH2	2.38	0.56
3:F:102:VAL:HG22	3:F:232:ILE:HB	1.87	0.56
3:F:206:THR:HG23	3:F:242:VAL:O	2.06	0.56
3:F:63:ASP:O	3:F:93:ALA:HA	2.06	0.56
1:H:12:VAL:HB	1:H:111:VAL:HG12	1.87	0.56
3:I:499:ARG:CG	3:I:499:ARG:HH21	2.09	0.55
3:I:73:ASP:HB3	3:I:76:CYS:SG	2.46	0.55
2:B:108:ARG:HG2	2:B:140:TYR:CG	2.40	0.55
3:F:412:TYR:CD1	3:F:413:VAL:N	2.73	0.55
3:I:10:THR:OG1	3:I:469:ILE:O	2.16	0.55
3:F:391:LYS:HE2	3:F:424:ASN:OD1	2.07	0.55
1:H:34:ALA:HB1	1:H:94:ARG:HD3	1.88	0.55
1:A:96:SER:OG	1:A:101:GLU:OE1	2.24	0.55
1:A:100(C):VAL:HG12	1:A:100(C):VAL:O	2.05	0.55
1:H:126:PRO:HG3	1:H:138:LEU:HB3	1.89	0.55
2:B:122:ASP:N	2:B:122:ASP:OD1	2.40	0.54
3:F:89:GLU:HB2	3:F:269:ARG:HG2	1.88	0.54
2:B:108:ARG:HH21	2:B:172:THR:CG2	2.20	0.54
3:F:436:THR:O	3:F:440:THR:HG22	2.07	0.54
3:F:350[A]:TRP:CZ3	3:F:374:ILE:HG22	2.43	0.54
2:B:105:GLU:HG3	2:B:105:GLU:O	2.05	0.54
1:A:12:VAL:O	1:A:111:VAL:HA	2.07	0.54
1:H:31:SER:OG	1:H:32:ASN:O	2.25	0.54
2:B:108:ARG:NH2	2:B:172:THR:CG2	2.71	0.53
3:F:455:LEU:HD11	3:F:481:ILE:HD13	1.89	0.53
1:H:124:LEU:HB2	1:H:139:GLY:O	2.08	0.53
2:B:158:ASN:HD22	2:B:158:ASN:N	2.02	0.53
1:H:215:SER:C	1:H:216:CYS:O	2.42	0.53
1:A:12:VAL:HG13	1:A:111:VAL:HG12	1.90	0.53
1:H:82(C):VAL:HG12	1:H:83:THR:H	1.74	0.53
2:L:6:GLN:O	2:L:100:GLN:NE2	2.42	0.53
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.90	0.53
1:A:100(D):ILE:CD1	1:A:100(D):ILE:H	2.22	0.53
1:H:100(D):ILE:CD1	3:F:347:ILE:HD12	2.38	0.53
3:F:410:GLU:O	3:F:411:LYS:HB2	2.09	0.52
1:A:67:ILE:HG12	1:A:68:THR:N	2.24	0.52
2:L:50:GLY:O	2:L:51:ALA:HB3	2.08	0.52
1:H:33:ARG:H	1:H:52(B):ARG:CZ	2.23	0.52
1:A:100(D):ILE:CD1	1:A:100(D):ILE:N	2.73	0.52
1:A:2:VAL:HG12	1:A:27:ASP:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:GLY:O	2:B:51:ALA:HB3	2.09	0.52
3:I:499:ARG:HG2	3:I:499:ARG:NH2	2.11	0.52
3:I:275:ASP:OD1	3:I:276:THR:N	2.42	0.52
1:H:21:THR:HG22	1:H:79:SER:HB3	1.91	0.52
1:H:124:LEU:HB2	1:H:139:GLY:C	2.31	0.51
1:A:63:VAL:CG1	1:A:82:MET:HE2	2.41	0.51
3:F:335:ILE:HG13	3:F:356:GLN:HB2	1.92	0.51
2:L:33:LEU:HD22	2:L:71:PHE:CG	2.45	0.51
1:A:100(C):VAL:HG22	2:B:32:TYR:CZ	2.46	0.51
3:F:412:TYR:HE1	3:F:413:VAL:HG22	1.76	0.51
3:I:97:CYS:O	3:I:98:TYR:C	2.50	0.51
3:I:402:VAL:O	3:I:402:VAL:HG13	2.11	0.51
3:F:71:LEU:HD11	3:F:232:ILE:CD1	2.41	0.50
1:H:6:GLN:OE1	1:H:92:CYS:HB3	2.11	0.50
3:F:412:TYR:HD1	3:F:412:TYR:C	2.15	0.50
1:H:6:GLN:OE1	1:H:92:CYS:CB	2.59	0.50
3:I:323:VAL:HG23	3:I:342:GLY:H	1.76	0.50
3:I:86:LEU:HD11	3:I:268:MET:HG2	1.92	0.50
3:I:28:THR:HG23	3:I:31:ASP:H	1.77	0.50
3:I:452:ARG:HG3	3:I:467:PHE:HE1	1.73	0.49
3:F:385:ILE:HA	3:F:388:THR:CG2	2.40	0.49
1:A:138:LEU:C	1:A:138:LEU:HD12	2.32	0.49
3:F:79:PHE:O	3:F:118:LEU:HD23	2.13	0.49
3:F:204:VAL:HG23	3:F:245:ILE:HG12	1.95	0.49
3:F:208:ARG:HD2	3:F:208:ARG:N	2.27	0.49
3:F:104:ASP:HB3	3:F:107:SER:HB2	1.95	0.49
1:H:16:GLN:O	1:H:82(C):VAL:HG23	2.12	0.49
3:F:132:GLN:CG	3:F:133:ASN:H	2.03	0.49
3:F:98:TYR:CE1	3:F:226:LEU:HD13	2.48	0.49
3:F:477:CYS:O	3:F:480:SER:OG	2.21	0.49
1:H:50:ARG:HG2	1:H:58:ASP:HB2	1.94	0.49
3:I:201:ARG:NH1	3:I:201:ARG:CB	2.75	0.49
3:I:399:PHE:O	3:I:399:PHE:HD1	1.96	0.49
1:A:63:VAL:HG13	1:A:82:MET:HE2	1.95	0.48
3:F:457:GLU:O	3:F:499:ARG:NH2	2.45	0.48
3:I:406:ILE:HG13	3:I:409:LEU:H	1.78	0.48
3:I:164:LEU:O	3:I:246:ASN:HA	2.14	0.48
1:H:199:ASN:HB2	1:H:206:LYS:HE2	1.95	0.48
2:L:119:PRO:HB3	2:L:209:PHE:CE2	2.48	0.48
3:F:329:ARG:NH1	3:F:329:ARG:CG	2.73	0.48
3:F:71:LEU:HD11	3:F:232:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:TYR:HB2	1:H:64:LYS:HD3	1.96	0.48
3:I:33:GLN:OE1	3:I:33:GLN:N	2.47	0.48
3:F:72:GLY:HA3	3:F:149:SER:HB3	1.96	0.47
3:F:326:LYS:HG3	3:F:327:GLN:HG2	1.95	0.47
3:I:460:GLU:HB3	3:I:499:ARG:NH1	2.29	0.47
3:F:323:VAL:HG23	3:F:323:VAL:O	2.13	0.47
3:I:402:VAL:HG13	3:I:404:GLY:O	2.14	0.47
1:H:214:LYS:NZ	2:L:119:PRO:HD2	2.29	0.47
3:I:35:GLU:HG2	3:I:322:ASN:HD22	1.80	0.47
3:I:44:GLN:H	3:I:295:GLN:HA	1.79	0.47
1:A:100(D):ILE:H	1:A:100(D):ILE:HD12	1.77	0.47
3:I:60:ASP:HA	3:I:88:VAL:HG22	1.97	0.47
3:F:412:TYR:C	3:F:412:TYR:CD1	2.87	0.47
3:F:385:ILE:CA	3:F:388:THR:HG22	2.42	0.47
3:F:412:TYR:CD1	3:F:413:VAL:HG23	2.50	0.47
3:I:74:PRO:HG2	3:I:139:CYS:HB3	1.95	0.47
2:B:30:SER:O	2:B:51:ALA:HB2	2.15	0.47
2:B:90:GLN:HE21	2:B:97:THR:CB	2.28	0.47
3:F:189:GLN:O	3:F:193:SER:OG	2.22	0.46
3:I:477:CYS:O	3:I:480:SER:OG	2.23	0.46
3:F:402:VAL:HG11	3:F:409:LEU:HD13	1.89	0.46
2:L:190:LYS:O	2:L:211:ARG:N	2.46	0.46
3:I:406:ILE:HG13	3:I:406:ILE:O	2.15	0.46
2:L:161:GLU:HA	2:L:177:SER:HA	1.98	0.46
1:H:163:VAL:HG22	1:H:182:VAL:HG22	1.98	0.46
2:B:13:LEU:HD13	2:B:78:LEU:HD11	1.97	0.46
1:H:125:ALA:HA	1:H:126:PRO:HD3	1.80	0.46
3:I:41:GLU:OE2	3:I:43:VAL:HG22	2.16	0.46
3:F:500:PHE:O	3:F:501:GLN:HB2	2.16	0.46
1:H:215:SER:O	1:H:216:CYS:C	2.52	0.46
3:I:52:CYS:SG	3:I:279:SER:HB2	2.56	0.46
1:A:105:GLN:HG3	1:A:105:GLN:H	1.42	0.45
2:L:149:LYS:NZ	2:L:154:LEU:HD21	2.32	0.45
3:I:346:MET:HE1	3:I:352:GLY:HA3	1.96	0.45
3:I:399:PHE:CD1	3:I:399:PHE:O	2.69	0.45
3:I:151:LEU:HA	3:I:151:LEU:HD23	1.79	0.45
2:L:34:ALA:HB3	2:L:89:GLN:HG2	1.97	0.45
2:B:108:ARG:HD3	2:B:140:TYR:HB2	1.98	0.45
3:I:205:SER:HB3	3:I:210:GLN:HG3	1.98	0.45
2:L:12:SER:O	2:L:107:LYS:NZ	2.50	0.45
2:B:24:ARG:NH2	2:L:69:THR:HG21	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:259:LYS:HE3	3:F:261:ARG:HG3	1.98	0.45
3:F:329:ARG:NH2	3:F:464:ASN:ND2	2.64	0.45
2:L:163:VAL:HG22	2:L:175:LEU:HD12	1.98	0.45
1:H:124:LEU:HD12	1:H:124:LEU:HA	1.69	0.45
1:H:212:GLU:HA	1:H:213:PRO:HD3	1.70	0.45
3:F:412:TYR:CE1	3:F:413:VAL:HG22	2.50	0.44
3:I:66:LEU:HD22	3:I:267:ILE:HD12	1.99	0.44
3:I:474:ASP:OD1	3:I:474:ASP:N	2.50	0.44
2:L:48:ILE:HD12	2:L:73:LEU:HD13	2.00	0.44
3:I:399:PHE:HZ	3:I:416:THR:CG2	2.29	0.44
1:A:11:LEU:HB2	1:A:147:PRO:HG3	1.98	0.44
3:I:499:ARG:CG	3:I:499:ARG:NH2	2.73	0.44
2:L:33:LEU:HD22	2:L:71:PHE:CD1	2.52	0.44
2:B:49:TYR:O	2:B:53:SER:HB2	2.17	0.44
3:I:377:ILE:HA	3:I:380:LYS:HG3	1.98	0.44
1:H:82(C):VAL:HG12	1:H:83:THR:N	2.33	0.44
1:A:40:SER:HB3	1:A:88:ALA:HB2	2.00	0.44
3:F:380:LYS:HZ2	3:F:436:THR:HG1	1.57	0.44
3:I:355:HIS:CG	3:I:478:ILE:HD13	2.53	0.44
2:B:1:GLU:HG3	2:B:95:GLN:NE2	2.32	0.44
3:F:283:THR:HG22	3:F:301:THR:HG22	1.99	0.44
1:A:35(A):TRP:HB3	1:A:78:PHE:CZ	2.53	0.44
3:F:108:LEU:O	3:F:112:VAL:HG12	2.18	0.44
3:F:207:ARG:HG3	3:F:208:ARG:N	2.33	0.44
1:A:63:VAL:HG11	1:A:82:MET:CE	2.47	0.43
3:F:128:THR:HA	3:F:129:GLY:HA2	1.59	0.43
3:F:384:VAL:O	3:F:388:THR:HG22	2.18	0.43
3:F:60:ASP:HB3	3:F:62:ILE:CD1	2.48	0.43
2:L:132:VAL:HG13	2:L:179:LEU:HB3	2.00	0.43
3:F:88:VAL:HA	3:F:268:MET:O	2.18	0.43
3:F:405:ARG:O	3:F:407:GLN:N	2.51	0.43
3:I:460:GLU:CD	3:I:499:ARG:HH12	2.12	0.43
3:F:329:ARG:HD2	3:F:329:ARG:HA	1.69	0.43
1:A:100(E):ILE:HD13	2:B:49:TYR:HB2	1.99	0.43
3:F:437:ILE:HA	3:F:440:THR:HG22	1.99	0.43
3:F:402:VAL:HG11	3:F:409:LEU:CD1	2.32	0.43
3:F:355:HIS:CG	3:F:478:ILE:HD13	2.54	0.43
3:I:496:LEU:O	3:I:499:ARG:O	2.36	0.43
2:B:85:VAL:HG22	2:B:103:LYS:HD3	2.01	0.43
2:B:108:ARG:CD	2:B:140:TYR:CB	2.92	0.43
3:F:259:LYS:HE2	3:F:259:LYS:HB3	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:314:LEU:HD23	3:F:314:LEU:HA	1.92	0.43
2:B:61:ARG:NH1	2:B:77:ARG:O	2.52	0.42
2:L:191:VAL:HG22	2:L:210:ASN:OD1	2.19	0.42
1:A:119:PRO:HB2	1:A:142:VAL:HG13	2.01	0.42
3:F:405:ARG:N	3:F:405:ARG:HD3	2.28	0.42
3:I:399:PHE:CZ	3:I:416:THR:HG23	2.49	0.42
3:F:403:GLU:O	3:F:403:GLU:HG3	2.20	0.42
3:F:455:LEU:HD23	3:F:459:ALA:HB3	2.00	0.42
3:F:170:ASN:HB2	3:F:176:LYS:HZ2	1.84	0.42
1:A:83:THR:HG23	1:A:85:GLU:H	1.85	0.42
2:B:11:LEU:HD23	2:B:104:LEU:HD13	2.01	0.42
3:F:60:ASP:HB3	3:F:62:ILE:HD11	2.02	0.42
1:H:126:PRO:HD2	1:H:213:PRO:HA	2.01	0.42
2:L:185:ASP:HA	2:L:188:LYS:HD2	2.00	0.42
2:B:150:VAL:HG11	2:B:155:GLN:OE1	2.18	0.42
2:B:66:GLY:HA3	2:B:71:PHE:HA	2.02	0.42
1:H:52(B):ARG:O	1:H:53:SER:OG	2.28	0.42
3:I:206:THR:CG2	3:I:237:VAL:CG1	2.85	0.42
2:L:186:TYR:O	2:L:192:TYR:OH	2.38	0.42
1:A:84:PRO:HA	1:A:111:VAL:HG23	2.02	0.42
2:L:138:ASN:HA	2:L:173:TYR:O	2.20	0.42
3:F:180:TRP:CZ2	3:F:204:VAL:HG11	2.54	0.42
3:F:180:TRP:CZ2	3:F:233:TYR:HB2	2.54	0.42
3:F:370:THR:O	3:F:374:ILE:HG23	2.20	0.42
3:I:29:ILE:HD11	3:I:431:LEU:CD2	2.50	0.42
1:A:143:LYS:NZ	1:A:144:ASP:CG	2.73	0.41
2:B:108:ARG:NH2	2:B:172:THR:HG22	2.33	0.41
3:F:156:LYS:CB	3:F:196:VAL:CG2	2.97	0.41
3:F:326:LYS:CG	3:F:327:GLN:N	2.75	0.41
3:F:403:GLU:H	3:F:403:GLU:HG2	1.69	0.41
1:A:87:THR:OG1	1:A:111:VAL:HG22	2.20	0.41
2:B:108:ARG:HG2	2:B:140:TYR:CD1	2.55	0.41
3:F:28:THR:HG23	3:F:30:THR:H	1.85	0.41
3:I:471:HIS:CD2	3:I:491:TYR:HB3	2.55	0.41
2:L:54:ARG:NH1	2:L:62:PHE:O	2.53	0.41
2:B:211:ARG:HG2	2:B:212:GLY:N	2.35	0.41
2:B:140:TYR:CG	2:B:141:PRO:HA	2.55	0.41
3:F:156:LYS:HB2	3:F:196:VAL:HG23	2.01	0.41
3:F:123:GLU:OE1	3:F:178:TYR:OH	2.27	0.41
3:I:409:LEU:CD1	3:I:411:LYS:HD3	2.43	0.41
3:I:409:LEU:C	3:I:409:LEU:CD1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:412:TYR:HE1	3:F:413:VAL:CG2	2.31	0.41
2:L:36:TYR:HE1	2:L:89:GLN:HG2	1.86	0.41
3:F:339:ILE:HD13	3:F:339:ILE:HA	1.92	0.41
3:I:398:GLU:C	3:I:400:SER:H	2.23	0.41
2:L:31:SER:OG	3:F:374:ILE:HD11	2.21	0.40
3:I:108:LEU:O	3:I:112:VAL:HG12	2.21	0.40
3:I:207:ARG:HG3	3:I:241:ASP:OD1	2.20	0.40
3:F:409:LEU:C	3:F:409:LEU:CD2	2.85	0.40
1:A:2:VAL:CG1	1:A:94:ARG:NH2	2.82	0.40
1:A:99:ILE:HD12	1:A:100(C):VAL:HG11	2.03	0.40
3:F:298:ASN:OD1	3:F:299:LYS:N	2.55	0.40
3:I:401:GLU:C	3:I:402:VAL:HG12	2.34	0.40
2:L:214:CYS:O	2:L:214:CYS:SG	2.79	0.40
3:F:164:LEU:O	3:F:246:ASN:HA	2.21	0.40
3:F:285:ASN:N	3:F:285:ASN:OD1	2.55	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	222/229 (97%)	210 (95%)	11 (5%)	1 (0%)	34 75
1	H	220/229 (96%)	207 (94%)	13 (6%)	0	100 100
2	B	213/215 (99%)	207 (97%)	6 (3%)	0	100 100
2	L	213/215 (99%)	208 (98%)	5 (2%)	0	100 100
3	F	494/503 (98%)	470 (95%)	24 (5%)	0	100 100
3	I	487/503 (97%)	467 (96%)	20 (4%)	0	100 100
All	All	1849/1894 (98%)	1769 (96%)	79 (4%)	1 (0%)	56 89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/200 (99%)	190 (96%)	8 (4%)	38	75
1	H	196/200 (98%)	187 (95%)	9 (5%)	33	71
2	B	185/185 (100%)	171 (92%)	14 (8%)	16	49
2	L	185/185 (100%)	177 (96%)	8 (4%)	35	74
3	F	435/440 (99%)	411 (94%)	24 (6%)	27	64
3	I	432/440 (98%)	412 (95%)	20 (5%)	33	71
All	All	1631/1650 (99%)	1548 (95%)	83 (5%)	29	67

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	65	SER
1	A	66	ARG
1	A	82(A)	LYS
1	A	96	SER
1	A	98	MET
1	A	105	GLN
1	A	196	CYS
2	B	26	SER
2	B	33	LEU
2	B	52	SER
2	B	89	GLN
2	B	94	SER
2	B	95	GLN
2	B	105	GLU
2	B	108	ARG
2	B	122	ASP
2	B	158	ASN

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Mol	Chain	Res	Type
2	B	159	SER
2	B	179	LEU
2	B	187	GLU
2	B	214	CYS
3	I	90	ARG
3	I	97	CYS
3	I	140	LYS
3	I	196	VAL
3	I	205	SER
3	I	208	ARG
3	I	209	SER
3	I	218	GLU
3	I	274	ILE
3	I	279	SER
3	I	326	LYS
3	I	328	THR
3	I	401	GLU
3	I	403	GLU
3	I	405	ARG
3	I	407	GLN
3	I	409	LEU
3	I	411	LYS
3	I	452	ARG
3	I	499	ARG
1	H	1	GLN
1	H	33	ARG
1	H	94	ARG
1	H	101	GLU
1	H	124	LEU
1	H	127	SER
1	H	140	CYS
1	H	175	LEU
1	H	187	SER
2	L	1	GLU
2	L	20	THR
2	L	70	ASP
2	L	89	GLN
2	L	94	SER
2	L	105	GLU
2	L	213	GLU
2	L	214	CYS
3	F	92	LYS

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Mol	Chain	Res	Type
3	F	98	TYR
3	F	130	VAL
3	F	133	ASN
3	F	155	THR
3	F	156	LYS
3	F	161	TYR
3	F	206	THR
3	F	208	ARG
3	F	210	GLN
3	F	222	TRP
3	F	228	SER
3	F	229	ARG
3	F	285	ASN
3	F	288	ILE
3	F	295	GLN
3	F	326	LYS
3	F	329	ARG
3	F	331	LEU
3	F	401	GLU
3	F	405	ARG
3	F	407	GLN
3	F	409	LEU
3	F	412	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	95	GLN
2	B	155	GLN
2	B	158	ASN
3	I	327	GLN
3	I	371	GLN
1	H	1	GLN
2	L	147	GLN
3	F	6	ASN
3	F	75	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

48 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	$\#\|Z\| > 2$
4	NAG	F	601	3	14,14,15	0.17	0	15,19,21	0.32	0
4	NAG	F	602	3,4	14,14,15	0.33	0	15,19,21	0.39	0
4	NAG	F	603	5,4	14,14,15	0.24	0	15,19,21	0.42	0
5	BMA	F	604	4,6	11,11,12	0.71	0	15,15,17	0.89	0
6	MAN	F	605	5	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
6	MAN	F	606	5	11,11,12	0.79	1 (9%)	15,15,17	1.30	2 (13%)
4	NAG	F	607	3,4	14,14,15	0.36	0	15,19,21	0.60	0
4	NAG	F	608	5,4	14,14,15	0.21	0	15,19,21	0.68	0
5	BMA	F	609	4,6	11,11,12	0.60	0	15,15,17	0.86	0
6	MAN	F	610	5	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
6	MAN	F	611	5,6	11,11,12	0.73	0	15,15,17	1.10	2 (13%)
6	MAN	F	612	6	11,11,12	0.73	0	15,15,17	0.96	1 (6%)
4	NAG	F	613	3,4	14,14,15	0.52	0	15,19,21	0.65	0
4	NAG	F	614	5,4	14,14,15	0.28	0	15,19,21	0.28	0
5	BMA	F	615	4	11,11,12	0.61	0	15,15,17	0.70	0
4	NAG	F	616	3,4	14,14,15	1.02	1 (7%)	15,19,21	0.83	0
4	NAG	F	617	5,4	14,14,15	0.20	0	15,19,21	0.45	0
5	BMA	F	618	4,6	11,11,12	0.55	0	15,15,17	0.76	0
6	MAN	F	619	5,6	11,11,12	0.67	0	15,15,17	0.91	1 (6%)
6	MAN	F	620	6	11,11,12	0.59	0	15,15,17	0.97	2 (13%)
4	NAG	F	621	3	14,14,15	0.25	0	15,19,21	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	F	622	3,4	14,14,15	0.36	0	15,19,21	0.42	0
4	NAG	F	623	5,4	14,14,15	0.33	0	15,19,21	0.68	0
5	BMA	F	624	4,6	11,11,12	0.85	0	15,15,17	1.42	1 (6%)
6	MAN	F	625	5	11,11,12	0.63	0	15,15,17	0.97	2 (13%)
6	MAN	F	626	5	11,11,12	0.88	0	15,15,17	0.90	1 (6%)
4	NAG	I	601	-	14,14,15	0.20	0	15,19,21	0.32	0
4	NAG	I	602	3	14,14,15	0.23	0	15,19,21	0.37	0
4	NAG	I	603	3,4	14,14,15	0.38	0	15,19,21	0.50	0
4	NAG	I	604	5,4	14,14,15	0.24	0	15,19,21	0.74	0
5	BMA	I	605	4,6	11,11,12	0.52	0	15,15,17	0.79	0
6	MAN	I	606	5	11,11,12	0.57	0	15,15,17	0.95	2 (13%)
6	MAN	I	607	5	11,11,12	0.60	0	15,15,17	1.00	2 (13%)
4	NAG	I	608	3,4	14,14,15	0.37	0	15,19,21	0.52	0
4	NAG	I	609	5,4	14,14,15	0.25	0	15,19,21	0.40	0
5	BMA	I	610	4	11,11,12	0.52	0	15,15,17	0.76	0
4	NAG	I	611	3,4	14,14,15	0.45	0	15,19,21	1.77	2 (13%)
4	NAG	I	612	4	14,14,15	0.26	0	15,19,21	0.41	0
4	NAG	I	613	3,4	14,14,15	0.30	0	15,19,21	0.42	0
4	NAG	I	614	5,4	14,14,15	0.37	0	15,19,21	0.79	1 (6%)
5	BMA	I	615	4,6	11,11,12	0.65	0	15,15,17	1.10	1 (6%)
6	MAN	I	616	5,6	11,11,12	0.74	0	15,15,17	0.94	1 (6%)
6	MAN	I	617	6	11,11,12	0.67	0	15,15,17	1.06	2 (13%)
4	NAG	I	618	3,4	14,14,15	0.38	0	15,19,21	0.73	0
4	NAG	I	619	5,4	14,14,15	0.20	0	15,19,21	0.51	0
5	BMA	I	620	4,6	11,11,12	1.71	2 (18%)	15,15,17	1.64	2 (13%)
6	MAN	I	621	5	11,11,12	0.71	0	15,15,17	1.12	2 (13%)
6	MAN	I	622	5	11,11,12	0.56	0	15,15,17	0.99	2 (13%)

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
4	NAG	F	601	3	-	0/6/23/26	0/1/1/1
4	NAG	F	602	3,4	-	0/6/23/26	0/1/1/1
4	NAG	F	603	5,4	-	0/6/23/26	0/1/1/1
5	BMA	F	604	4,6	-	0/2/19/22	0/1/1/1
6	MAN	F	605	5	-	0/2/19/22	0/1/1/1
6	MAN	F	606	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	607	3,4	-	0/6/23/26	0/1/1/1
4	NAG	F	608	5,4	-	0/6/23/26	0/1/1/1
5	BMA	F	609	4,6	-	0/2/19/22	0/1/1/1
6	MAN	F	610	5	-	0/2/19/22	0/1/1/1
6	MAN	F	611	5,6	-	0/2/19/22	0/1/1/1
6	MAN	F	612	6	-	0/2/19/22	0/1/1/1
4	NAG	F	613	3,4	-	0/6/23/26	0/1/1/1
4	NAG	F	614	5,4	-	0/6/23/26	0/1/1/1
5	BMA	F	615	4	-	0/2/19/22	0/1/1/1
4	NAG	F	616	3,4	-	0/6/23/26	0/1/1/1
4	NAG	F	617	5,4	-	0/6/23/26	0/1/1/1
5	BMA	F	618	4,6	-	0/2/19/22	0/1/1/1
6	MAN	F	619	5,6	-	0/2/19/22	0/1/1/1
6	MAN	F	620	6	-	0/2/19/22	0/1/1/1
4	NAG	F	621	3	-	0/6/23/26	0/1/1/1
4	NAG	F	622	3,4	-	0/6/23/26	0/1/1/1
4	NAG	F	623	5,4	-	0/6/23/26	0/1/1/1
5	BMA	F	624	4,6	-	0/2/19/22	1/1/1/1
6	MAN	F	625	5	-	0/2/19/22	0/1/1/1
6	MAN	F	626	5	-	0/2/19/22	1/1/1/1
4	NAG	I	601	-	-	0/6/23/26	0/1/1/1
4	NAG	I	602	3	-	0/6/23/26	0/1/1/1
4	NAG	I	603	3,4	-	0/6/23/26	0/1/1/1
4	NAG	I	604	5,4	-	0/6/23/26	0/1/1/1
5	BMA	I	605	4,6	-	0/2/19/22	0/1/1/1
6	MAN	I	606	5	-	0/2/19/22	0/1/1/1
6	MAN	I	607	5	-	0/2/19/22	0/1/1/1
4	NAG	I	608	3,4	-	0/6/23/26	0/1/1/1
4	NAG	I	609	5,4	-	0/6/23/26	0/1/1/1
5	BMA	I	610	4	-	0/2/19/22	0/1/1/1
4	NAG	I	611	3,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	I	612	4	-	0/6/23/26	0/1/1/1
4	NAG	I	613	3,4	-	0/6/23/26	0/1/1/1
4	NAG	I	614	5,4	-	0/6/23/26	0/1/1/1
5	BMA	I	615	4,6	-	0/2/19/22	0/1/1/1
6	MAN	I	616	5,6	-	0/2/19/22	0/1/1/1
6	MAN	I	617	6	-	0/2/19/22	1/1/1/1
4	NAG	I	618	3,4	-	0/6/23/26	0/1/1/1
4	NAG	I	619	5,4	-	0/6/23/26	0/1/1/1
5	BMA	I	620	4,6	-	0/2/19/22	0/1/1/1
6	MAN	I	621	5	-	0/2/19/22	1/1/1/1
6	MAN	I	622	5	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	616	NAG	O5-C1	-3.57	1.37	1.43
6	F	606	MAN	C1-C2	2.27	1.57	1.52
5	I	620	BMA	C2-C3	3.68	1.57	1.52
5	I	620	BMA	C1-C2	3.96	1.61	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	620	BMA	O5-C5-C4	-3.29	104.68	110.13
6	I	606	MAN	O2-C2-C3	-2.37	105.40	110.19
6	F	610	MAN	O2-C2-C3	-2.33	105.48	110.19
6	F	606	MAN	O2-C2-C3	-2.29	105.56	110.19
6	I	607	MAN	O2-C2-C3	-2.29	105.57	110.19
6	F	605	MAN	O2-C2-C3	-2.29	105.57	110.19
6	F	611	MAN	O2-C2-C3	-2.29	105.58	110.19
6	I	621	MAN	O2-C2-C3	-2.28	105.59	110.19
6	I	622	MAN	O2-C2-C3	-2.27	105.60	110.19
6	F	625	MAN	O2-C2-C3	-2.27	105.60	110.19
6	I	617	MAN	O2-C2-C3	-2.26	105.62	110.19
6	F	620	MAN	O2-C2-C3	-2.24	105.68	110.19
6	F	619	MAN	O2-C2-C3	-2.18	105.80	110.19
6	F	626	MAN	O2-C2-C3	-2.17	105.81	110.19
6	I	616	MAN	O2-C2-C3	-2.14	105.88	110.19
6	F	612	MAN	O2-C2-C3	-2.14	105.88	110.19
6	F	610	MAN	C1-O5-C5	2.02	115.11	112.14
4	I	614	NAG	C1-O5-C5	2.02	115.11	112.14
6	I	606	MAN	C1-O5-C5	2.17	115.33	112.14
6	F	620	MAN	C1-O5-C5	2.29	115.51	112.14
6	F	605	MAN	C1-O5-C5	2.33	115.56	112.14
6	I	607	MAN	C1-O5-C5	2.35	115.60	112.14
6	F	625	MAN	C1-O5-C5	2.35	115.60	112.14
6	I	622	MAN	C1-O5-C5	2.51	115.84	112.14
4	I	611	NAG	C4-C3-C2	2.66	115.47	111.34
6	F	611	MAN	C1-O5-C5	2.69	116.10	112.14
5	I	615	BMA	C1-O5-C5	2.73	116.15	112.14
6	I	617	MAN	C1-O5-C5	2.85	116.32	112.14
6	I	621	MAN	C1-O5-C5	3.02	116.57	112.14
6	F	606	MAN	C1-O5-C5	3.46	117.22	112.14
5	F	624	BMA	C1-O5-C5	4.14	118.23	112.14
5	I	620	BMA	C1-C2-C3	4.17	114.60	109.55
4	I	611	NAG	C1-O5-C5	5.63	120.42	112.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	I	611	NAG	C1

There are no torsion outliers.

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	624	BMA	C1-C2-C3-C4-C5-O5
6	F	626	MAN	C1-C2-C3-C4-C5-O5
6	I	617	MAN	C1-C2-C3-C4-C5-O5
6	I	621	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	610	MAN	1	0
4	I	618	NAG	3	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	226/229 (98%)	0.37	7 (3%) 52 31	37, 63, 98, 162	1 (0%)
1	H	224/229 (97%)	0.33	3 (1%) 79 59	24, 65, 94, 155	0
2	B	215/215 (100%)	0.31	4 (1%) 70 48	45, 68, 97, 149	1 (0%)
2	L	215/215 (100%)	0.41	8 (3%) 45 26	37, 61, 100, 162	1 (0%)
3	F	497/503 (98%)	0.68	47 (9%) 10 5	39, 85, 137, 182	2 (0%)
3	I	490/503 (97%)	0.44	29 (5%) 26 13	49, 70, 117, 168	4 (0%)
All	All	1867/1894 (98%)	0.46	98 (5%) 31 16	24, 70, 122, 182	9 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	CYS	10.2
3	I	6	ASN	10.1
3	F	4	PRO	9.5
3	F	5	GLY	7.0
3	F	128	THR	5.8
3	F	127	TRP	5.7
3	I	403	GLU	5.7
3	F	147	PHE	5.6
3	F	71	LEU	5.3
3	F	155	THR	5.1
3	F	243	LEU	4.8
3	F	66	LEU	4.6
3	I	470	TYR	4.6
3	F	125	PHE	4.4
3	I	457	GLU	4.3
2	L	214	CYS	4.3
1	A	130	SER	4.1
3	F	332	PHE	4.0
3	F	236	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
3	I	7	ASP	3.9
3	I	408	ASP	3.8
1	A	216	CYS	3.8
3	F	177	LEU	3.7
3	F	245	ILE	3.4
3	I	101	ASP	3.4
3	F	154	LEU	3.4
3	F	159	SER	3.4
3	F	218	GLU	3.3
1	A	92	CYS	3.2
1	H	216	CYS	3.2
2	B	181	LEU	3.1
3	F	87	PHE	3.1
3	F	205	SER	3.1
3	F	143	PRO	3.1
3	F	254	PRO	2.9
3	I	314	LEU	2.8
2	L	147	GLN	2.8
1	A	138	LEU	2.7
3	F	65	THR	2.7
3	I	456	ARG	2.7
3	F	231	SER	2.7
3	F	153	TRP	2.6
3	I	340	GLU	2.6
3	F	64	CYS	2.6
3	I	481	ILE	2.6
3	F	333	GLY	2.6
3	I	501	GLN	2.6
2	L	154	LEU	2.5
2	L	152	ASN	2.5
2	L	192	TYR	2.5
3	F	280	GLU	2.5
3	I	317	ALA	2.5
3	F	94	PHE	2.5
3	F	350[A]	TRP	2.5
3	I	318	THR	2.5
3	F	194	LEU	2.4
3	F	304	ALA	2.4
3	I	472	LYS	2.4
3	F	70	LEU	2.4
3	F	412	TYR	2.4
3	I	345	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	104	LEU	2.3
2	B	106	ILE	2.3
3	I	166	VAL	2.3
3	I	70	LEU	2.3
3	I	283	THR	2.3
3	F	148	PHE	2.3
3	I	167	THR	2.3
3	I	350[A]	TRP	2.3
3	I	282	ILE	2.2
2	L	123	GLU	2.2
3	F	258	PHE	2.2
3	F	118	LEU	2.2
3	F	84	TRP	2.2
3	F	242	VAL	2.2
3	F	6	ASN	2.2
1	H	156	SER	2.2
3	I	15	LEU	2.2
1	H	137	ALA	2.1
3	F	327	GLN	2.1
3	F	481	ILE	2.1
3	I	471	HIS	2.1
3	I	24	THR	2.1
1	A	194	TYR	2.1
3	I	13	LEU	2.1
3	I	245	ILE	2.1
3	F	122	THR	2.0
1	A	181	VAL	2.0
3	F	33	GLN	2.0
3	I	32	ASP	2.0
3	F	199	SER	2.0
3	F	144	GLY	2.0
3	F	501	GLN	2.0
2	L	195	GLU	2.0
3	F	67	ILE	2.0
3	I	127	TRP	2.0
1	A	2	VAL	2.0
2	L	196	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	I	618	14/15	0.88	0.24	0.39	68,85,104,107	0
4	NAG	I	613	14/15	0.85	0.20	0.15	59,83,90,100	0
6	MAN	I	606	11/12	0.80	0.23	-0.60	77,80,86,92	0
6	MAN	F	610	11/12	0.87	0.21	-0.69	96,101,115,118	0
4	NAG	I	603	14/15	0.94	0.13	-1.12	29,35,60,70	0
4	NAG	F	607	14/15	0.93	0.16	-1.16	26,38,57,61	0
4	NAG	F	616	14/15	0.89	0.19	-1.22	63,81,93,96	0
4	NAG	I	608	14/15	0.84	0.22	-	87,99,121,129	0
4	NAG	I	601	14/15	0.64	0.58	-	128,134,148,150	0
4	NAG	F	601	14/15	0.52	0.79	-	127,140,147,149	0
6	MAN	F	619	11/12	0.59	0.24	-	150,158,162,163	0
4	NAG	I	614	14/15	0.86	0.22	-	81,100,113,121	0
5	BMA	F	618	11/12	0.70	0.32	-	128,131,151,154	0
5	BMA	I	610	11/12	0.24	0.48	-	134,151,164,164	0
6	MAN	F	605	11/12	0.38	0.75	-	171,189,191,193	0
6	MAN	F	626	11/12	0.62	0.41	-	105,126,133,133	0
6	MAN	I	621	11/12	0.75	0.28	-	117,124,127,130	0
4	NAG	F	608	14/15	0.88	0.17	-	32,51,58,72	0
4	NAG	F	622	14/15	0.90	0.20	-	60,71,93,97	0
6	MAN	I	616	11/12	0.44	0.38	-	140,153,157,163	0
5	BMA	I	615	11/12	0.62	0.25	-	127,131,145,151	0
6	MAN	F	620	11/12	0.71	0.42	-	150,154,156,161	0
6	MAN	F	612	11/12	0.78	0.31	-	127,130,136,137	0
4	NAG	I	602	14/15	0.37	0.59	-	118,133,151,151	0
5	BMA	F	604	11/12	0.50	0.73	-	194,195,199,199	0
4	NAG	I	619	14/15	0.80	0.28	-	108,115,138,139	0
4	NAG	I	612	14/15	0.77	0.37	-	127,145,172,173	0
4	NAG	I	611	14/15	0.77	0.46	-	103,136,165,170	0
6	MAN	F	611	11/12	0.69	0.26	-	114,121,126,127	0
5	BMA	F	615	11/12	0.42	0.56	-	168,171,173,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MAN	I	617	11/12	0.43	0.83	-	159,168,173,177	0
6	MAN	I	607	11/12	0.62	0.24	-	82,102,117,121	0
4	NAG	F	603	14/15	0.45	0.79	-	185,188,196,197	0
4	NAG	F	614	14/15	0.44	0.51	-	131,148,158,165	0
4	NAG	F	613	14/15	0.59	0.32	-	109,135,142,144	0
6	MAN	F	606	11/12	0.32	1.05	-	187,191,196,197	0
4	NAG	I	609	14/15	0.59	0.46	-	121,147,156,161	0
5	BMA	I	605	11/12	0.90	0.12	-	63,70,79,89	0
6	MAN	F	625	11/12	0.66	0.43	-	140,143,146,148	0
5	BMA	I	620	11/12	0.73	0.24	-	129,146,152,155	0
5	BMA	F	624	11/12	0.74	0.24	-	128,134,137,139	0
4	NAG	F	623	14/15	0.87	0.18	-	86,96,108,118	0
4	NAG	I	604	14/15	0.93	0.14	-	32,41,56,56	0
4	NAG	F	617	14/15	0.81	0.27	-	73,107,115,121	0
4	NAG	F	602	14/15	0.58	0.68	-	124,150,158,173	0
4	NAG	F	621	14/15	0.74	0.34	-	96,110,124,127	0
5	BMA	F	609	11/12	0.89	0.11	-	59,75,97,106	0
6	MAN	I	622	11/12	0.63	0.37	-	149,153,156,164	0

6.5 Other polymers (i)

There are no such residues in this entry.