



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:55 AM GMT

PDB ID : 3NGB
Title : Crystal structure of broadly and potently neutralizing antibody VRC01 in complex with HIV-1 gp120
Authors : Zhou, T.; Kwong, P.D.
Deposited on : 2010-06-11
Resolution : 2.68 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

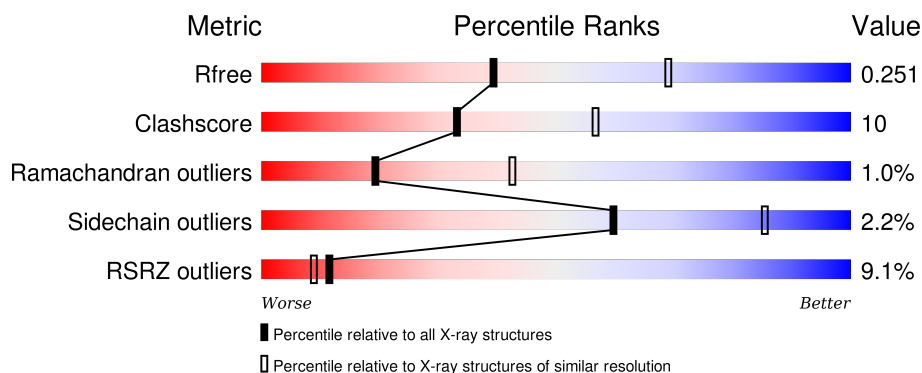
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	353	<div> <div>2%</div> <div>74%</div> <div>23%</div> <div>..</div> </div>
1	D	353	<div> <div>3%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	G	353	<div> <div>4%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	I	353	<div> <div>8%</div> <div>77%</div> <div>21%</div> <div>..</div> </div>
2	B	224	<div> <div>7%</div> <div>74%</div> <div>25%</div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
2	E	224	
2	H	224	
2	J	224	
3	C	210	
3	F	210	
3	K	210	
3	L	210	

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	A	948	-	-	-	X
4	NAG	D	588	-	-	-	X
5	BGC	A	506	-	-	-	X
5	BGC	A	508	-	-	-	X
5	BGC	D	505	-	-	-	X
5	BGC	G	503	-	-	-	X
5	BGC	I	401	-	-	-	X
7	TRS	K	405	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25808 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 gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	347	Total	C	N	O	S	0	0	0
			2713	1700	472	518	23			
1	A	349	Total	C	N	O	S	0	0	0
			2723	1705	474	521	23			
1	D	350	Total	C	N	O	S	0	0	0
			2727	1707	475	522	23			
1	I	349	Total	C	N	O	S	0	0	0
			2721	1704	474	520	23			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	124	GLY	-	LINKER	UNP Q0ED31
G	198	GLY	-	LINKER	UNP Q0ED31
G	318	GLY	-	LINKER	UNP Q0ED31
G	319	GLY	-	LINKER	UNP Q0ED31
G	320	SER	-	LINKER	UNP Q0ED31
G	321	GLY	-	LINKER	UNP Q0ED31
G	322	SER	-	LINKER	UNP Q0ED31
G	323	GLY	-	LINKER	UNP Q0ED31
A	124	GLY	-	LINKER	UNP Q0ED31
A	198	GLY	-	LINKER	UNP Q0ED31
A	318	GLY	-	LINKER	UNP Q0ED31
A	319	GLY	-	LINKER	UNP Q0ED31
A	320	SER	-	LINKER	UNP Q0ED31
A	321	GLY	-	LINKER	UNP Q0ED31
A	322	SER	-	LINKER	UNP Q0ED31
A	323	GLY	-	LINKER	UNP Q0ED31
D	124	GLY	-	LINKER	UNP Q0ED31
D	198	GLY	-	LINKER	UNP Q0ED31
D	318	GLY	-	LINKER	UNP Q0ED31
D	319	GLY	-	LINKER	UNP Q0ED31
D	320	SER	-	LINKER	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
D	321	GLY	-	LINKER	UNP Q0ED31
D	322	SER	-	LINKER	UNP Q0ED31
D	323	GLY	-	LINKER	UNP Q0ED31
I	124	GLY	-	LINKER	UNP Q0ED31
I	198	GLY	-	LINKER	UNP Q0ED31
I	302	GLY	-	LINKER	UNP Q0ED31
I	319	GLY	-	LINKER	UNP Q0ED31
I	320	SER	-	LINKER	UNP Q0ED31
I	321	GLY	-	LINKER	UNP Q0ED31
I	322	SER	-	LINKER	UNP Q0ED31
I	323	GLY	-	LINKER	UNP Q0ED31

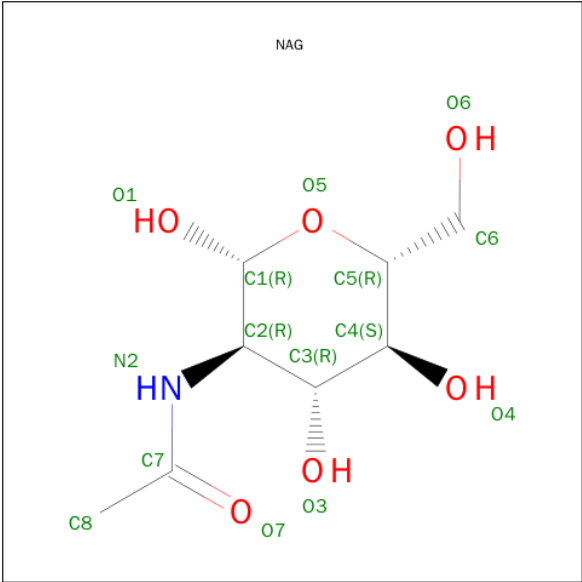
- Molecule 2 is a protein called Antigen binding fragment of heavy chain: Antibody VRC01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1710	1077	297	325	11			
2	B	224	Total	C	N	O	S	0	0	0
			1710	1077	297	325	11			
2	E	224	Total	C	N	O	S	0	0	0
			1710	1077	297	325	11			
2	J	224	Total	C	N	O	S	0	0	0
			1710	1077	297	325	11			

- Molecule 3 is a protein called Antigen binding fragment of light chain: Antibody VRC01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	208	Total	C	N	O	S	0	0	0
			1615	1011	277	322	5			
3	C	210	Total	C	N	O	S	0	0	0
			1632	1022	279	326	5			
3	F	208	Total	C	N	O	S	0	0	0
			1615	1011	277	322	5			
3	K	210	Total	C	N	O	S	0	0	0
			1632	1022	279	326	5			

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



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

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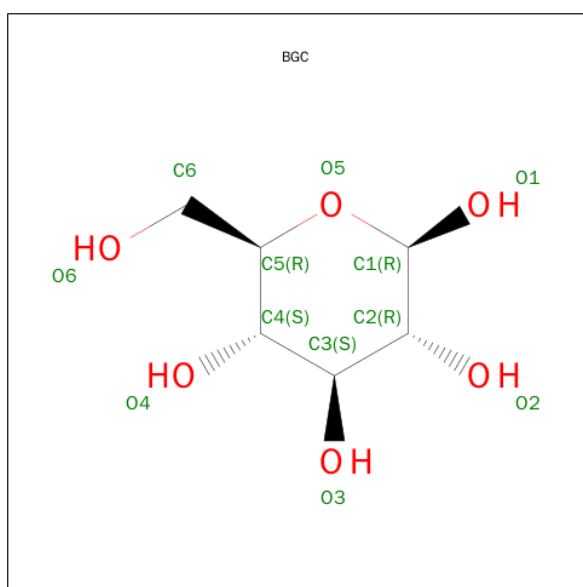
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1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

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

- Molecule 5 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C₆H₁₂O₆).

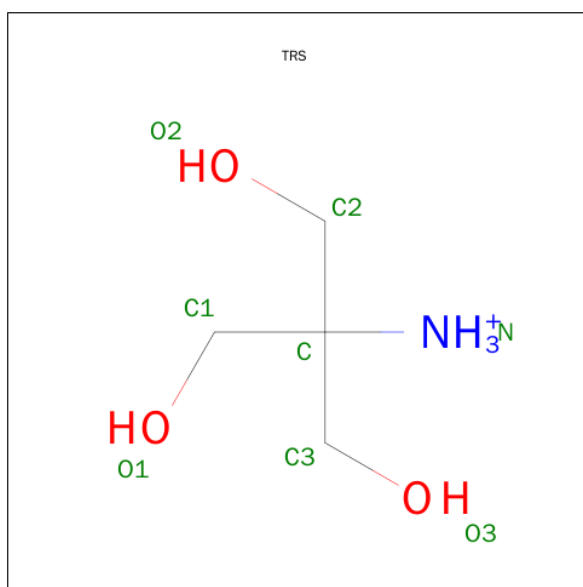


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			12	6	6		
5	A	1	Total	C	O	0	0
			12	6	6		
5	A	1	Total	C	O	0	0
			12	6	6		
5	A	1	Total	C	O	0	0
			12	6	6		
5	B	1	Total	C	O	0	0
			12	6	6		
5	B	1	Total	C	O	0	0
			12	6	6		
5	C	1	Total	C	O	0	0
			12	6	6		
5	D	1	Total	C	O	0	0
			12	6	6		
5	E	1	Total	C	O	0	0
			12	6	6		
5	I	1	Total	C	O	0	0
			12	6	6		
5	I	1	Total	C	O	0	0
			12	6	6		
5	J	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	5	Total	C	N	O	0	0
			61	34	2	25		
6	C	5	Total	C	N	O	0	0
			61	34	2	25		
6	K	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	D	1	Total	C	N	O	0	0
			8	4	1	3		
7	D	1	Total	C	N	O	0	0
			8	4	1	3		
7	I	1	Total	C	N	O	0	0
			8	4	1	3		
7	J	1	Total	C	N	O	0	0
			8	4	1	3		
7	K	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	68	Total	O	0	0
			68	68		

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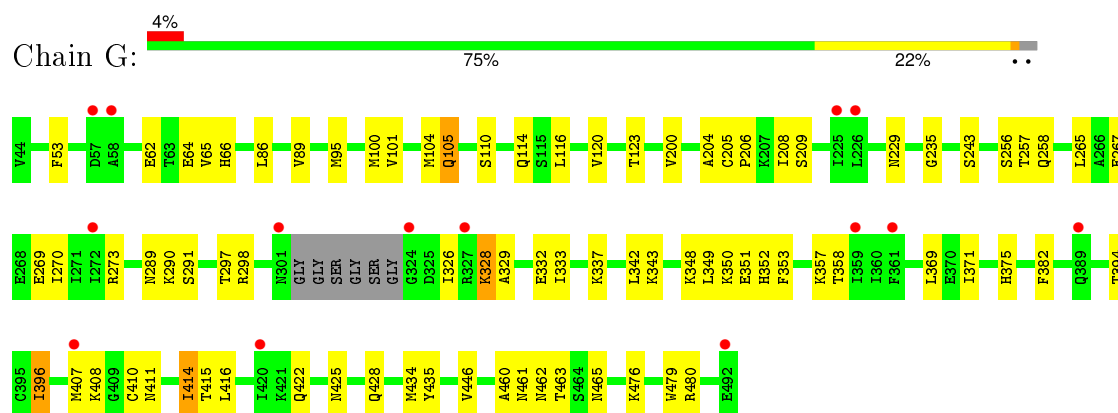
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	52	Total 52	O 52	0	0
9	L	44	Total 44	O 44	0	0
9	A	89	Total 89	O 89	0	0
9	B	46	Total 46	O 46	0	0
9	C	33	Total 33	O 33	0	0
9	D	60	Total 60	O 60	0	0
9	E	29	Total 29	O 29	0	0
9	F	7	Total 7	O 7	0	0
9	I	44	Total 44	O 44	0	0
9	J	24	Total 24	O 24	0	0
9	K	27	Total 27	O 27	0	0

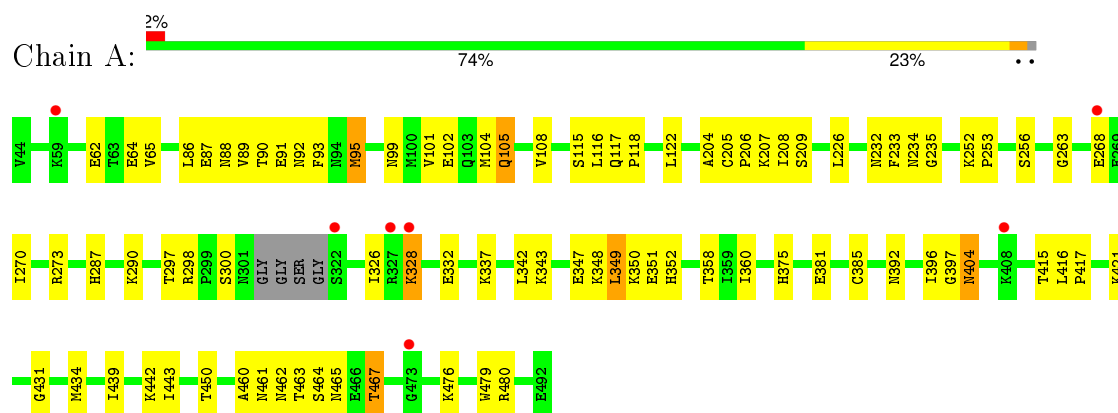
3 Residue-property plots

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.

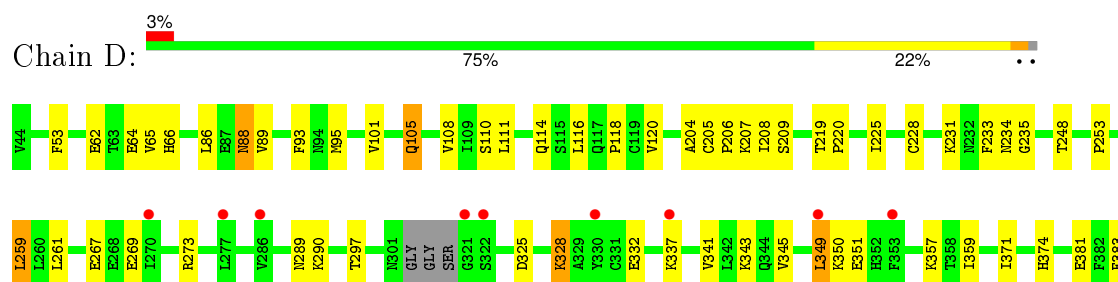
• Molecule 1: Envelope glycoprotein gp160

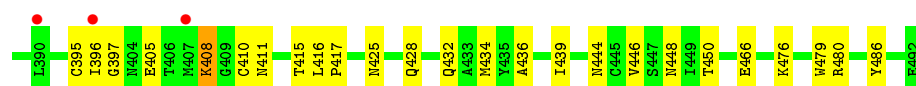


• Molecule 1: Envelope glycoprotein gp160

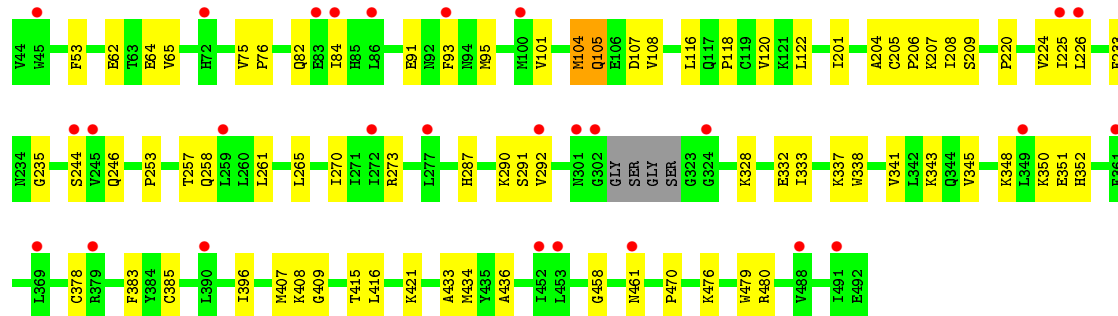
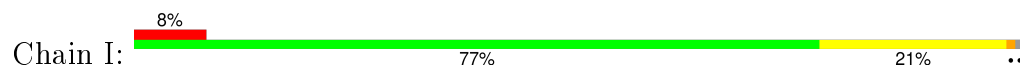


• Molecule 1: Envelope glycoprotein gp160

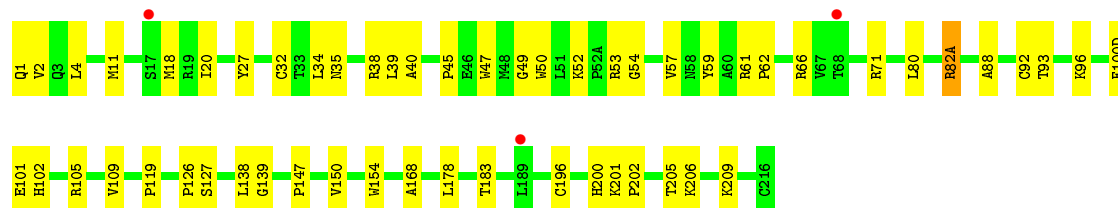
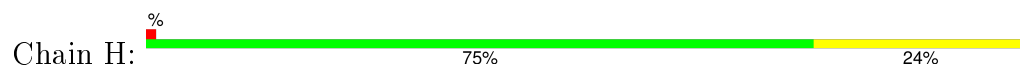




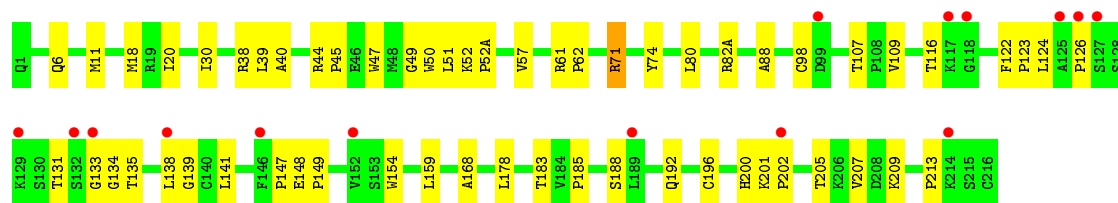
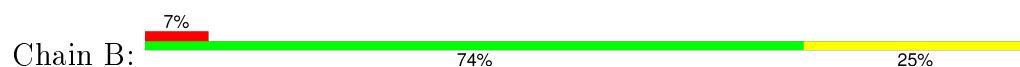
- Molecule 1: Envelope glycoprotein gp160



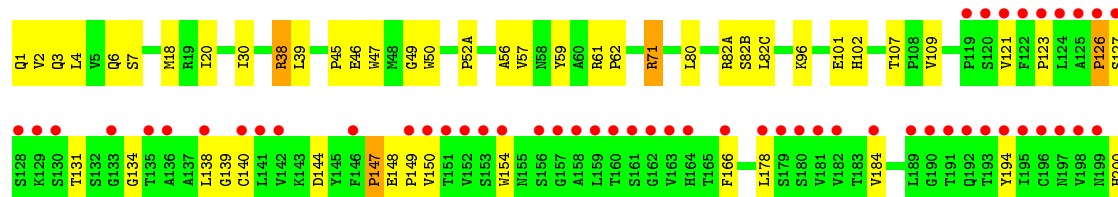
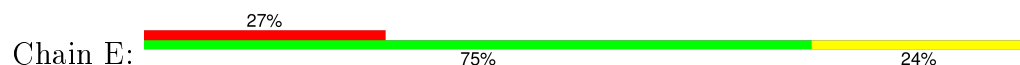
- Molecule 2: Antigen binding fragment of heavy chain: Antibody VRC01

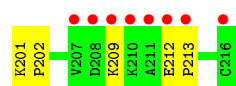


- Molecule 2: Antigen binding fragment of heavy chain: Antibody VRC01

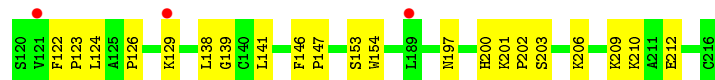
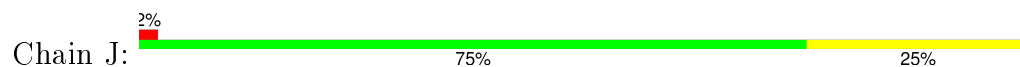


- Molecule 2: Antigen binding fragment of heavy chain: Antibody VRC01

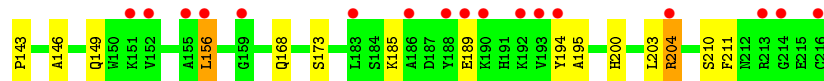
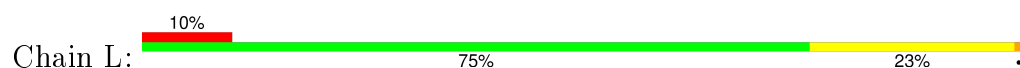




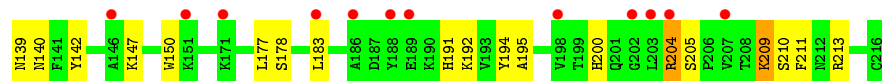
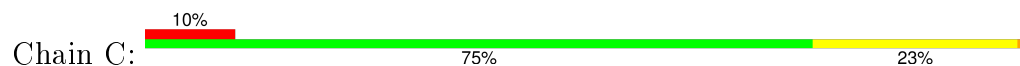
- Molecule 2: Antigen binding fragment of heavy chain: Antibody VRC01



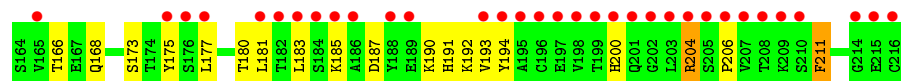
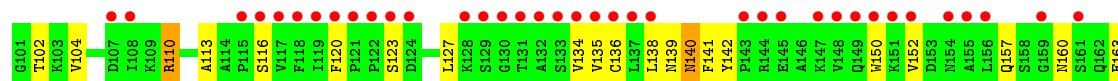
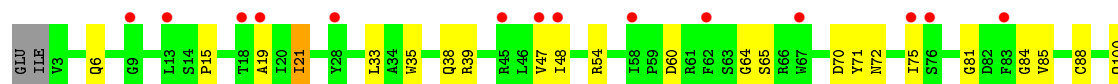
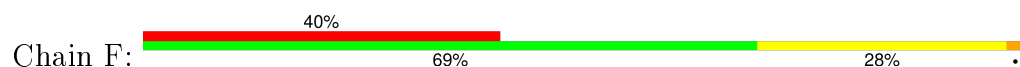
- Molecule 3: Antigen binding fragment of light chain: Antibody VRC01



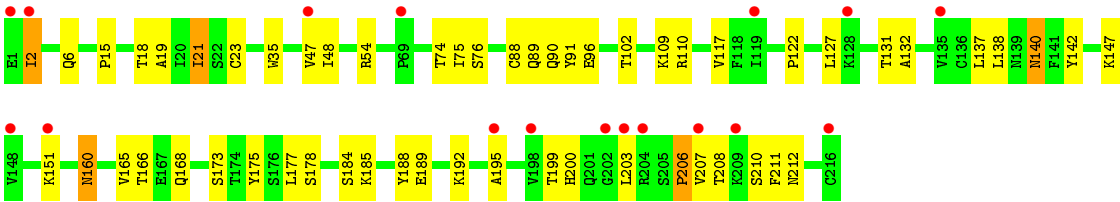
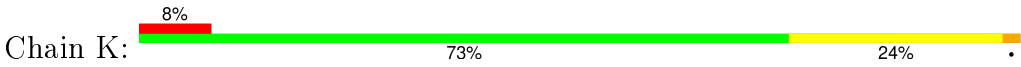
- Molecule 3: Antigen binding fragment of light chain: Antibody VRC01



- Molecule 3: Antigen binding fragment of light chain: Antibody VRC01



- Molecule 3: Antigen binding fragment of light chain: Antibody VRC01



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.63 Å 98.28 Å 205.26 Å 90.00° 99.68° 90.00°	Depositor
Resolution (Å)	49.73 – 2.68 49.73 – 2.68	Depositor EDS
% Data completeness (in resolution range)	94.8 (49.73-2.68) 81.3 (49.73-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.69 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.197 , 0.256 0.194 , 0.251	Depositor DCC
R_{free} test set	4868 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	82.6	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 97172 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25808	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, TRS, 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	0.21	0/2780	0.39	0/3773
1	D	0.21	0/2784	0.38	0/3778
1	G	0.21	0/2770	0.39	0/3760
1	I	0.21	0/2778	0.37	0/3770
2	B	0.21	0/1755	0.40	0/2387
2	E	0.21	0/1755	0.39	0/2387
2	H	0.22	0/1755	0.41	0/2387
2	J	0.21	0/1755	0.40	0/2387
3	C	0.21	0/1669	0.38	0/2265
3	F	0.20	0/1652	0.36	0/2242
3	K	0.21	0/1669	0.38	0/2265
3	L	0.21	0/1652	0.37	0/2242
All	All	0.21	0/24774	0.39	0/33643

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	2723	0	2649	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2727	0	2652	56	0
1	G	2713	0	2642	53	0
1	I	2721	0	2648	56	0
2	B	1710	0	1680	45	0
2	E	1710	0	1680	34	0
2	H	1710	0	1680	34	0
2	J	1710	0	1680	44	0
3	C	1632	0	1573	38	0
3	F	1615	0	1553	41	0
3	K	1632	0	1573	40	0
3	L	1615	0	1553	35	0
4	A	168	0	156	2	0
4	D	168	0	156	1	0
4	G	154	0	143	1	0
4	I	154	0	142	1	0
5	A	48	0	48	6	0
5	B	24	0	24	1	0
5	C	12	0	12	0	0
5	D	12	0	12	0	0
5	E	12	0	12	0	0
5	G	12	0	12	1	0
5	I	24	0	24	1	0
5	J	12	0	12	1	0
6	C	61	0	52	1	0
6	K	61	0	52	0	0
6	L	61	0	52	0	0
7	A	16	0	24	0	0
7	D	16	0	24	1	0
7	I	8	0	12	2	0
7	J	8	0	12	0	0
7	K	8	0	12	1	0
8	F	28	0	25	1	0
9	A	89	0	0	1	0
9	B	46	0	0	1	0
9	C	33	0	0	2	0
9	D	60	0	0	0	0
9	E	29	0	0	1	0
9	F	7	0	0	0	0
9	G	68	0	0	2	0
9	H	52	0	0	2	0
9	I	44	0	0	2	0
9	J	24	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	27	0	0	0	0
9	L	44	0	0	1	0
All	All	25808	0	24581	514	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 (514) 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)
1:G:105:GLN:HG3	1:G:476:LYS:HG2	1.47	0.96
1:A:342:LEU:HD23	1:A:396:ILE:HD11	1.54	0.88
1:I:105:GLN:HG3	1:I:476:LYS:HG2	1.56	0.87
1:A:95:MET:HE1	1:A:235:GLY:HA3	1.56	0.86
3:F:6:GLN:HE21	3:F:21:ILE:HD11	1.42	0.85
1:D:349:LEU:HB3	1:D:359:ILE:HG12	1.63	0.79
1:I:408:LYS:HG2	1:I:409:GLY:H	1.48	0.78
2:B:20:ILE:HD11	2:B:80:LEU:HD23	1.66	0.77
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.68	0.76
2:J:39:LEU:HD21	2:J:45:PRO:HG3	1.66	0.74
1:I:62:GLU:HG3	1:I:64:GLU:H	1.51	0.74
1:D:65:VAL:HG21	1:D:208:ILE:HD12	1.70	0.74
1:G:65:VAL:HG21	1:G:208:ILE:HD12	1.71	0.73
1:I:84:ILE:HB	1:I:244:SER:HB3	1.71	0.72
2:J:126:PRO:HG3	2:J:138:LEU:HB3	1.73	0.70
2:H:39:LEU:HD21	2:H:45:PRO:HG3	1.71	0.70
3:F:204:ARG:H	3:F:204:ARG:HD3	1.54	0.70
5:A:506:BGC:H6C1	2:B:74:TYR:HB2	1.71	0.70
2:B:11:MET:HG2	1:I:122:LEU:HD12	1.74	0.69
1:I:95:MET:HE1	1:I:235:GLY:HA3	1.73	0.69
2:B:126:PRO:HD2	2:B:213:PRO:HA	1.74	0.69
1:A:460:ALA:HB3	2:B:61:ARG:HD2	1.75	0.69
2:J:18:MET:HE3	2:J:82(C):LEU:HD21	1.74	0.68
3:C:195:ALA:HB2	3:C:210:SER:HB3	1.75	0.68
1:G:62:GLU:HG3	1:G:64:GLU:H	1.58	0.68
1:A:62:GLU:HG3	1:A:64:GLU:H	1.59	0.67
3:F:163:GLU:HB3	3:F:177:LEU:HD11	1.77	0.67
2:E:126:PRO:HG3	2:E:138:LEU:HD23	1.76	0.67
1:A:350:LYS:O	1:A:351:GLU:HB3	1.96	0.66
1:G:95:MET:HE1	1:G:235:GLY:HA3	1.77	0.66
1:A:332:GLU:HG2	1:A:415:THR:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:O	1:A:89:VAL:HG12	1.97	0.65
3:L:47:VAL:HG12	3:L:48:ILE:HG12	1.77	0.65
1:D:332:GLU:HG2	1:D:415:THR:HG22	1.77	0.65
1:G:265:LEU:HD21	1:G:291:SER:HB3	1.80	0.64
2:E:6:GLN:HE21	2:E:107:THR:HG23	1.62	0.64
2:J:35:ASN:OD1	2:J:50:TRP:HB3	1.98	0.64
1:D:120:VAL:HG12	1:D:434:MET:HB3	1.80	0.64
2:J:201:LYS:HB2	2:J:202:PRO:HD3	1.80	0.63
1:I:332:GLU:HG2	1:I:415:THR:HG22	1.81	0.62
1:D:95:MET:HE1	1:D:235:GLY:HA3	1.80	0.62
1:G:332:GLU:HG2	1:G:415:THR:HG22	1.81	0.62
1:D:371:ILE:HD13	2:E:56:ALA:HB2	1.82	0.62
1:I:207:LYS:HE2	1:I:436:ALA:HB3	1.82	0.62
1:A:205:CYS:N	1:A:206:PRO:HD3	2.15	0.61
3:K:110:ARG:HD2	3:K:173:SER:HB2	1.81	0.61
3:F:187:ASP:HA	3:F:190:LYS:HE3	1.81	0.61
3:F:21:ILE:HD12	3:F:102:THR:HB	1.81	0.61
1:I:350:LYS:O	1:I:351:GLU:HB3	2.00	0.61
3:C:47:VAL:HG12	3:C:48:ILE:HG12	1.81	0.61
3:K:21:ILE:HD12	3:K:102:THR:HB	1.82	0.61
2:H:126:PRO:HG3	2:H:138:LEU:HB3	1.82	0.61
1:G:446:VAL:HG21	4:G:795:NAG:H82	1.82	0.61
1:G:105:GLN:CG	1:G:476:LYS:HG2	2.27	0.61
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.36	0.60
2:J:30:ILE:HA	2:J:52(A):PRO:HB2	1.83	0.60
2:J:17:SER:OG	5:J:507:BGC:H5	2.02	0.60
1:G:105:GLN:HG3	1:G:476:LYS:CG	2.29	0.60
1:A:431:GLY:HA2	5:A:506:BGC:O4	2.02	0.60
1:I:265:LEU:HD21	1:I:291:SER:HB3	1.84	0.60
1:G:358:THR:O	1:G:465:ASN:HB2	2.02	0.60
1:I:204:ALA:C	1:I:206:PRO:HD3	2.21	0.60
3:F:152:VAL:HG23	3:F:157:GLN:HG3	1.83	0.59
2:E:61:ARG:HB2	2:E:62:PRO:HD3	1.84	0.59
1:D:405:GLU:O	1:D:408:LYS:HG3	2.03	0.59
1:A:381:GLU:HG3	1:A:443:ILE:HD13	1.84	0.59
1:G:342:LEU:HD23	1:G:396:ILE:HD11	1.84	0.59
1:G:204:ALA:C	1:G:206:PRO:HD3	2.23	0.59
1:I:246:GLN:HB2	9:I:1183:HOH:O	2.02	0.58
4:A:776:NAG:H5	3:C:28:TYR:OH	2.03	0.58
1:D:350:LYS:O	1:D:351:GLU:HB3	2.03	0.58
1:G:290:LYS:HE2	1:G:337:LYS:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:105:GLN:HG2	1:I:479:TRP:HE1	1.67	0.57
3:C:192:LYS:HA	3:C:213:ARG:HB3	1.86	0.57
3:F:47:VAL:HG12	3:F:48:ILE:HG12	1.85	0.57
2:J:20:ILE:HD11	2:J:80:LEU:HD23	1.87	0.57
3:K:195:ALA:HA	3:K:210:SER:HB3	1.86	0.57
5:A:506:BGC:C6	2:B:74:TYR:HB2	2.34	0.57
3:F:192:LYS:HG3	3:F:193:VAL:HG23	1.86	0.57
3:K:203:LEU:HD13	3:K:207:VAL:HG23	1.87	0.57
1:A:65:VAL:HG21	1:A:208:ILE:HD12	1.85	0.57
1:D:101:VAL:HG21	1:D:480:ARG:HG2	1.87	0.57
1:G:357:LYS:HB3	1:G:465:ASN:HA	1.86	0.57
1:A:290:LYS:HE2	1:A:337:LYS:HE3	1.86	0.57
2:E:82(A):ARG:NH1	2:E:82(A):ARG:HB3	2.20	0.57
2:J:63:LEU:HD23	2:J:66:ARG:HH12	1.71	0.56
3:K:117:VAL:HG22	3:K:138:LEU:HG	1.88	0.56
3:K:177:LEU:HD23	3:K:178:SER:N	2.21	0.56
1:I:105:GLN:HG3	1:I:476:LYS:CG	2.33	0.56
1:D:207:LYS:HG2	1:D:439:ILE:HG23	1.86	0.56
2:E:148:GLU:HB3	2:E:149:PRO:HA	1.87	0.56
2:J:18:MET:CE	2:J:109:VAL:HG11	2.36	0.56
1:G:350:LYS:O	1:G:351:GLU:HB3	2.06	0.56
2:J:5:VAL:HG13	2:J:105:ARG:HH22	1.69	0.56
1:I:65:VAL:HG21	1:I:208:ILE:HD12	1.86	0.56
1:I:101:VAL:HG21	1:I:480:ARG:HG2	1.87	0.55
2:E:30:ILE:HA	2:E:52(A):PRO:HB2	1.87	0.55
3:K:185:LYS:O	3:K:189:GLU:HG2	2.07	0.55
2:H:82(A):ARG:HB3	2:H:82(A):ARG:HH11	1.71	0.55
2:J:47:TRP:CZ2	2:J:49:GLY:HA2	2.41	0.55
3:L:146:ALA:HB2	3:L:200:HIS:HD2	1.72	0.55
1:G:104:MET:HE2	1:G:479:TRP:HB3	1.88	0.55
3:F:194:TYR:HB2	3:F:211:PHE:HE2	1.72	0.55
1:I:270:ILE:HB	1:I:348:LYS:HG3	1.89	0.55
1:D:207:LYS:HG2	1:D:439:ILE:CG2	2.36	0.55
1:A:463:THR:O	1:A:464:SER:HB3	2.07	0.55
2:E:47:TRP:CH2	2:E:49:GLY:HA2	2.42	0.55
1:A:95:MET:CE	1:A:235:GLY:HA3	2.34	0.54
1:G:205:CYS:N	1:G:206:PRO:HD3	2.22	0.54
2:E:18:MET:HE3	2:E:82(C):LEU:HD21	1.89	0.54
3:C:21:ILE:HD11	3:C:35:TRP:HZ3	1.72	0.54
1:I:105:GLN:HG2	1:I:479:TRP:NE1	2.22	0.54
3:K:140:ASN:ND2	7:K:405:TRS:H21	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:VAL:O	1:D:345:VAL:HG23	2.06	0.54
1:A:116:LEU:O	1:A:118:PRO:HD3	2.07	0.54
3:C:209:LYS:HB2	3:C:209:LYS:NZ	2.22	0.54
2:H:105:ARG:HD2	9:E:1415:HOH:O	2.06	0.54
1:G:64:GLU:HA	1:G:209:SER:HB3	1.88	0.54
8:F:570:NAG:O3	8:F:571:NAG:H2	2.07	0.54
2:B:51:LEU:HD21	2:B:71:ARG:HB3	1.89	0.54
1:I:53:PHE:HA	7:I:502:TRS:H21	1.89	0.54
1:D:53:PHE:HA	7:D:402:TRS:H31	1.89	0.54
3:L:195:ALA:HB2	3:L:210:SER:HB3	1.89	0.53
3:C:54:ARG:NE	3:C:60:ASP:HA	2.23	0.53
3:C:2:ILE:HG22	3:C:3:VAL:H	1.73	0.53
1:D:116:LEU:O	1:D:118:PRO:HD3	2.09	0.53
1:I:273:ARG:HH12	1:I:287:HIS:CG	2.27	0.53
2:J:200:HIS:CD2	2:J:202:PRO:HD2	2.44	0.53
2:B:82(A):ARG:HB3	2:B:82(A):ARG:NH1	2.22	0.53
1:A:463:THR:HG22	9:A:1258:HOH:O	2.08	0.53
1:D:205:CYS:N	1:D:206:PRO:HD3	2.23	0.53
3:F:194:TYR:HB2	3:F:211:PHE:CE2	2.44	0.53
2:B:98:CYS:HB2	5:B:407:BGC:H6C2	1.91	0.53
3:L:168:GLN:HE21	3:L:173:SER:HB3	1.73	0.53
3:K:6:GLN:NE2	3:K:21:ILE:HD11	2.24	0.53
2:H:66:ARG:HD3	9:H:1240:HOH:O	2.08	0.52
3:F:38:GLN:HB3	3:F:85:VAL:HG13	1.92	0.52
3:F:6:GLN:NE2	3:F:21:ILE:HD11	2.20	0.52
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.45	0.52
1:D:204:ALA:C	1:D:206:PRO:HD3	2.30	0.52
2:B:131:THR:HG23	2:B:133:GLY:H	1.74	0.52
2:J:82(A):ARG:NH1	2:J:82(A):ARG:HB3	2.25	0.52
1:D:261:LEU:HD21	1:D:374:HIS:CE1	2.45	0.52
1:G:95:MET:CE	1:G:235:GLY:HA3	2.40	0.52
2:H:82(A):ARG:HB3	2:H:82(A):ARG:NH1	2.24	0.52
1:A:105:GLN:HG3	1:A:476:LYS:HG2	1.90	0.52
1:G:101:VAL:HG21	1:G:480:ARG:HG2	1.92	0.52
3:K:137:LEU:C	3:K:138:LEU:HD12	2.31	0.52
1:D:62:GLU:HG3	1:D:64:GLU:H	1.75	0.52
3:L:79:GLU:H	3:L:82:ASP:HB2	1.75	0.52
2:E:20:ILE:HD11	2:E:80:LEU:HD23	1.91	0.52
1:G:86:LEU:HB2	1:G:89:VAL:HG11	1.92	0.51
2:H:35:ASN:HB2	2:H:93:THR:OG1	2.10	0.51
1:D:105:GLN:HG3	1:D:476:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:116:LEU:HD13	1:I:208:ILE:HD11	1.92	0.51
2:B:47:TRP:HZ2	2:B:50:TRP:CD1	2.28	0.51
2:B:18:MET:CE	2:B:109:VAL:HG11	2.41	0.51
1:I:385:CYS:SG	1:I:416:LEU:HB2	2.51	0.51
1:A:87:GLU:O	1:A:88:ASN:HB2	2.10	0.51
2:J:139:GLY:HA2	2:J:154:TRP:CH2	2.46	0.51
1:I:292:VAL:HG21	1:I:338:TRP:HE3	1.75	0.51
3:L:204:ARG:H	3:L:204:ARG:HE	1.57	0.51
3:L:77:ASN:HB2	9:L:1349:HOH:O	2.10	0.51
3:F:168:GLN:HB2	3:F:175:TYR:CE1	2.46	0.51
1:I:101:VAL:HG13	1:I:479:TRP:HB2	1.92	0.51
3:C:109:LYS:HA	3:C:142:TYR:OH	2.11	0.51
1:A:105:GLN:CG	1:A:476:LYS:HG2	2.41	0.50
3:F:110:ARG:HH12	3:F:113:ALA:HB2	1.75	0.50
3:L:27:GLN:HG3	3:L:28:TYR:N	2.27	0.50
1:G:463:THR:HG21	2:H:61:ARG:NH2	2.25	0.50
3:C:79:GLU:H	3:C:82:ASP:HB2	1.77	0.50
1:G:350:LYS:C	1:G:352:HIS:H	2.14	0.50
3:K:142:TYR:O	3:K:200:HIS:HE1	1.94	0.50
1:I:64:GLU:HA	1:I:209:SER:HB3	1.94	0.50
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.46	0.50
2:B:44:ARG:HG2	3:C:100:GLN:HA	1.94	0.50
3:L:185:LYS:O	3:L:189:GLU:HG2	2.12	0.50
3:K:35:TRP:CZ3	3:K:88:CYS:HB3	2.46	0.50
2:B:201:LYS:HA	2:B:201:LYS:HE2	1.93	0.50
3:F:191:HIS:HB2	3:F:194:TYR:OH	2.11	0.50
2:E:18:MET:CE	2:E:109:VAL:HG11	2.42	0.50
2:B:139:GLY:HA2	2:B:154:TRP:CH2	2.46	0.50
1:A:421:LYS:NZ	5:A:508:BGC:H3	2.26	0.50
1:D:231:LYS:HD2	1:D:267:GLU:HB3	1.94	0.50
3:C:21:ILE:HD12	3:C:102:THR:HB	1.93	0.49
3:L:110:ARG:HH12	3:L:113:ALA:HB2	1.76	0.49
2:B:134:GLY:HA3	9:B:1383:HOH:O	2.13	0.49
1:A:108:VAL:HG22	1:A:253:PRO:HB3	1.94	0.49
1:I:290:LYS:HD2	4:I:789:NAG:H82	1.95	0.49
1:A:350:LYS:C	1:A:352:HIS:H	2.16	0.49
2:B:200:HIS:CE1	2:B:202:PRO:HB2	2.48	0.49
3:F:65:SER:OG	3:F:72:ASN:HB2	2.13	0.49
1:I:95:MET:SD	1:I:273:ARG:HD3	2.53	0.49
1:D:261:LEU:HD21	1:D:374:HIS:HE1	1.78	0.49
1:G:371:ILE:HD11	2:H:54:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:MET:HB3	1:D:95:MET:HE2	1.69	0.48
2:B:30:ILE:HA	2:B:52(A):PRO:HB2	1.94	0.48
2:B:124:LEU:HD11	2:B:141:LEU:HB2	1.95	0.48
2:E:7:SER:O	2:E:107:THR:HG22	2.12	0.48
2:J:124:LEU:HD11	2:J:141:LEU:HB2	1.95	0.48
1:D:328:LYS:HD3	1:D:328:LYS:O	2.13	0.48
2:B:11:MET:CE	1:I:434:MET:HB2	2.43	0.48
2:J:210:LYS:NZ	2:J:212:GLU:HG2	2.28	0.48
2:B:135:THR:HG22	2:B:185:PRO:HA	1.95	0.48
2:B:124:LEU:HB3	3:C:120:PHE:CD1	2.48	0.48
2:E:123:PRO:HG3	2:E:209:LYS:HD2	1.95	0.48
3:K:131:THR:HG22	3:K:184:SER:HA	1.96	0.48
2:E:139:GLY:HA2	2:E:154:TRP:HH2	1.79	0.48
3:L:89:GLN:HG2	3:L:90:GLN:N	2.27	0.48
3:K:48:ILE:HD13	3:K:54:ARG:HA	1.96	0.48
3:K:165:VAL:HG12	3:K:166:THR:O	2.14	0.48
1:D:86:LEU:HB2	1:D:89:VAL:HG11	1.96	0.48
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.79	0.48
1:D:408:LYS:HD2	1:D:408:LYS:C	2.34	0.48
3:L:127:LEU:O	3:L:185:LYS:HD2	2.14	0.48
2:B:126:PRO:HG3	2:B:138:LEU:HD23	1.95	0.48
1:D:325:ASP:O	1:D:328:LYS:HG3	2.13	0.48
2:H:50:TRP:CZ3	2:H:52:LYS:HG3	2.49	0.48
2:E:150:VAL:HG23	2:E:178:LEU:HD21	1.96	0.48
1:A:95:MET:HE1	1:A:234:ASN:O	2.14	0.47
1:A:256:SER:HA	1:A:375:HIS:O	2.14	0.47
3:C:137:LEU:C	3:C:138:LEU:HD12	2.34	0.47
3:C:191:HIS:O	3:C:213:ARG:HD3	2.13	0.47
3:L:204:ARG:H	3:L:204:ARG:NE	2.12	0.47
3:C:77:ASN:HB2	9:C:1197:HOH:O	2.14	0.47
1:A:273:ARG:HH12	1:A:287:HIS:CG	2.33	0.47
1:I:341:VAL:O	1:I:345:VAL:HG23	2.14	0.47
1:D:108:VAL:HG22	1:D:253:PRO:HB3	1.96	0.47
3:K:147:LYS:HB3	3:K:199:THR:OG1	2.15	0.47
2:J:129:LYS:NZ	3:K:211:PHE:HA	2.29	0.47
1:I:93:PHE:HB2	1:I:233:PHE:CZ	2.50	0.47
3:K:199:THR:HG22	3:K:206:PRO:HB3	1.95	0.47
2:B:61:ARG:HB2	2:B:62:PRO:HD3	1.96	0.47
3:F:110:ARG:HD2	3:F:173:SER:HB2	1.96	0.47
2:B:116:THR:HG22	2:B:147:PRO:HD3	1.96	0.47
1:D:446:VAL:HG11	4:D:795:NAG:H82	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:89:GLN:HG2	3:K:90:GLN:N	2.29	0.47
2:E:96:LYS:HG3	2:E:101:GLU:OE1	2.14	0.47
3:C:131:THR:HB	3:C:183:LEU:O	2.14	0.47
3:F:160:ASN:HD22	3:F:183:LEU:HD21	1.80	0.47
1:A:263:GLY:O	1:A:450:THR:HG21	2.14	0.47
2:H:178:LEU:C	2:H:178:LEU:HD12	2.34	0.47
3:C:177:LEU:HD23	3:C:178:SER:N	2.30	0.47
1:I:104:MET:HG2	1:I:479:TRP:CG	2.49	0.47
2:J:63:LEU:HD23	2:J:66:ARG:NH1	2.29	0.47
3:C:2:ILE:HD13	3:C:97:PHE:HD2	1.79	0.47
1:G:256:SER:HA	1:G:375:HIS:O	2.15	0.47
2:H:11:MET:CE	1:D:434:MET:HB2	2.45	0.47
2:J:123:PRO:HG3	2:J:209:LYS:HD2	1.96	0.47
3:L:18:THR:HG22	3:L:76:SER:O	2.14	0.47
1:A:207:LYS:HG2	1:A:439:ILE:CG2	2.45	0.47
3:C:17:GLU:O	3:C:78:LEU:HD13	2.14	0.47
3:F:75:ILE:N	3:F:75:ILE:HD12	2.30	0.47
1:I:458:GLY:O	2:J:60:ALA:HA	2.15	0.46
3:L:33:LEU:HD13	3:L:71:TYR:CG	2.50	0.46
1:D:95:MET:SD	1:D:273:ARG:HD3	2.55	0.46
2:E:201:LYS:N	2:E:202:PRO:CD	2.78	0.46
1:G:394:THR:HB	9:G:1607:HOH:O	2.15	0.46
3:K:23:CYS:HB2	3:K:35:TRP:CH2	2.50	0.46
2:H:119:PRO:HD2	2:H:205:THR:HG21	1.98	0.46
1:I:116:LEU:O	1:I:118:PRO:HD3	2.15	0.46
1:D:259:LEU:HB2	1:D:374:HIS:CE1	2.51	0.46
2:B:178:LEU:C	2:B:178:LEU:HD12	2.35	0.46
2:H:40:ALA:HB2	2:H:88:ALA:HB2	1.97	0.46
1:I:333:ILE:N	1:I:333:ILE:HD12	2.30	0.46
1:D:408:LYS:C	1:D:410:CYS:H	2.18	0.46
1:G:414:ILE:HD11	1:G:416:LEU:HD21	1.98	0.46
1:A:298:ARG:HD2	1:A:326:ILE:O	2.14	0.46
2:H:20:ILE:HD11	2:H:80:LEU:HD23	1.97	0.46
1:D:343:LYS:NZ	1:D:343:LYS:HB3	2.30	0.46
2:E:39:LEU:HD21	2:E:45:PRO:HG3	1.96	0.46
1:G:349:LEU:O	1:G:353:PHE:HD2	1.98	0.46
1:A:392:ASN:O	1:A:396:ILE:HD13	2.15	0.46
1:D:207:LYS:HE2	1:D:436:ALA:HB3	1.97	0.46
3:L:66:ARG:HG3	3:L:71:TYR:CZ	2.51	0.46
1:A:360:ILE:O	1:A:467:THR:HA	2.14	0.46
2:B:39:LEU:HD22	2:B:45:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:160:ASN:H	3:K:160:ASN:HD22	1.64	0.46
1:G:120:VAL:HG12	1:G:434:MET:HB3	1.98	0.46
2:E:121:VAL:HG13	2:E:140:CYS:HB3	1.98	0.46
3:L:12:SER:HB3	3:L:107:ASP:HB2	1.98	0.46
1:I:350:LYS:C	1:I:352:HIS:H	2.19	0.46
1:A:358:THR:HB	1:A:465:ASN:HB3	1.96	0.46
3:F:54:ARG:NE	3:F:60:ASP:HA	2.31	0.46
3:K:127:LEU:O	3:K:185:LYS:HD2	2.16	0.45
2:E:200:HIS:CE1	2:E:202:PRO:HB2	2.50	0.45
2:B:126:PRO:HG3	2:B:138:LEU:HB3	1.98	0.45
3:L:110:ARG:HD2	3:L:173:SER:HB2	1.98	0.45
3:L:83:PHE:HA	3:L:104:VAL:HG23	1.98	0.45
2:E:131:THR:HG23	2:E:134:GLY:H	1.81	0.45
2:H:57:VAL:HG21	2:H:59:TYR:CE1	2.52	0.45
3:F:116:SER:OG	3:F:139:ASN:HB3	2.16	0.45
1:A:351:GLU:OE2	5:A:495:BGC:H6C1	2.15	0.45
3:L:194:TYR:HB2	3:L:211:PHE:CE2	2.51	0.45
2:H:183:THR:HG21	3:L:139:ASN:ND2	2.32	0.45
1:D:425:ASN:ND2	1:D:432:GLN:HG2	2.31	0.45
3:F:204:ARG:H	3:F:204:ARG:CD	2.19	0.45
2:B:148:GLU:HB3	2:B:149:PRO:HA	1.98	0.45
1:D:248:THR:HA	1:D:486:TYR:CE1	2.51	0.45
4:A:795:NAG:H2	4:A:795:NAG:H82	1.87	0.45
2:J:57:VAL:HG21	2:J:59:TYR:CE1	2.52	0.45
1:I:120:VAL:HG12	1:I:434:MET:HB3	1.99	0.45
2:E:147:PRO:HB2	2:E:148:GLU:H	1.44	0.45
2:H:61:ARG:HB2	2:H:62:PRO:HD3	1.99	0.45
1:A:232:ASN:OD1	1:A:268:GLU:HB3	2.17	0.45
1:A:91:GLU:HG3	1:A:226:LEU:HD13	1.99	0.45
1:G:95:MET:HE2	1:G:95:MET:HB3	1.79	0.45
3:L:168:GLN:NE2	3:L:173:SER:HB3	2.32	0.45
2:E:3:GLN:C	2:E:4:LEU:HD12	2.37	0.45
1:I:105:GLN:HG2	1:I:479:TRP:CD1	2.51	0.45
1:I:205:CYS:N	1:I:206:PRO:HD3	2.32	0.45
2:E:82(A):ARG:HB3	2:E:82(A):ARG:HH11	1.81	0.45
3:K:18:THR:HG22	3:K:76:SER:O	2.17	0.45
3:L:65:SER:OG	3:L:72:ASN:HB2	2.17	0.45
2:J:18:MET:HE1	2:J:109:VAL:HG11	1.99	0.45
1:D:101:VAL:HG13	1:D:479:TRP:HB2	1.98	0.45
1:I:108:VAL:HG22	1:I:253:PRO:HB3	1.97	0.45
1:G:104:MET:CE	1:G:479:TRP:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:TYR:O	3:C:200:HIS:HE1	2.00	0.45
1:I:290:LYS:HE2	1:I:337:LYS:HE3	1.99	0.45
1:A:434:MET:HB2	2:J:11:MET:CE	2.47	0.45
1:D:93:PHE:HB2	1:D:233:PHE:HZ	1.82	0.45
1:G:95:MET:SD	1:G:273:ARG:HD3	2.57	0.44
2:B:154:TRP:HB2	2:B:159:LEU:HB3	1.98	0.44
3:F:33:LEU:HD13	3:F:71:TYR:CD1	2.52	0.44
3:K:21:ILE:HD12	3:K:102:THR:CB	2.47	0.44
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.52	0.44
2:J:44:ARG:NH1	3:K:2:ILE:HD11	2.31	0.44
3:F:138:LEU:HB2	3:F:177:LEU:HB3	2.00	0.44
3:F:142:TYR:O	3:F:200:HIS:HE1	2.00	0.44
3:F:120:PHE:HB2	3:F:135:VAL:HB	1.99	0.44
2:H:53:ARG:HB3	9:H:1215:HOH:O	2.16	0.44
1:I:421:LYS:HB3	1:I:421:LYS:HE2	1.85	0.44
1:D:381:GLU:HB2	1:D:383:PHE:HE2	1.82	0.44
1:G:65:VAL:HG12	1:G:66:HIS:N	2.32	0.44
3:F:139:ASN:O	3:F:141:PHE:HD1	2.01	0.44
2:B:40:ALA:HB2	2:B:88:ALA:HB2	2.00	0.44
3:K:47:VAL:HG12	3:K:48:ILE:HG12	2.00	0.44
1:A:104:MET:HE2	1:A:479:TRP:HB3	2.00	0.44
3:K:6:GLN:HE21	3:K:21:ILE:HD11	1.82	0.44
1:D:290:LYS:HE2	1:D:337:LYS:HE3	2.00	0.44
2:H:18:MET:CE	2:H:109:VAL:HG11	2.48	0.44
2:H:11:MET:HE3	1:D:434:MET:HB2	1.98	0.44
2:J:66:ARG:HD3	9:J:1660:HOH:O	2.17	0.44
2:E:47:TRP:HZ2	2:E:50:TRP:CD1	2.35	0.44
3:C:147:LYS:HE3	9:C:1115:HOH:O	2.18	0.44
3:C:2:ILE:HD13	3:C:97:PHE:CD2	2.53	0.44
1:I:461:ASN:OD1	3:K:2:ILE:HG22	2.17	0.44
1:D:357:LYS:HD3	1:D:466:GLU:HG2	1.98	0.44
3:C:114:ALA:HA	3:C:115:PRO:HD3	1.76	0.44
1:A:64:GLU:HA	1:A:209:SER:HB3	1.99	0.44
2:J:82(A):ARG:HH11	2:J:82(A):ARG:HB3	1.83	0.44
3:K:151:LYS:HB2	3:K:195:ALA:HB3	1.99	0.44
1:G:269:GLU:HA	1:G:289:ASN:ND2	2.32	0.44
1:A:99:ASN:HA	1:A:102:GLU:HG2	2.00	0.44
1:I:378:CYS:HB3	1:I:383:PHE:CE2	2.53	0.44
2:B:82(A):ARG:HB3	2:B:82(A):ARG:HH11	1.83	0.43
3:L:203:LEU:HD22	3:L:204:ARG:HH21	1.82	0.43
1:G:269:GLU:HA	1:G:289:ASN:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:O	1:A:348:LYS:HE2	2.17	0.43
3:L:75:ILE:N	3:L:75:ILE:HD12	2.33	0.43
2:J:47:TRP:CH2	2:J:49:GLY:HA2	2.53	0.43
3:F:39:ARG:HD3	3:F:81:GLY:O	2.17	0.43
1:G:53:PHE:HB2	9:G:1460:HOH:O	2.17	0.43
1:I:118:PRO:HB3	1:I:433:ALA:HB1	1.99	0.43
2:H:2:VAL:HB	2:H:102:HIS:CD2	2.53	0.43
1:G:229:ASN:HD21	1:G:243:SER:HB3	1.82	0.43
1:I:408:LYS:HG2	1:I:409:GLY:N	2.25	0.43
1:A:93:PHE:HB2	1:A:233:PHE:CZ	2.53	0.43
1:D:93:PHE:CE2	1:D:228:CYS:HB2	2.54	0.43
1:G:408:LYS:N	1:G:408:LYS:HD2	2.34	0.43
3:F:6:GLN:H	3:F:100:GLN:HE22	1.67	0.43
1:G:460:ALA:HB3	2:H:61:ARG:HD3	2.00	0.43
3:K:109:LYS:HA	3:K:142:TYR:OH	2.18	0.43
2:E:38:ARG:HG3	2:E:46:GLU:HB3	2.00	0.43
1:A:252:LYS:HA	1:A:253:PRO:HD3	1.83	0.43
2:H:205:THR:C	2:H:206:LYS:HD2	2.38	0.43
2:H:139:GLY:HA2	2:H:154:TRP:CH2	2.54	0.43
3:K:207:VAL:HG12	3:K:208:THR:N	2.34	0.43
3:C:135:VAL:HG12	3:C:136:CYS:N	2.33	0.43
3:C:136:CYS:HB2	3:C:150:TRP:CZ2	2.54	0.43
1:G:461:ASN:HD22	3:L:3:VAL:HG13	1.84	0.43
1:G:100:MET:HE2	1:G:100:MET:HB3	1.93	0.43
2:B:123:PRO:HG3	2:B:209:LYS:HD2	2.00	0.43
2:J:18:MET:HE2	2:J:109:VAL:HG11	2.00	0.43
2:H:27:TYR:HE2	2:H:32:CYS:HB2	1.83	0.43
1:G:110:SER:O	1:G:114:GLN:HG2	2.18	0.43
1:A:349:LEU:HA	1:A:349:LEU:HD12	1.82	0.43
2:H:168:ALA:HA	2:H:178:LEU:HB3	2.01	0.43
1:A:122:LEU:HD12	2:J:11:MET:HG2	2.01	0.43
2:B:196:CYS:SG	2:B:209:LYS:HB3	2.59	0.43
2:B:188:SER:O	2:B:192:GLN:HB2	2.18	0.43
1:G:422:GLN:HB3	1:G:435:TYR:O	2.19	0.43
1:D:64:GLU:HA	1:D:209:SER:HB3	2.00	0.43
2:B:168:ALA:HA	2:B:178:LEU:HB3	2.00	0.43
2:E:184:VAL:HG21	2:E:194:TYR:CE1	2.54	0.43
2:J:116:THR:HG22	2:J:147:PRO:HD3	2.01	0.43
2:H:196:CYS:SG	2:H:209:LYS:HB3	2.58	0.43
2:J:51:LEU:C	2:J:51:LEU:HD23	2.39	0.43
1:I:95:MET:HE2	1:I:95:MET:HB3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:59:TYR:HB2	2:J:64:GLN:HG2	2.01	0.42
3:C:78:LEU:HD23	3:C:83:PHE:CZ	2.54	0.42
1:G:257:THR:O	1:G:258:GLN:HB2	2.19	0.42
1:A:204:ALA:C	1:A:206:PRO:HD3	2.40	0.42
2:J:19:ARG:HA	2:J:80:LEU:O	2.19	0.42
2:E:57:VAL:HG21	2:E:59:TYR:CE1	2.53	0.42
2:E:2:VAL:HB	2:E:102:HIS:NE2	2.34	0.42
2:E:212:GLU:HA	2:E:213:PRO:HD3	1.92	0.42
3:F:136:CYS:HB2	3:F:150:TRP:CH2	2.54	0.42
1:I:201:ILE:N	1:I:201:ILE:HD12	2.34	0.42
1:G:333:ILE:N	1:G:333:ILE:HD12	2.35	0.42
3:C:65:SER:OG	3:C:72:ASN:HB2	2.18	0.42
2:H:35:ASN:O	2:H:92:CYS:HA	2.19	0.42
6:C:572:BMA:H61	6:C:574:MAN:H2	1.68	0.42
1:A:65:VAL:HG13	1:A:115:SER:OG	2.20	0.42
1:I:107:ASP:OD2	7:I:502:TRS:H32	2.20	0.42
2:H:206:LYS:HD2	2:H:206:LYS:N	2.34	0.42
2:H:96:LYS:HG3	2:H:101:GLU:OE1	2.20	0.42
3:C:64:GLY:HA2	3:C:72:ASN:O	2.19	0.42
3:F:104:VAL:O	3:F:104:VAL:HG23	2.20	0.42
3:C:75:ILE:HD12	3:C:75:ILE:N	2.35	0.42
3:K:160:ASN:N	3:K:160:ASN:HD22	2.17	0.42
1:A:104:MET:CE	1:A:479:TRP:HB3	2.49	0.42
2:J:61:ARG:HB2	2:J:62:PRO:HD3	2.01	0.42
3:K:19:ALA:O	3:K:74:THR:HA	2.19	0.42
2:B:6:GLN:HE21	2:B:107:THR:HG23	1.84	0.42
1:G:343:LYS:HB3	1:G:343:LYS:NZ	2.34	0.42
2:J:206:LYS:HD3	2:J:206:LYS:N	2.34	0.42
3:C:195:ALA:HB2	3:C:210:SER:CB	2.46	0.42
3:F:35:TRP:CZ3	3:F:88:CYS:HB3	2.54	0.42
3:K:75:ILE:N	3:K:75:ILE:HD12	2.34	0.42
2:J:122:PHE:HA	2:J:123:PRO:HD3	1.82	0.42
3:C:83:PHE:HA	3:C:104:VAL:HG23	2.02	0.42
3:F:139:ASN:O	3:F:140:ASN:C	2.59	0.42
1:D:93:PHE:HB2	1:D:233:PHE:CZ	2.55	0.42
3:K:192:LYS:O	3:K:212:ASN:HA	2.20	0.42
1:G:297:THR:O	1:G:329:ALA:HB1	2.20	0.42
1:I:95:MET:CE	1:I:235:GLY:HA3	2.47	0.42
3:K:127:LEU:HD23	3:K:132:ALA:HB2	2.02	0.42
1:D:88:ASN:OD1	1:D:88:ASN:N	2.52	0.42
2:J:29:PHE:O	2:J:52(A):PRO:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:150:VAL:HG12	2:H:200:HIS:CD2	2.55	0.41
3:L:149:GLN:CD	3:L:156:LEU:HD21	2.40	0.41
1:I:82:GLN:HB3	9:I:1183:HOH:O	2.18	0.41
2:J:146:PHE:HA	2:J:147:PRO:HA	1.88	0.41
3:C:204:ARG:HG2	3:C:205:SER:N	2.35	0.41
1:A:115:SER:O	1:A:117:GLN:HG3	2.19	0.41
2:B:50:TRP:CZ3	2:B:52:LYS:HG3	2.55	0.41
2:B:38:ARG:C	2:B:39:LEU:HD23	2.41	0.41
1:D:416:LEU:HA	1:D:417:PRO:HD3	1.88	0.41
1:A:343:LYS:NZ	1:A:343:LYS:HB3	2.34	0.41
1:A:416:LEU:HA	1:A:417:PRO:HD3	1.84	0.41
3:F:64:GLY:HA2	3:F:72:ASN:O	2.20	0.41
1:A:300:SER:HB3	1:A:442:LYS:N	2.36	0.41
1:D:66:HIS:CD2	1:D:111:LEU:HD11	2.56	0.41
1:D:269:GLU:HA	1:D:289:ASN:ND2	2.35	0.41
2:J:35:ASN:HD21	2:J:100(A):ASN:ND2	2.18	0.41
3:L:27:GLN:HG3	3:L:28:TYR:H	1.84	0.41
3:L:66:ARG:HG3	3:L:71:TYR:CE2	2.55	0.41
3:L:84:GLY:H	3:L:104:VAL:HG23	1.85	0.41
3:L:149:GLN:OE1	3:L:156:LEU:HD21	2.20	0.41
1:A:328:LYS:HD3	1:A:328:LYS:O	2.21	0.41
1:D:349:LEU:HA	1:D:349:LEU:HD12	1.86	0.41
1:G:342:LEU:HA	1:G:342:LEU:HD12	1.95	0.41
3:C:6:GLN:H	3:C:100:GLN:NE2	2.18	0.41
2:B:201:LYS:N	2:B:202:PRO:CD	2.83	0.41
2:B:122:PHE:HA	2:B:123:PRO:HD3	1.84	0.41
2:H:201:LYS:N	2:H:202:PRO:CD	2.83	0.41
1:I:343:LYS:NZ	1:I:343:LYS:HB3	2.36	0.41
1:G:298:ARG:HD2	1:G:326:ILE:O	2.20	0.41
1:I:480:ARG:NH1	5:I:401:BGC:H2	2.35	0.41
3:K:91:TYR:HB3	3:K:96:GLU:OE1	2.20	0.41
2:J:153:SER:OG	2:J:197:ASN:HB2	2.20	0.41
3:K:122:PRO:HG2	3:K:188:TYR:CZ	2.56	0.41
1:D:297:THR:HB	1:D:444:ASN:OD1	2.21	0.41
1:G:328:LYS:O	1:G:328:LYS:HD3	2.21	0.41
1:A:86:LEU:HB2	1:A:89:VAL:HG11	2.02	0.41
3:F:190:LYS:NZ	3:F:190:LYS:HB2	2.35	0.41
2:J:17:SER:HB3	9:J:1139:HOH:O	2.19	0.41
1:I:91:GLU:HG3	1:I:226:LEU:HD13	2.01	0.41
1:G:270:ILE:O	1:G:348:LYS:HE2	2.21	0.41
1:I:257:THR:O	1:I:258:GLN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:118:GLY:HA2	2:J:119:PRO:HD3	1.81	0.41
2:E:166:PHE:HA	3:F:166:THR:HG22	2.02	0.41
1:A:461:ASN:HD21	3:C:2:ILE:HA	1.85	0.41
1:A:421:LYS:HE2	1:A:421:LYS:HB3	1.87	0.41
3:F:127:LEU:HB3	3:F:185:LYS:NZ	2.36	0.41
1:I:75:VAL:HB	1:I:76:PRO:HD2	2.03	0.41
2:J:17:SER:CB	2:J:82(A):ARG:HA	2.51	0.40
3:L:142:TYR:CG	3:L:143:PRO:HA	2.56	0.40
3:F:19:ALA:HB3	3:F:75:ILE:HD13	2.04	0.40
2:B:183:THR:HG21	3:C:139:ASN:HD22	1.86	0.40
2:B:205:THR:HG22	2:B:207:VAL:HG23	2.02	0.40
1:D:234:ASN:O	1:D:273:ARG:HG2	2.21	0.40
3:L:142:TYR:O	3:L:200:HIS:HE1	2.04	0.40
3:C:78:LEU:HD23	3:C:83:PHE:CE1	2.56	0.40
3:K:160:ASN:ND2	3:K:160:ASN:N	2.69	0.40
3:F:134:VAL:O	3:F:180:THR:HA	2.20	0.40
1:D:219:THR:HA	1:D:220:PRO:HD3	1.87	0.40
1:D:448:ASN:O	1:D:450:THR:HG23	2.21	0.40
1:G:425:ASN:HD21	5:G:503:BGC:H1	1.85	0.40
1:D:110:SER:O	1:D:114:GLN:HG2	2.21	0.40
1:G:116:LEU:HD13	1:G:382:PHE:HZ	1.86	0.40
2:B:50:TRP:CH2	2:B:52:LYS:HE3	2.56	0.40
2:E:123:PRO:O	3:F:123:SER:HB3	2.22	0.40
1:D:225:ILE:HG21	1:D:486:TYR:HD1	1.86	0.40
3:K:168:GLN:HB2	3:K:175:TYR:CE1	2.56	0.40
1:A:421:LYS:HZ3	5:A:508:BGC:H3	1.87	0.40
3:F:84:GLY:H	3:F:104:VAL:HG23	1.86	0.40
3:C:194:TYR:HB2	3:C:211:PHE:CE2	2.57	0.40
1:I:224:VAL:HG22	1:I:225:ILE:N	2.37	0.40
2:E:71:ARG:O	2:E:71:ARG:HD3	2.21	0.40
1:A:397:GLY:O	1:A:404:ASN:HB2	2.22	0.40
3:L:17:GLU:OE1	3:L:109:LYS:HE3	2.22	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	345/353 (98%)	312 (90%)	30 (9%)	3 (1%)	21	46
1	D	346/353 (98%)	314 (91%)	30 (9%)	2 (1%)	30	56
1	G	343/353 (97%)	315 (92%)	25 (7%)	3 (1%)	21	46
1	I	345/353 (98%)	311 (90%)	31 (9%)	3 (1%)	21	46
2	B	222/224 (99%)	203 (91%)	19 (9%)	0	100	100
2	E	222/224 (99%)	192 (86%)	25 (11%)	5 (2%)	8	19
2	H	222/224 (99%)	201 (90%)	19 (9%)	2 (1%)	21	46
2	J	222/224 (99%)	206 (93%)	14 (6%)	2 (1%)	21	46
3	C	208/210 (99%)	178 (86%)	28 (14%)	2 (1%)	19	42
3	F	206/210 (98%)	176 (85%)	26 (13%)	4 (2%)	10	23
3	K	208/210 (99%)	188 (90%)	16 (8%)	4 (2%)	10	23
3	L	206/210 (98%)	192 (93%)	12 (6%)	2 (1%)	19	42
All	All	3095/3148 (98%)	2788 (90%)	275 (9%)	32 (1%)	19	42

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	127	SER
2	E	147	PRO
1	G	410	CYS
2	H	100(D)	PHE
3	L	140	ASN
1	A	404	ASN
3	C	140	ASN
1	D	397	GLY
1	D	411	ASN
3	K	2	ILE
3	K	140	ASN
1	G	267	GLU
1	G	411	ASN
2	E	127	SER
3	F	140	ASN
1	I	396	ILE
2	J	203	SER
1	A	467	THR

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Mol	Chain	Res	Type
3	F	110	ARG
2	J	100(D)	PHE
1	A	462	ASN
2	E	82(B)	SER
2	E	144	ASP
3	F	15	PRO
3	K	15	PRO
3	L	15	PRO
1	I	470	PRO
3	K	206	PRO
3	C	2	ILE
3	F	206	PRO
1	I	220	PRO
2	E	126	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/311 (100%)	301 (97%)	9 (3%)	50	78
1	D	310/311 (100%)	301 (97%)	9 (3%)	50	78
1	G	309/311 (99%)	299 (97%)	10 (3%)	46	75
1	I	309/311 (99%)	304 (98%)	5 (2%)	70	90
2	B	192/192 (100%)	190 (99%)	2 (1%)	82	94
2	E	192/192 (100%)	189 (98%)	3 (2%)	70	90
2	H	192/192 (100%)	185 (96%)	7 (4%)	42	71
2	J	192/192 (100%)	191 (100%)	1 (0%)	92	98
3	C	182/182 (100%)	178 (98%)	4 (2%)	60	85
3	F	180/182 (99%)	175 (97%)	5 (3%)	51	79
3	K	182/182 (100%)	180 (99%)	2 (1%)	80	94
3	L	180/182 (99%)	177 (98%)	3 (2%)	68	89
All	All	2730/2740 (100%)	2670 (98%)	60 (2%)	60	85

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	105	GLN
1	G	123	THR
1	G	200	VAL
1	G	328	LYS
1	G	369	LEU
1	G	396	ILE
1	G	407	MET
1	G	414	ILE
1	G	428	GLN
1	G	462	ASN
2	H	1	GLN
2	H	4	LEU
2	H	34	LEU
2	H	38	ARG
2	H	71	ARG
2	H	82(A)	ARG
2	H	147	PRO
3	L	74	THR
3	L	156	LEU
3	L	204	ARG
1	A	90	THR
1	A	92	ASN
1	A	95	MET
1	A	105	GLN
1	A	297	THR
1	A	328	LYS
1	A	347	GLU
1	A	349	LEU
1	A	385	CYS
2	B	57	VAL
2	B	71	ARG
3	C	21	ILE
3	C	74	THR
3	C	204	ARG
3	C	209	LYS
1	D	88	ASN
1	D	105	GLN
1	D	259	LEU
1	D	328	LYS
1	D	349	LEU
1	D	395	CYS
1	D	396	ILE

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Mol	Chain	Res	Type
1	D	408	LYS
1	D	428	GLN
2	E	1	GLN
2	E	38	ARG
2	E	71	ARG
3	F	21	ILE
3	F	70	ASP
3	F	181	LEU
3	F	204	ARG
3	F	211	PHE
1	I	104	MET
1	I	105	GLN
1	I	261	LEU
1	I	328	LYS
1	I	407	MET
2	J	71	ARG
3	K	21	ILE
3	K	160	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	389	GLN
1	A	92	ASN
1	A	362	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

17 carbohydrates 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	$\# Z > 2$
6	NAG	C	570	3,6	14,14,15	0.56	0	15,19,21	0.73	0
6	NAG	C	571	6	14,14,15	0.56	0	15,19,21	0.66	0
6	BMA	C	572	6	11,11,12	0.60	0	14,15,17	0.80	1 (7%)
6	MAN	C	573	6	11,11,12	0.61	0	14,15,17	0.54	0
6	MAN	C	574	6	11,11,12	0.64	0	14,15,17	0.65	0
8	NAG	F	570	8,3	14,14,15	0.46	0	15,19,21	0.92	1 (6%)
8	NAG	F	571	8	14,14,15	0.50	0	15,19,21	0.63	0
6	NAG	K	570	3,6	14,14,15	0.55	0	15,19,21	0.75	0
6	NAG	K	571	6	14,14,15	0.53	0	15,19,21	0.81	0
6	BMA	K	572	6	11,11,12	0.66	0	14,15,17	1.04	1 (7%)
6	MAN	K	573	6	11,11,12	0.59	0	14,15,17	0.59	0
6	MAN	K	574	6	11,11,12	0.63	0	14,15,17	0.67	0
6	NAG	L	570	3,6	14,14,15	0.54	0	15,19,21	0.72	0
6	NAG	L	571	6	14,14,15	0.51	0	15,19,21	0.76	0
6	BMA	L	572	6	11,11,12	0.61	0	14,15,17	0.83	1 (7%)
6	MAN	L	573	6	11,11,12	0.65	0	14,15,17	0.63	0
6	MAN	L	574	6	11,11,12	0.60	0	14,15,17	0.64	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
6	NAG	C	570	3,6	-	0/6/23/26	0/1/1/1
6	NAG	C	571	6	-	0/6/23/26	0/1/1/1
6	BMA	C	572	6	-	0/2/19/22	0/1/1/1
6	MAN	C	573	6	-	0/2/19/22	0/1/1/1
6	MAN	C	574	6	-	0/2/19/22	0/1/1/1
8	NAG	F	570	8,3	-	0/6/23/26	0/1/1/1
8	NAG	F	571	8	-	0/6/23/26	0/1/1/1
6	NAG	K	570	3,6	-	0/6/23/26	0/1/1/1
6	NAG	K	571	6	-	0/6/23/26	0/1/1/1
6	BMA	K	572	6	-	0/2/19/22	0/1/1/1
6	MAN	K	573	6	-	0/2/19/22	0/1/1/1
6	MAN	K	574	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	L	570	3,6	-	0/6/23/26	0/1/1/1
6	NAG	L	571	6	-	0/6/23/26	0/1/1/1
6	BMA	L	572	6	-	0/2/19/22	0/1/1/1
6	MAN	L	573	6	-	0/2/19/22	0/1/1/1
6	MAN	L	574	6	-	0/2/19/22	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	F	570	NAG	O5-C5-C6	2.06	111.81	107.35
6	C	572	BMA	C1-C2-C3	2.07	111.99	109.54
6	L	572	BMA	C1-C2-C3	2.55	112.56	109.54
6	K	572	BMA	C1-C2-C3	3.36	113.51	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	572	BMA	1	0
6	C	574	MAN	1	0
8	F	570	NAG	1	0
8	F	571	NAG	1	0

5.6 Ligand geometry ⓘ

66 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
7	TRS	A	403	-	7,7,7	0.96	1 (14%)	9,9,9	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TRS	A	493	-	7,7,7	0.97	1 (14%)	9,9,9	0.51	0
5	BGC	A	494	-	12,12,12	0.54	0	17,17,17	0.50	0
5	BGC	A	495	-	12,12,12	0.53	0	17,17,17	0.52	0
5	BGC	A	506	-	12,12,12	0.53	0	17,17,17	0.45	0
5	BGC	A	508	-	12,12,12	0.55	0	17,17,17	0.57	0
4	NAG	A	588	1	14,14,15	0.53	0	15,19,21	0.65	0
4	NAG	A	734	1	14,14,15	0.51	0	15,19,21	0.73	0
4	NAG	A	741	1	14,14,15	0.50	0	15,19,21	0.71	0
4	NAG	A	762	1	14,14,15	0.53	0	15,19,21	0.96	1 (6%)
4	NAG	A	776	1	14,14,15	0.51	0	15,19,21	0.80	1 (6%)
4	NAG	A	789	1	14,14,15	0.51	0	15,19,21	0.84	1 (6%)
4	NAG	A	795	1	14,14,15	0.48	0	15,19,21	0.82	0
4	NAG	A	834	1	14,14,15	0.51	0	15,19,21	0.65	0
4	NAG	A	855	1	14,14,15	0.53	0	15,19,21	0.53	0
4	NAG	A	886	1	14,14,15	0.54	0	15,19,21	0.77	0
4	NAG	A	892	1	14,14,15	0.50	0	15,19,21	0.76	0
4	NAG	A	948	1	14,14,15	0.51	0	15,19,21	0.65	0
5	BGC	B	406	-	12,12,12	0.54	0	17,17,17	0.49	0
5	BGC	B	407	-	12,12,12	0.54	0	17,17,17	0.47	0
5	BGC	C	504	-	12,12,12	0.54	0	17,17,17	0.49	0
7	TRS	D	402	-	7,7,7	0.95	1 (14%)	9,9,9	0.56	0
7	TRS	D	500	-	7,7,7	0.99	1 (14%)	9,9,9	0.47	0
5	BGC	D	505	-	12,12,12	0.53	0	17,17,17	0.43	0
4	NAG	D	588	1	14,14,15	0.52	0	15,19,21	0.60	0
4	NAG	D	734	1	14,14,15	0.52	0	15,19,21	0.62	0
4	NAG	D	741	1	14,14,15	0.51	0	15,19,21	0.62	0
4	NAG	D	762	1	14,14,15	0.57	0	15,19,21	0.75	0
4	NAG	D	776	1	14,14,15	0.56	0	15,19,21	0.53	0
4	NAG	D	789	1	14,14,15	0.53	0	15,19,21	0.65	0
4	NAG	D	795	1	14,14,15	0.54	0	15,19,21	0.68	0
4	NAG	D	834	1	14,14,15	0.51	0	15,19,21	0.74	1 (6%)
4	NAG	D	855	1	14,14,15	0.53	0	15,19,21	0.63	0
4	NAG	D	886	1	14,14,15	0.54	0	15,19,21	0.69	0
4	NAG	D	892	1	14,14,15	0.52	0	15,19,21	0.74	0
4	NAG	D	948	1	14,14,15	0.52	0	15,19,21	0.57	0
5	BGC	E	511	-	12,12,12	0.53	0	17,17,17	0.50	0
5	BGC	G	503	-	12,12,12	0.54	0	17,17,17	0.48	0
4	NAG	G	588	1	14,14,15	0.50	0	15,19,21	0.59	0
4	NAG	G	734	1	14,14,15	0.51	0	15,19,21	0.66	0
4	NAG	G	741	1	14,14,15	0.51	0	15,19,21	0.73	0
4	NAG	G	762	1	14,14,15	0.51	0	15,19,21	1.12	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	776	1	14,14,15	0.51	0	15,19,21	0.88	1 (6%)
4	NAG	G	789	1	14,14,15	0.46	0	15,19,21	0.99	1 (6%)
4	NAG	G	795	1	14,14,15	0.51	0	15,19,21	0.72	0
4	NAG	G	834	1	14,14,15	0.53	0	15,19,21	0.71	0
4	NAG	G	886	1	14,14,15	0.56	0	15,19,21	0.65	0
4	NAG	G	892	1	14,14,15	0.52	0	15,19,21	0.67	0
4	NAG	G	948	1	14,14,15	0.53	0	15,19,21	0.61	0
5	BGC	I	400	-	12,12,12	0.55	0	17,17,17	0.50	0
5	BGC	I	401	-	12,12,12	0.55	0	17,17,17	0.55	0
7	TRS	I	502	-	7,7,7	0.96	1 (14%)	9,9,9	0.59	0
4	NAG	I	588	1	14,14,15	0.51	0	15,19,21	0.92	1 (6%)
4	NAG	I	734	1	14,14,15	0.49	0	15,19,21	0.73	0
4	NAG	I	741	1	14,14,15	0.53	0	15,19,21	0.54	0
4	NAG	I	762	1	14,14,15	0.52	0	15,19,21	0.73	0
4	NAG	I	776	1	14,14,15	0.54	0	15,19,21	0.56	0
4	NAG	I	789	1	14,14,15	0.48	0	15,19,21	1.03	1 (6%)
4	NAG	I	795	1	14,14,15	0.52	0	15,19,21	0.55	0
4	NAG	I	834	1	14,14,15	0.54	0	15,19,21	0.55	0
4	NAG	I	886	1	14,14,15	0.53	0	15,19,21	0.72	0
4	NAG	I	892	1	14,14,15	0.50	0	15,19,21	0.84	1 (6%)
4	NAG	I	948	1	14,14,15	0.56	0	15,19,21	1.36	1 (6%)
7	TRS	J	501	-	7,7,7	0.97	1 (14%)	9,9,9	0.51	0
5	BGC	J	507	-	12,12,12	0.54	0	17,17,17	0.52	0
7	TRS	K	405	-	7,7,7	0.99	1 (14%)	9,9,9	0.49	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
7	TRS	A	403	-	-	0/9/9/9	0/0/0/0
7	TRS	A	493	-	-	0/9/9/9	0/0/0/0
5	BGC	A	494	-	-	0/2/22/22	0/1/1/1
5	BGC	A	495	-	-	0/2/22/22	0/1/1/1
5	BGC	A	506	-	-	0/2/22/22	0/1/1/1
5	BGC	A	508	-	-	0/2/22/22	0/1/1/1
4	NAG	A	588	1	-	0/6/23/26	0/1/1/1
4	NAG	A	734	1	-	0/6/23/26	0/1/1/1
4	NAG	A	741	1	-	0/6/23/26	0/1/1/1
4	NAG	A	762	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	776	1	-	0/6/23/26	0/1/1/1
4	NAG	A	789	1	-	0/6/23/26	0/1/1/1
4	NAG	A	795	1	-	0/6/23/26	0/1/1/1
4	NAG	A	834	1	-	0/6/23/26	0/1/1/1
4	NAG	A	855	1	-	0/6/23/26	0/1/1/1
4	NAG	A	886	1	-	0/6/23/26	0/1/1/1
4	NAG	A	892	1	-	0/6/23/26	0/1/1/1
4	NAG	A	948	1	-	0/6/23/26	0/1/1/1
5	BGC	B	406	-	-	0/2/22/22	0/1/1/1
5	BGC	B	407	-	-	0/2/22/22	0/1/1/1
5	BGC	C	504	-	-	0/2/22/22	0/1/1/1
7	TRS	D	402	-	-	0/9/9/9	0/0/0/0
7	TRS	D	500	-	-	0/9/9/9	0/0/0/0
5	BGC	D	505	-	-	0/2/22/22	0/1/1/1
4	NAG	D	588	1	-	0/6/23/26	0/1/1/1
4	NAG	D	734	1	-	0/6/23/26	0/1/1/1
4	NAG	D	741	1	-	0/6/23/26	0/1/1/1
4	NAG	D	762	1	-	0/6/23/26	0/1/1/1
4	NAG	D	776	1	-	0/6/23/26	0/1/1/1
4	NAG	D	789	1	-	0/6/23/26	0/1/1/1
4	NAG	D	795	1	-	0/6/23/26	0/1/1/1
4	NAG	D	834	1	-	0/6/23/26	0/1/1/1
4	NAG	D	855	1	-	0/6/23/26	0/1/1/1
4	NAG	D	886	1	-	0/6/23/26	0/1/1/1
4	NAG	D	892	1	-	0/6/23/26	0/1/1/1
4	NAG	D	948	1	-	0/6/23/26	0/1/1/1
5	BGC	E	511	-	-	0/2/22/22	0/1/1/1
5	BGC	G	503	-	-	0/2/22/22	0/1/1/1
4	NAG	G	588	1	-	0/6/23/26	0/1/1/1
4	NAG	G	734	1	-	0/6/23/26	0/1/1/1
4	NAG	G	741	1	-	0/6/23/26	0/1/1/1
4	NAG	G	762	1	-	0/6/23/26	0/1/1/1
4	NAG	G	776	1	-	0/6/23/26	0/1/1/1
4	NAG	G	789	1	-	0/6/23/26	0/1/1/1
4	NAG	G	795	1	-	0/6/23/26	0/1/1/1
4	NAG	G	834	1	-	0/6/23/26	0/1/1/1
4	NAG	G	886	1	-	0/6/23/26	0/1/1/1
4	NAG	G	892	1	-	0/6/23/26	0/1/1/1
4	NAG	G	948	1	-	2/6/23/26	0/1/1/1
5	BGC	I	400	-	-	0/2/22/22	0/1/1/1
5	BGC	I	401	-	-	0/2/22/22	0/1/1/1
7	TRS	I	502	-	-	0/9/9/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	588	1	-	0/6/23/26	0/1/1/1
4	NAG	I	734	1	-	0/6/23/26	0/1/1/1
4	NAG	I	741	1	-	0/6/23/26	0/1/1/1
4	NAG	I	762	1	-	0/6/23/26	0/1/1/1
4	NAG	I	776	1	-	0/6/23/26	0/1/1/1
4	NAG	I	789	1	-	0/6/23/26	0/1/1/1
4	NAG	I	795	1	-	0/6/23/26	0/1/1/1
4	NAG	I	834	1	-	0/6/23/26	0/1/1/1
4	NAG	I	886	1	-	0/6/23/26	0/1/1/1
4	NAG	I	892	1	-	0/6/23/26	0/1/1/1
4	NAG	I	948	1	-	0/6/23/26	0/1/1/1
7	TRS	J	501	-	-	0/9/9/9	0/0/0/0
5	BGC	J	507	-	-	0/2/22/22	0/1/1/1
7	TRS	K	405	-	-	0/9/9/9	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	500	TRS	C-N	-2.58	1.46	1.50
7	K	405	TRS	C-N	-2.58	1.46	1.50
7	J	501	TRS	C-N	-2.53	1.47	1.50
7	A	493	TRS	C-N	-2.52	1.47	1.50
7	A	403	TRS	C-N	-2.51	1.47	1.50
7	I	502	TRS	C-N	-2.50	1.47	1.50
7	D	402	TRS	C-N	-2.48	1.47	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	789	NAG	C2-N2-C7	-2.03	120.43	123.04
4	D	834	NAG	C1-O5-C5	2.13	114.95	112.25
4	A	776	NAG	C1-O5-C5	2.33	115.20	112.25
4	G	776	NAG	C1-O5-C5	2.40	115.29	112.25
4	A	762	NAG	C1-O5-C5	2.43	115.33	112.25
4	I	892	NAG	C1-O5-C5	2.59	115.53	112.25
4	G	789	NAG	C1-O5-C5	2.68	115.64	112.25
4	I	588	NAG	C1-O5-C5	2.95	115.99	112.25
4	G	762	NAG	C1-O5-C5	3.08	116.16	112.25
4	I	789	NAG	C1-O5-C5	3.24	116.35	112.25
4	I	948	NAG	C1-O5-C5	4.63	118.13	112.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	948	NAG	C8-C7-N2-C2
4	G	948	NAG	O7-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	495	BGC	1	0
5	A	506	BGC	3	0
5	A	508	BGC	2	0
4	A	776	NAG	1	0
4	A	795	NAG	1	0
5	B	407	BGC	1	0
7	D	402	TRS	1	0
4	D	795	NAG	1	0
5	G	503	BGC	1	0
4	G	795	NAG	1	0
5	I	401	BGC	1	0
7	I	502	TRS	2	0
4	I	789	NAG	1	0
5	J	507	BGC	1	0
7	K	405	TRS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	349/353 (98%)	0.19	7 (2%) 68 68	55, 89, 141, 225	0
1	D	350/353 (99%)	0.25	12 (3%) 49 48	64, 97, 168, 273	0
1	G	347/353 (98%)	0.41	14 (4%) 42 40	68, 103, 160, 241	0
1	I	349/353 (98%)	0.44	28 (8%) 15 12	74, 118, 181, 249	0
2	B	224/224 (100%)	0.36	15 (6%) 21 19	59, 102, 172, 208	0
2	E	224/224 (100%)	1.89	61 (27%) 1 0	70, 118, 264, 292	0
2	H	224/224 (100%)	0.48	3 (1%) 79 79	59, 85, 117, 165	0
2	J	224/224 (100%)	0.19	4 (1%) 71 71	66, 101, 134, 202	0
3	C	210/210 (100%)	0.59	20 (9%) 10 8	61, 116, 173, 216	0
3	F	208/210 (99%)	2.12	84 (40%) 0 0	88, 181, 245, 270	0
3	K	210/210 (100%)	0.52	17 (8%) 15 12	78, 114, 163, 210	0
3	L	208/210 (99%)	0.44	21 (10%) 9 6	71, 112, 154, 228	0
All	All	3127/3148 (99%)	0.60	286 (9%) 11 9	55, 105, 206, 292	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	181	VAL	15.1
3	F	155	ALA	15.1
2	E	125	ALA	13.7
2	E	141	LEU	13.0
2	E	210	LYS	12.4
2	E	129	LYS	12.2
2	E	127	SER	12.0
2	E	194	TYR	11.9
2	E	180	SER	10.8
3	F	150	TRP	10.7
3	F	134	VAL	10.1

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Mol	Chain	Res	Type	RSRZ
3	F	183	LEU	10.1
3	F	151	LYS	9.9
3	F	119	ILE	9.8
3	F	207	VAL	9.2
3	F	135	VAL	9.0
3	F	120	PHE	8.9
2	E	136	ALA	8.9
3	F	206	PRO	8.8
3	F	198	VAL	8.7
2	E	158	ALA	8.5
2	E	211	ALA	8.4
2	E	184	VAL	8.3
2	E	191	THR	8.2
2	E	152	VAL	8.1
3	F	117	VAL	8.1
3	C	1	GLU	8.0
2	E	126	PRO	7.8
3	F	185	LYS	7.8
3	F	122	PRO	7.6
2	E	198	VAL	7.3
2	E	195	ILE	7.1
3	F	214	GLY	7.1
2	E	130	SER	6.8
3	K	2	ILE	6.8
2	E	122	PHE	6.6
2	E	128	SER	6.6
2	E	164	HIS	6.5
3	F	196	CYS	6.5
3	F	208	THR	6.5
3	F	182	THR	6.4
2	E	189	LEU	6.4
3	F	136	CYS	6.2
2	E	212	GLU	6.1
3	F	197	GLU	6.0
2	E	159	LEU	6.0
3	F	205	SER	6.0
1	I	379	ARG	6.0
3	F	210	SER	5.9
3	F	118	PHE	5.9
2	E	142	VAL	5.8
3	K	1	GLU	5.8
3	F	123	SER	5.8

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Mol	Chain	Res	Type	RSRZ
3	F	124	ASP	5.7
2	E	124	LEU	5.6
3	F	156	LEU	5.6
3	F	133	SER	5.5
2	E	196	CYS	5.5
2	E	207	VAL	5.5
3	F	154	ASN	5.3
2	E	208	ASP	5.3
2	E	120	SER	5.3
2	E	190	GLY	5.3
2	E	209	LYS	5.3
2	E	156	SER	5.3
2	E	179	SER	5.2
3	L	204	ARG	5.2
3	F	193	VAL	5.2
3	C	186	ALA	5.1
2	E	197	ASN	5.1
3	F	121	PRO	5.0
3	F	138	LEU	4.9
2	E	162	GLY	4.8
3	C	171	LYS	4.8
1	G	407	MET	4.7
2	E	193	THR	4.7
2	B	125	ALA	4.7
3	K	135	VAL	4.7
3	C	203	LEU	4.6
3	L	216	CYS	4.6
3	F	148	VAL	4.6
3	F	209	LYS	4.5
2	E	150	VAL	4.5
2	E	160	THR	4.5
3	F	204	ARG	4.5
3	F	177	LEU	4.5
2	B	132	SER	4.4
3	F	129	SER	4.4
2	E	140	CYS	4.4
3	F	152	VAL	4.4
2	B	138	LEU	4.3
2	E	199	ASN	4.3
3	F	144	ARG	4.3
3	L	156	LEU	4.3
3	K	203	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
2	E	133	GLY	4.2
3	F	203	LEU	4.2
3	K	148	VAL	4.2
2	E	123	PRO	4.2
3	K	198	VAL	4.2
3	L	186	ALA	4.1
3	F	199	THR	4.1
1	I	349	LEU	4.1
3	K	151	LYS	4.1
3	F	184	SER	4.1
3	F	194	TYR	4.0
3	K	207	VAL	4.0
1	I	452	ILE	4.0
3	F	195	ALA	3.9
3	C	204	ARG	3.9
2	E	121	VAL	3.9
1	I	259	LEU	3.8
2	E	178	LEU	3.8
3	C	188	TYR	3.8
1	A	322	SER	3.7
3	K	119	ILE	3.7
2	B	146	PHE	3.7
3	F	147	LYS	3.7
2	E	154	TRP	3.7
1	I	302	GLY	3.6
3	F	202	GLY	3.6
3	F	165	VAL	3.6
3	F	128	LYS	3.6
2	E	149	PRO	3.5
3	F	116	SER	3.5
2	E	182	VAL	3.5
1	D	322	SER	3.5
3	C	146	ALA	3.5
3	C	151	LYS	3.4
1	I	93	PHE	3.4
3	F	201	GLN	3.4
2	E	161	SER	3.4
3	C	120	PHE	3.4
1	I	491	ILE	3.4
3	F	159	GLY	3.4
3	F	145	GLU	3.3
1	I	272	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	45	TRP	3.3
2	E	138	LEU	3.3
3	K	216	CYS	3.3
1	D	349	LEU	3.2
3	C	189	GLU	3.2
1	I	277	LEU	3.2
3	L	213	ARG	3.1
3	F	130	GLY	3.1
3	F	175	TYR	3.1
3	F	137	LEU	3.1
3	L	192	LYS	3.0
1	G	492	GLU	3.0
3	F	18	THR	3.0
3	C	137	LEU	3.0
3	F	47	VAL	3.0
2	E	213	PRO	3.0
1	D	337	LYS	2.9
3	F	132	ALA	2.9
3	L	188	TYR	2.9
3	F	67	TRP	2.9
1	D	407	MET	2.9
3	L	152	VAL	2.9
1	D	321	GLY	2.9
3	F	19	ALA	2.9
1	A	408	LYS	2.9
1	D	396	ILE	2.8
3	F	188	TYR	2.8
3	F	107	ASP	2.8
3	C	202	GLY	2.8
2	E	166	PHE	2.8
3	F	28	TYR	2.8
3	F	13	LEU	2.8
3	F	58	ILE	2.8
3	F	181	LEU	2.8
3	L	214	GLY	2.8
2	B	202	PRO	2.8
3	F	115	PRO	2.8
3	L	190	LYS	2.8
3	F	189	GLU	2.8
2	E	216	CYS	2.8
3	C	2	ILE	2.7
3	F	215	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	192	GLN	2.7
3	F	131	THR	2.7
3	K	202	GLY	2.7
3	L	183	LEU	2.7
3	F	200	HIS	2.7
2	B	126	PRO	2.7
3	L	78	LEU	2.7
2	E	163	VAL	2.7
1	I	86	LEU	2.7
2	B	152	VAL	2.6
2	J	189	LEU	2.6
1	D	353	PHE	2.6
3	C	207	VAL	2.6
3	F	149	GLN	2.6
1	G	361	PHE	2.6
3	K	195	ALA	2.6
1	I	453	LEU	2.5
1	A	328	LYS	2.5
2	E	119	PRO	2.5
2	E	157	GLY	2.5
1	G	57	ASP	2.5
2	B	129	LYS	2.5
3	K	204	ARG	2.5
1	I	226	LEU	2.5
1	I	461	ASN	2.5
1	G	420	ILE	2.5
1	I	225	ILE	2.5
1	I	390	LEU	2.5
3	F	143	PRO	2.5
2	B	117	LYS	2.4
3	F	108	ILE	2.4
2	B	133	GLY	2.4
3	F	161	SER	2.4
2	B	214	LYS	2.4
2	E	146	PHE	2.4
3	F	83	PHE	2.4
1	I	245	VAL	2.4
3	C	135	VAL	2.4
1	G	324	GLY	2.4
3	C	113	ALA	2.4
3	F	9	GLY	2.4
1	I	84	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	361	PHE	2.3
1	I	369	LEU	2.3
1	I	244	SER	2.3
2	J	121	VAL	2.3
3	F	48	ILE	2.3
1	I	324	GLY	2.3
3	C	67	TRP	2.3
3	F	176	SER	2.3
1	G	389	GLN	2.3
1	G	225	ILE	2.3
1	G	327	ARG	2.3
2	B	118	GLY	2.3
3	L	159	GLY	2.3
1	I	488	VAL	2.3
3	C	198	VAL	2.3
1	G	301	ASN	2.3
1	I	301	ASN	2.3
1	A	473	GLY	2.3
2	J	63	LEU	2.2
3	C	183	LEU	2.2
3	F	62	PHE	2.2
2	B	127	SER	2.2
3	L	189	GLU	2.2
3	F	216	CYS	2.2
2	H	68	THR	2.2
3	L	155	ALA	2.2
3	L	4	LEU	2.2
3	L	21	ILE	2.2
2	E	135	THR	2.2
2	E	151	THR	2.2
1	D	286	VAL	2.2
1	I	292	VAL	2.2
3	K	47	VAL	2.2
1	G	272	ILE	2.2
1	G	359	ILE	2.2
3	K	69	PRO	2.2
1	G	58	ALA	2.2
1	G	226	LEU	2.1
2	J	129	LYS	2.1
3	F	76	SER	2.1
1	A	268	GLU	2.1
3	K	128	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	186	ALA	2.1
1	I	100	MET	2.1
3	F	75	ILE	2.1
1	A	59	LYS	2.1
1	D	330	TYR	2.1
3	L	47	VAL	2.1
3	L	193	VAL	2.1
3	C	47	VAL	2.1
1	I	72	HIS	2.1
1	D	270	ILE	2.1
3	L	151	LYS	2.1
2	B	189	LEU	2.1
2	E	153	SER	2.1
2	H	17	SER	2.1
3	L	194	TYR	2.1
1	D	277	LEU	2.0
1	D	390	LEU	2.0
2	H	189	LEU	2.0
1	A	327	ARG	2.0
1	I	83	GLU	2.0
2	B	99	ASP	2.0
3	F	45	ARG	2.0
3	K	209	LYS	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](#)

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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	K	570	14/15	0.86	0.21	0.34	116,142,167,186	0
8	NAG	F	570	14/15	0.90	0.25	0.25	144,174,187,199	0
6	NAG	L	570	14/15	0.92	0.17	-0.47	125,143,162,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	C	570	14/15	0.94	0.13	-0.93	102,112,125,146	0
6	MAN	C	573	11/12	0.79	0.27	-	188,198,216,216	0
6	MAN	C	574	11/12	0.80	0.15	-	202,209,216,216	0
6	NAG	L	571	14/15	0.88	0.17	-	158,179,191,206	0
6	BMA	L	572	11/12	0.52	0.33	-	211,219,224,230	0
6	NAG	C	571	14/15	0.87	0.23	-	125,168,183,204	0
6	MAN	K	574	11/12	0.79	0.27	-	216,236,238,239	0
6	MAN	L	574	11/12	0.58	0.44	-	209,235,239,239	0
6	BMA	K	572	11/12	0.24	0.23	-	230,237,239,242	0
6	NAG	K	571	14/15	0.70	0.30	-	118,182,200,219	0
8	NAG	F	571	14/15	0.89	0.27	-	190,206,214,217	0
6	MAN	L	573	11/12	0.75	0.29	-	159,191,200,207	0
6	MAN	K	573	11/12	0.78	0.38	-	217,221,232,232	0
6	BMA	C	572	11/12	0.65	0.22	-	211,218,224,225	0

6.4 Ligands

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
7	TRS	K	405	8/8	0.59	0.42	34.75	164,183,188,188	0
4	NAG	A	948	14/15	0.91	0.29	8.03	152,166,176,182	0
5	BGC	A	506	12/12	0.63	0.49	6.20	179,199,203,205	0
5	BGC	D	505	12/12	0.61	0.35	4.32	162,179,185,185	0
5	BGC	A	508	12/12	0.85	0.34	3.61	141,162,172,177	0
5	BGC	I	401	12/12	0.77	0.27	2.88	136,156,176,178	0
4	NAG	D	588	14/15	0.69	0.46	2.51	193,207,215,219	0
5	BGC	G	503	12/12	0.75	0.27	2.27	92,146,155,156	0
5	BGC	B	406	12/12	0.80	0.25	1.90	140,182,188,189	0
7	TRS	D	500	8/8	0.83	0.28	1.49	108,137,143,151	0
5	BGC	A	494	12/12	0.66	0.28	1.40	161,182,188,188	0
4	NAG	A	776	14/15	0.84	0.27	1.37	98,128,144,144	0
4	NAG	G	886	14/15	0.91	0.24	0.94	94,111,128,136	0
7	TRS	J	501	8/8	0.89	0.22	0.79	125,145,154,155	0
4	NAG	I	948	14/15	0.90	0.21	0.64	152,171,176,185	0
4	NAG	I	892	14/15	0.93	0.21	0.63	149,165,177,179	0
4	NAG	D	892	14/15	0.90	0.22	0.53	134,145,164,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	I	795	14/15	0.92	0.22	0.41	98,133,154,155	0
4	NAG	A	795	14/15	0.91	0.16	0.39	109,120,136,142	0
4	NAG	D	776	14/15	0.88	0.23	0.33	126,154,166,168	0
4	NAG	A	734	14/15	0.96	0.25	0.26	79,103,109,113	0
7	TRS	D	402	8/8	0.94	0.17	0.12	84,102,120,123	0
7	TRS	A	403	8/8	0.95	0.18	0.02	98,108,120,124	0
4	NAG	I	741	14/15	0.81	0.19	-0.00	149,180,190,191	0
4	NAG	G	762	14/15	0.97	0.20	-0.13	80,91,111,118	0
4	NAG	I	762	14/15	0.96	0.22	-0.17	98,113,118,123	0
4	NAG	D	734	14/15	0.96	0.19	-0.19	108,119,137,140	0
4	NAG	I	776	14/15	0.89	0.19	-0.27	146,173,183,184	0
4	NAG	G	776	14/15	0.93	0.16	-0.28	120,140,150,156	0
4	NAG	A	892	14/15	0.89	0.17	-0.31	123,151,163,164	0
4	NAG	D	762	14/15	0.95	0.16	-0.37	79,88,99,100	0
4	NAG	G	892	14/15	0.96	0.14	-0.41	71,107,123,133	0
4	NAG	D	795	14/15	0.97	0.16	-0.48	86,107,115,121	0
4	NAG	A	834	14/15	0.92	0.14	-0.58	122,135,148,151	0
4	NAG	I	734	14/15	0.93	0.17	-0.59	116,136,144,147	0
5	BGC	C	504	12/12	0.60	0.20	-0.71	197,212,216,216	0
4	NAG	A	762	14/15	0.97	0.13	-0.74	80,90,107,107	0
4	NAG	I	789	14/15	0.93	0.18	-0.76	120,132,137,142	0
5	BGC	B	407	12/12	0.88	0.18	-0.79	114,145,150,152	0
4	NAG	G	834	14/15	0.95	0.12	-0.86	136,145,179,186	0
4	NAG	G	734	14/15	0.96	0.13	-0.88	91,106,120,120	0
4	NAG	G	588	14/15	0.86	0.28	-0.89	159,171,176,177	0
4	NAG	D	789	14/15	0.94	0.17	-0.93	105,121,137,138	0
4	NAG	G	789	14/15	0.93	0.16	-1.08	110,116,129,134	0
4	NAG	A	588	14/15	0.97	0.12	-1.11	63,79,89,90	0
7	TRS	I	502	8/8	0.94	0.13	-1.16	113,126,128,130	0
4	NAG	A	789	14/15	0.96	0.15	-1.24	79,90,111,126	0
4	NAG	G	795	14/15	0.91	0.13	-1.42	97,123,136,139	0
5	BGC	E	511	12/12	0.68	0.30	-	162,194,197,198	0
4	NAG	D	855	14/15	0.85	0.22	-	170,185,192,193	0
4	NAG	D	948	14/15	0.90	0.15	-	129,149,163,168	0
4	NAG	A	855	14/15	0.77	0.43	-	191,212,221,221	0
4	NAG	D	741	14/15	0.79	0.47	-	176,190,202,207	0
4	NAG	D	886	14/15	0.93	0.17	-	82,103,121,122	0
4	NAG	I	886	14/15	0.95	0.14	-	102,127,140,149	0
5	BGC	J	507	12/12	0.38	0.29	-	197,218,223,223	0
5	BGC	A	495	12/12	0.85	0.13	-	113,153,160,160	0
4	NAG	I	834	14/15	0.89	0.17	-	124,151,159,166	0
4	NAG	A	886	14/15	0.93	0.18	-	72,86,111,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	D	834	14/15	0.89	0.23	-	116,132,139,144	0
5	BGC	I	400	12/12	0.83	0.33	-	208,216,220,220	0
7	TRS	A	493	8/8	0.66	0.21	-	156,167,171,172	0
4	NAG	G	948	14/15	0.86	0.22	-	153,173,179,179	0
4	NAG	G	741	14/15	0.88	0.18	-	143,160,167,171	0
4	NAG	A	741	14/15	0.90	0.12	-	105,126,137,138	0
4	NAG	I	588	14/15	0.78	0.33	-	167,178,186,187	0

6.5 Other polymers [i](#)

There are no such residues in this entry.