Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:00 PM GMT

PDB ID	:	4NCO
Title	:	Crystal Structure of the BG505 SOSIP gp140 HIV-1 Env trimer in Complex with the Broadly Neutralizing Fab PGT122
Authors	:	Julien, J.-P.; Stanfield, R.L.; Lyumkis, D.; Ward, A.B.; Wilson, I.A.
Deposited on	:	2013-10-24
Resolution	:	4.70 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:

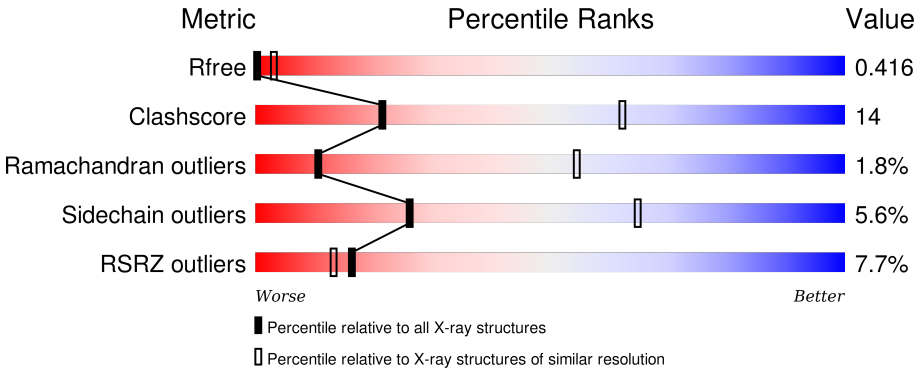
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.70 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	1095 (5.80-3.60)
Clashscore	102246	1010 (5.76-3.64)
Ramachandran outliers	100387	1137 (5.80-3.60)
Sidechain outliers	100360	1118 (5.80-3.60)
RSRZ outliers	91569	1098 (5.80-3.60)

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	475	2% 51% 33% 5% 12%
1	E	475	4% 51% 33% 5% 12%
1	I	475	4% 50% 33% 5% 12%
2	B	78	95%
2	F	78	95%

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Mol	Chain	Length	Quality of chain
2	J	78	92% 6%
3	C	211	9% 82% 13%
3	G	211	12% 82% 13%
3	K	211	18% 80% 13%
4	D	235	10% 78% 17%
4	H	235	7% 78% 17%
4	L	235	11% 76% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	1295	-	-	-	X
5	NAG	A	1386	-	-	-	X
5	NAG	E	1295	-	-	-	X
5	NAG	E	1386	-	-	-	X
5	NAG	I	1295	-	-	-	X
5	NAG	I	1386	-	-	-	X
6	NAG	A	1131	-	-	-	X
6	NAG	A	1261	-	-	-	X
6	NAG	E	1131	-	-	-	X
6	NAG	E	1261	-	-	-	X
6	NAG	I	1131	-	-	-	X
6	NAG	I	1261	-	-	-	X
7	NAG	A	1331	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22014 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 BG505 SOSIP gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3096	1937	544	590	25			
1	E	420	Total	C	N	O	S	0	0	0
			3096	1937	544	590	25			
1	I	420	Total	C	N	O	S	0	0	0
			3096	1937	544	590	25			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	ENGINEERED MUTATION	UNP Q2N0S6
A	501	CYS	ALA	ENGINEERED MUTATION	UNP Q2N0S6
E	332	ASN	THR	ENGINEERED MUTATION	UNP Q2N0S6
E	501	CYS	ALA	ENGINEERED MUTATION	UNP Q2N0S6
I	332	ASN	THR	ENGINEERED MUTATION	UNP Q2N0S6
I	501	CYS	ALA	ENGINEERED MUTATION	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIP gp41.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	77	Total	C	N	O	0	0	0
			385	231	77	77			
2	F	77	Total	C	N	O	0	0	0
			385	231	77	77			
2	J	77	Total	C	N	O	0	0	0
			385	231	77	77			

- Molecule 3 is a protein called PGT122 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	202	Total	C	N	O	S	0	0	0
			1530	964	255	307	4			

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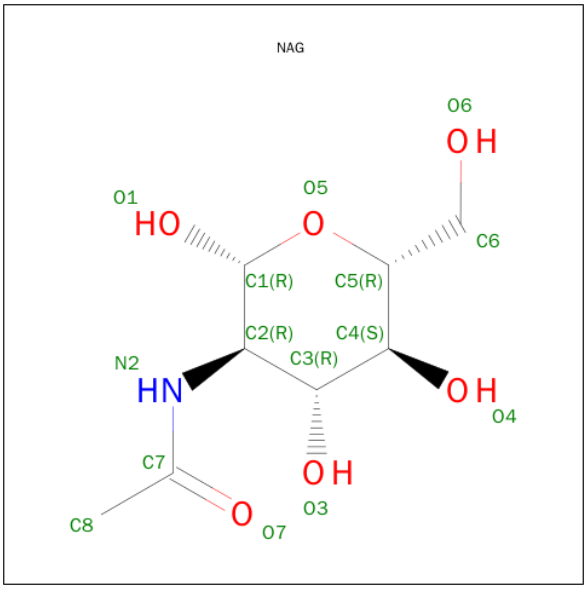
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	202	Total	C	N	O	S	0	0	0
			1530	964	255	307	4			
3	K	202	Total	C	N	O	S	0	0	0
			1530	964	255	307	4			

- Molecule 4 is a protein called PGT122 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	226	Total	C	N	O	S	0	0	0
			1728	1100	293	330	5			
4	H	226	Total	C	N	O	S	0	0	0
			1728	1100	293	330	5			
4	L	226	Total	C	N	O	S	0	0	0
			1728	1100	293	330	5			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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

- Molecule 6 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total C N O 83 46 2 35	0	0
6	A	7	Total C N O 83 46 2 35	0	0
6	A	7	Total C N O 83 46 2 35	0	0
6	A	7	Total C N O 83 46 2 35	0	0
6	E	7	Total C N O 83 46 2 35	0	0
6	E	7	Total C N O 83 46 2 35	0	0
6	E	7	Total C N O 83 46 2 35	0	0
6	E	7	Total C N O 83 46 2 35	0	0
6	I	7	Total C N O 83 46 2 35	0	0
6	I	7	Total C N O 83 46 2 35	0	0
6	I	7	Total C N O 83 46 2 35	0	0
6	I	7	Total C N O 83 46 2 35	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	9	Total	C	N	O	0	0
			105	58	2	45		
7	E	9	Total	C	N	O	0	0
			105	58	2	45		
7	I	9	Total	C	N	O	0	0
			105	58	2	45		

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

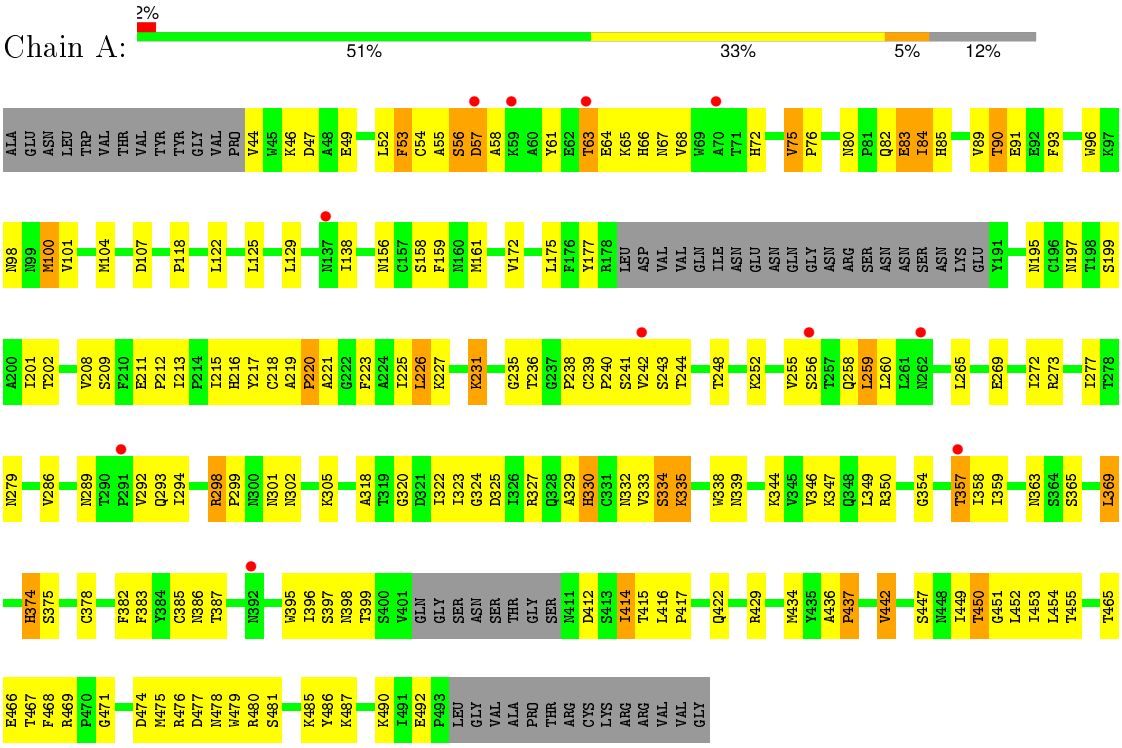
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	2	Total	C	O	0	0
			22	12	10		
8	G	2	Total	C	O	0	0
			22	12	10		
8	K	2	Total	C	O	0	0
			22	12	10		

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.

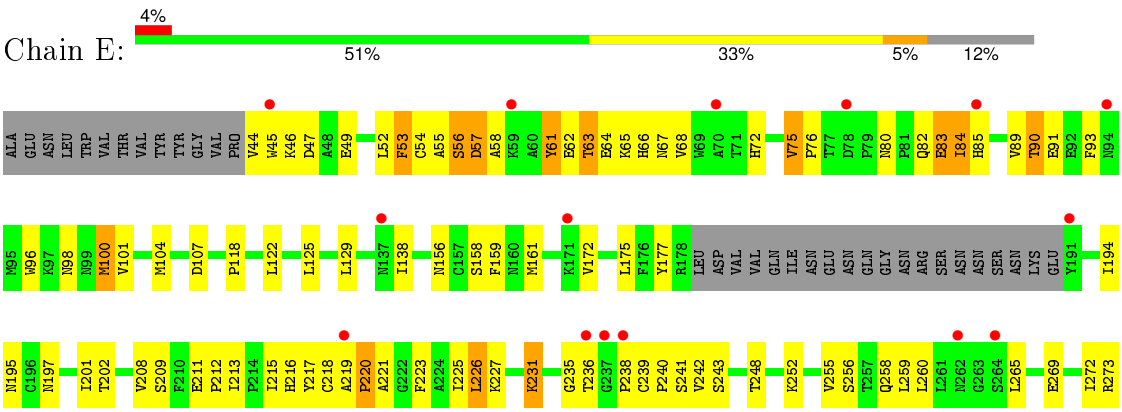
- Molecule 1: BG505 SOSIP gp120

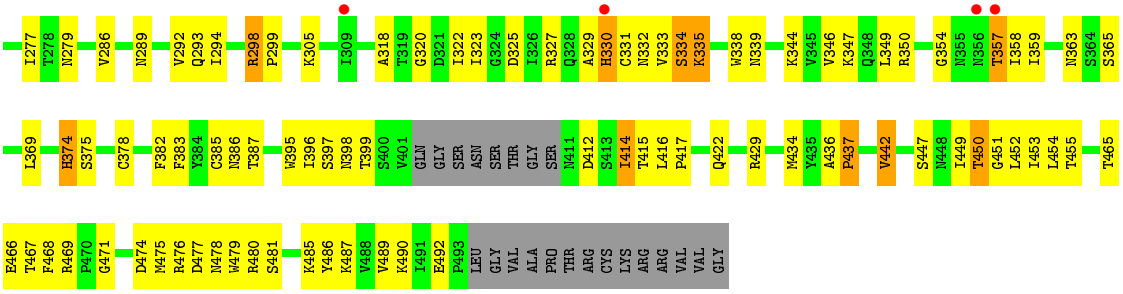
Chain A:



- Molecule 1: BG505 SOSIP gp120

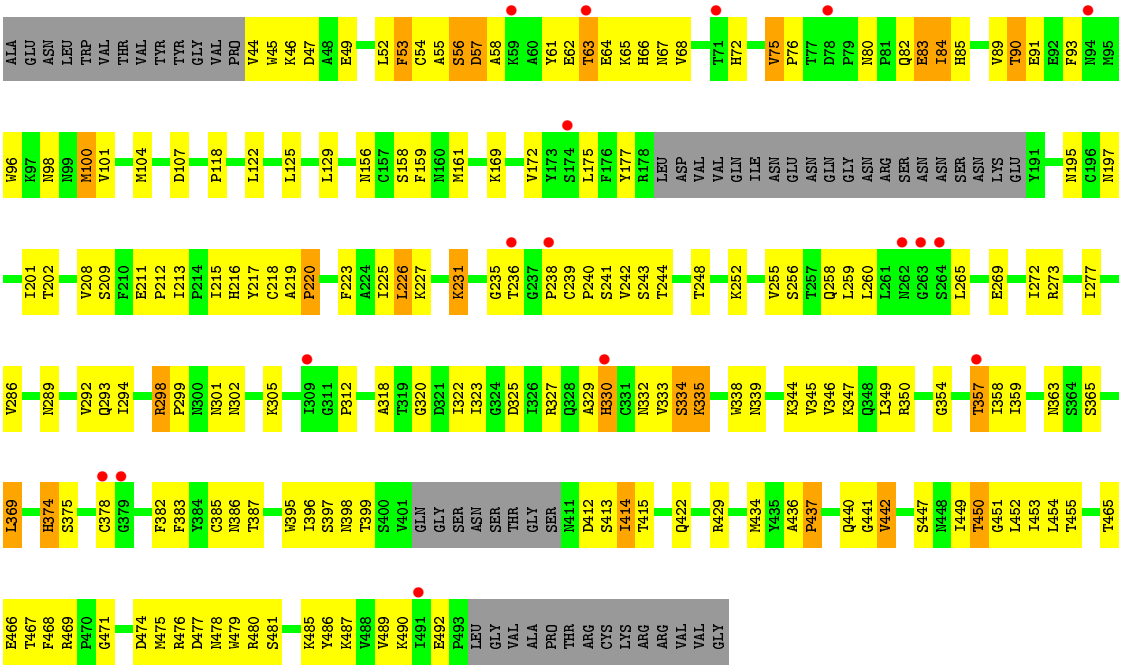
Chain E:





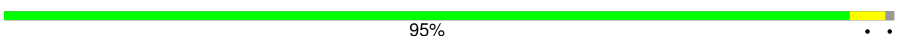
• Molecule 1: BG505 SOSIP gp120

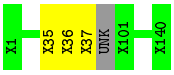
Chain I:



• Molecule 2: BG505 SOSIP gp41

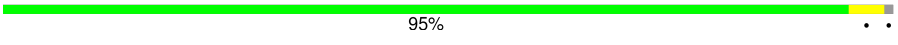
Chain B:

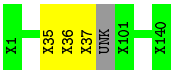




• Molecule 2: BG505 SOSIP gp41

Chain F:



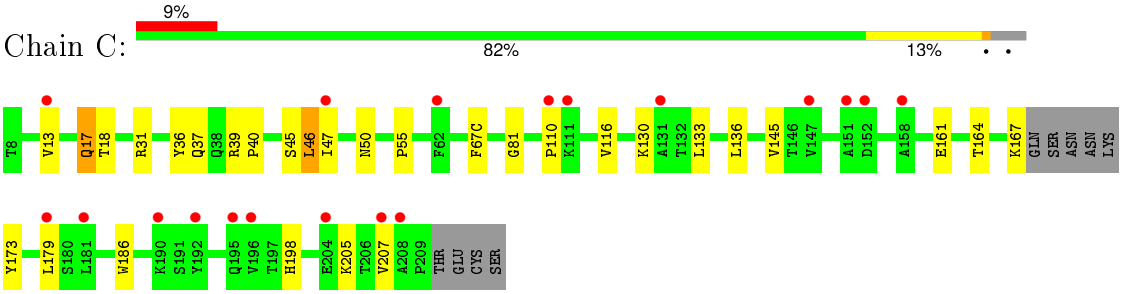


• Molecule 2: BG505 SOSIP gp41

Chain J:

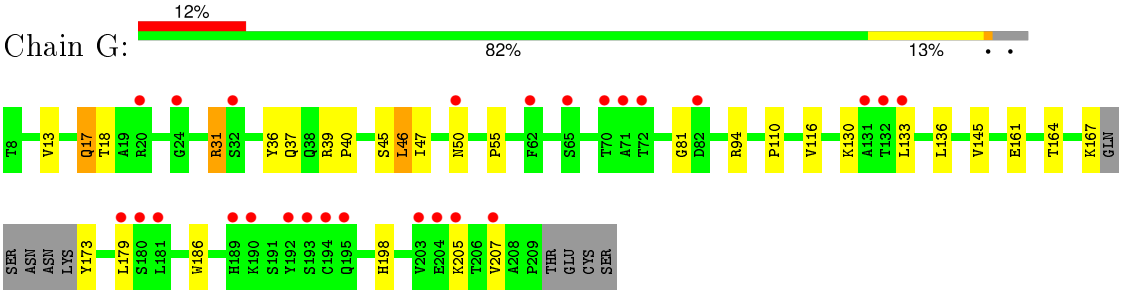
- Molecule 3: PGT122 light chain

Chain C:



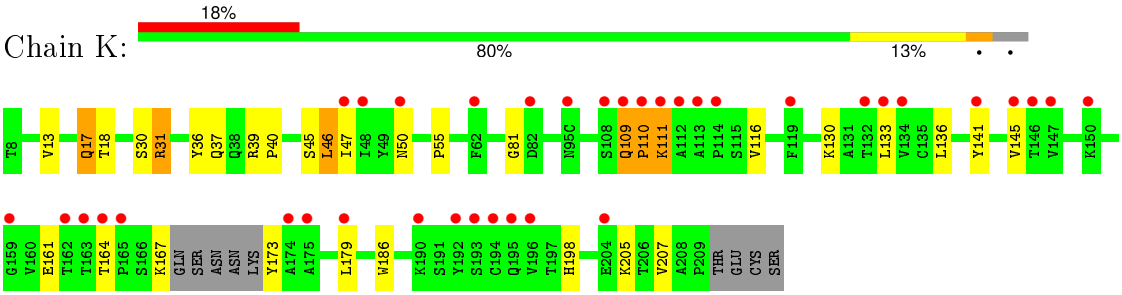
- Molecule 3: PGT122 light chain

Chain G:



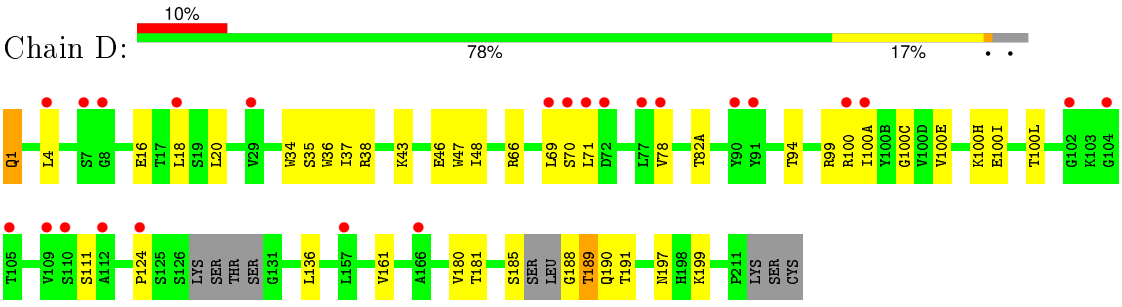
- Molecule 3: PGT122 light chain

Chain K:



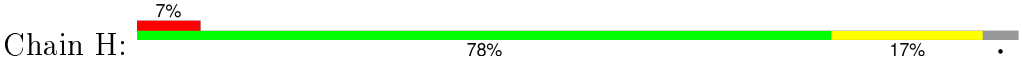
- Molecule 4: PGT122 heavy chain

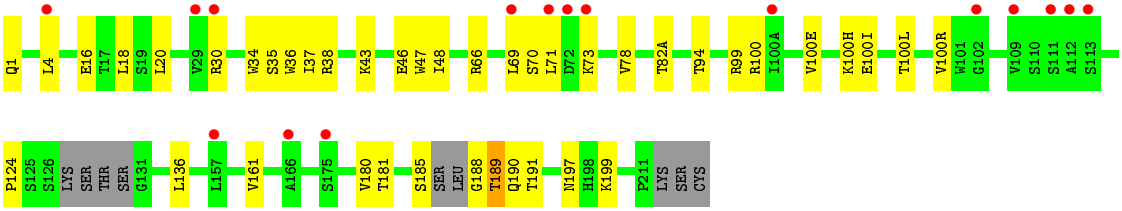
Chain D:



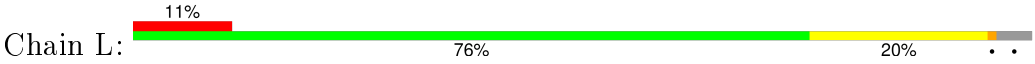
- Molecule 4: PGT122 heavy chain

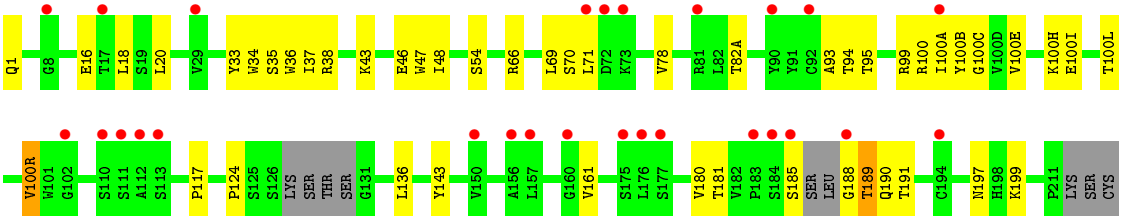
Chain H:





- Molecule 4: PGT122 heavy chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.20Å 260.72Å 283.18Å 90.00° 99.56° 90.00°	Depositor
Resolution (Å)	39.89 – 4.70 39.89 – 4.70	Depositor EDS
% Data completeness (in resolution range)	89.0 (39.89-4.70) 89.1 (39.89-4.70)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 4.63Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.375 , 0.389 0.399 , 0.416	Depositor DCC
R_{free} test set	2621 reflections (5.48%)	DCC
Wilson B-factor (Å^2)	136.6	Xtriage
Anisotropy	1.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 374.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.31$, $< L^2 > = 0.15$	Xtriage
Outliers	0 of 50382 reflections	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	22014	wwPDB-VP
Average B, all atoms (Å^2)	262.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, 0.375 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: 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	0.33	0/3161	0.71	4/4306 (0.1%)
1	E	0.35	0/3161	0.71	3/4306 (0.1%)
1	I	0.33	0/3161	0.71	3/4306 (0.1%)
3	C	0.27	0/1571	0.54	1/2151 (0.0%)
3	G	0.27	0/1571	0.55	1/2151 (0.0%)
3	K	0.28	0/1571	0.58	2/2151 (0.1%)
4	D	0.30	0/1774	0.57	0/2421
4	H	0.34	1/1774 (0.1%)	0.57	0/2421
4	L	0.45	1/1774 (0.1%)	0.59	1/2421 (0.0%)
All	All	0.33	2/19518 (0.0%)	0.64	15/26634 (0.1%)

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
1	A	0	3
1	E	0	3
1	I	0	3
3	C	0	1
3	G	0	1
3	K	0	1
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	100(R)	VAL	C-N	13.91	1.66	1.34
4	H	100(R)	VAL	C-N	6.19	1.48	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	335	LYS	N-CA-C	6.21	127.77	111.00
1	A	335	LYS	N-CA-C	6.18	127.69	111.00
1	I	335	LYS	N-CA-C	6.10	127.48	111.00
1	I	450	THR	C-N-CA	-6.05	109.59	122.30
4	L	100(R)	VAL	O-C-N	6.04	132.37	122.70
1	E	450	THR	C-N-CA	-5.98	109.73	122.30
1	A	450	THR	C-N-CA	-5.97	109.75	122.30
1	E	334	SER	C-N-CA	5.65	135.84	121.70
3	K	111	LYS	N-CA-C	5.61	126.14	111.00
1	A	334	SER	C-N-CA	5.51	135.48	121.70
3	C	46	LEU	CA-CB-CG	5.35	127.61	115.30
3	K	46	LEU	CA-CB-CG	5.35	127.61	115.30
3	G	46	LEU	CA-CB-CG	5.35	127.60	115.30
1	I	334	SER	C-N-CA	5.32	134.99	121.70
1	A	259	LEU	C-N-CA	-5.00	109.19	121.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	THR	Peptide
1	A	56	SER	Peptide
1	A	80	ASN	Peptide
3	C	110	PRO	Peptide
1	E	236	THR	Peptide
1	E	56	SER	Peptide
1	E	80	ASN	Peptide
3	G	110	PRO	Peptide
1	I	236	THR	Peptide
1	I	56	SER	Peptide
1	I	80	ASN	Peptide
3	K	110	PRO	Peptide

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	3096	0	2821	142	0
1	E	3096	0	2821	144	0
1	I	3096	0	2821	145	0
2	B	385	0	82	2	0
2	F	385	0	82	2	0
2	J	385	0	82	3	0
3	C	1530	0	1472	21	0
3	G	1530	0	1472	20	0
3	K	1530	0	1472	23	0
4	D	1728	0	1699	36	0
4	H	1728	0	1699	30	0
4	L	1728	0	1699	44	0
5	A	140	0	130	3	0
5	E	140	0	130	3	0
5	I	140	0	130	2	0
6	A	332	0	280	6	0
6	E	332	0	280	6	0
6	I	332	0	280	5	0
7	A	105	0	88	2	0
7	E	105	0	88	0	0
7	I	105	0	88	4	0
8	C	22	0	19	3	0
8	G	22	0	19	1	0
8	K	22	0	19	2	0
All	All	22014	0	19773	590	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 14.

All (590) 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:I:293:GLN:HB2	1:I:334:SER:HB3	1.33	1.11
1:E:293:GLN:HB2	1:E:334:SER:HB3	1.33	1.09
1:A:293:GLN:HB2	1:A:334:SER:HB3	1.33	1.08
1:I:91:GLU:HA	1:I:239:CYS:O	1.74	0.88
1:E:91:GLU:HA	1:E:239:CYS:O	1.74	0.86
1:A:91:GLU:HA	1:A:239:CYS:O	1.74	0.86
1:I:358:ILE:HB	1:I:465:THR:HG22	1.58	0.84
1:E:358:ILE:HB	1:E:465:THR:HG22	1.58	0.84
1:A:358:ILE:HB	1:A:465:THR:HG22	1.58	0.84
1:A:260:LEU:HB2	1:A:450:THR:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:260:LEU:HB2	1:I:450:THR:O	1.79	0.83
4:D:38:ARG:N	4:D:46:GLU:O	2.12	0.83
4:H:38:ARG:N	4:H:46:GLU:O	2.12	0.82
4:L:38:ARG:N	4:L:46:GLU:O	2.12	0.81
1:E:260:LEU:HB2	1:E:450:THR:O	1.79	0.81
4:H:38:ARG:O	4:H:46:GLU:N	2.15	0.79
4:D:38:ARG:O	4:D:46:GLU:N	2.15	0.78
1:A:269:GLU:HA	1:A:289:ASN:HD22	1.48	0.78
1:I:269:GLU:HA	1:I:289:ASN:HD22	1.48	0.78
1:E:269:GLU:HA	1:E:289:ASN:HD22	1.48	0.77
4:L:38:ARG:O	4:L:46:GLU:N	2.15	0.76
1:E:335:LYS:HD3	1:E:414:ILE:HD11	1.67	0.76
4:D:99:ARG:HG2	4:D:100(L):THR:HG22	1.68	0.76
1:I:335:LYS:HD3	1:I:414:ILE:HD11	1.68	0.75
1:A:335:LYS:HD3	1:A:414:ILE:HD11	1.67	0.75
1:I:101:VAL:HG13	1:I:479:TRP:HB2	1.69	0.75
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.68	0.75
4:L:35:SER:HB3	4:L:47:TRP:HE1	1.51	0.74
1:E:101:VAL:HG13	1:E:479:TRP:HB2	1.69	0.74
1:A:101:VAL:HG13	1:A:479:TRP:HB2	1.69	0.74
1:E:55:ALA:HB3	1:E:216:HIS:HB2	1.68	0.74
4:H:99:ARG:HG2	4:H:100(L):THR:HG22	1.68	0.74
4:L:99:ARG:HG2	4:L:100(L):THR:HG22	1.68	0.74
1:I:55:ALA:HB3	1:I:216:HIS:HB2	1.68	0.74
1:A:436:ALA:HB3	1:A:437:PRO:HD3	1.70	0.73
1:I:436:ALA:HB3	1:I:437:PRO:HD3	1.69	0.73
1:E:436:ALA:HB3	1:E:437:PRO:HD3	1.70	0.73
1:A:327:ARG:HA	4:D:100(H):LYS:HD2	1.71	0.72
1:E:327:ARG:HA	4:H:100(H):LYS:HD2	1.70	0.72
1:E:227:LYS:HE3	1:E:485:LYS:HD2	1.75	0.69
1:I:227:LYS:HE3	1:I:485:LYS:HD2	1.75	0.69
7:A:1332:NAG:H4	4:D:100(C):GLY:HA3	1.74	0.69
1:A:227:LYS:HE3	1:A:485:LYS:HD2	1.75	0.69
4:L:37:ILE:HG23	4:L:47:TRP:HA	1.76	0.68
4:D:37:ILE:HG23	4:D:47:TRP:HA	1.76	0.68
4:H:38:ARG:O	4:H:46:GLU:O	2.12	0.68
1:E:294:ILE:HG23	1:E:447:SER:HB2	1.76	0.68
4:H:37:ILE:HG23	4:H:47:TRP:HA	1.76	0.67
1:E:477:ASP:OD1	1:E:480:ARG:NH1	2.27	0.67
1:A:294:ILE:HG23	1:A:447:SER:HB2	1.76	0.67
1:I:477:ASP:OD1	1:I:480:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:38:ARG:O	4:D:46:GLU:O	2.12	0.67
2:F:35:UNK:O	2:F:37:UNK:O	2.12	0.67
2:B:35:UNK:O	2:B:37:UNK:O	2.12	0.67
3:G:39:ARG:HG3	3:G:40:PRO:HD2	1.77	0.67
1:A:477:ASP:OD1	1:A:480:ARG:NH1	2.27	0.67
4:L:38:ARG:O	4:L:46:GLU:O	2.12	0.67
2:J:35:UNK:O	2:J:37:UNK:O	2.12	0.67
3:K:39:ARG:HG3	3:K:40:PRO:HD2	1.77	0.66
1:I:294:ILE:HG23	1:I:447:SER:HB2	1.78	0.66
3:C:39:ARG:HG3	3:C:40:PRO:HD2	1.77	0.66
1:A:350:ARG:NH2	1:A:397:SER:O	2.29	0.66
1:I:350:ARG:NH2	1:I:397:SER:O	2.29	0.65
4:D:35:SER:HB3	4:D:47:TRP:HE1	1.62	0.65
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.79	0.65
1:I:327:ARG:HA	4:L:100(H):LYS:HD2	1.78	0.65
1:I:101:VAL:HG21	1:I:480:ARG:HG2	1.79	0.65
8:K:1340:MAN:H3	4:L:100(A):ILE:HB	1.78	0.65
1:E:350:ARG:NH2	1:E:397:SER:O	2.29	0.64
3:K:37:GLN:N	3:K:45:SER:O	2.31	0.64
1:E:359:ILE:HD12	1:E:468:PHE:HE1	1.63	0.64
1:A:68:VAL:O	1:A:72:HIS:ND1	2.31	0.63
1:E:330:HIS:HE1	1:E:415:THR:HG21	1.63	0.63
1:A:359:ILE:HD12	1:A:468:PHE:HE1	1.63	0.63
1:I:91:GLU:O	1:I:238:PRO:HA	1.99	0.63
1:E:91:GLU:O	1:E:238:PRO:HA	1.99	0.63
1:E:68:VAL:O	1:E:72:HIS:ND1	2.31	0.63
1:E:101:VAL:HG21	1:E:480:ARG:HG2	1.79	0.63
1:I:359:ILE:HD12	1:I:468:PHE:HE1	1.63	0.63
4:H:34:TRP:CZ3	4:H:94:THR:HG22	2.34	0.63
3:G:37:GLN:N	3:G:45:SER:O	2.31	0.62
3:C:37:GLN:N	3:C:45:SER:O	2.31	0.62
1:E:330:HIS:CG	4:H:100(E):VAL:HG23	2.34	0.62
1:A:91:GLU:O	1:A:238:PRO:HA	1.99	0.62
1:A:83:GLU:HG3	1:A:84:ILE:H	1.65	0.62
1:I:68:VAL:O	1:I:72:HIS:ND1	2.31	0.62
1:A:363:ASN:O	1:A:469:ARG:NH1	2.33	0.62
1:I:363:ASN:O	1:I:469:ARG:NH1	2.33	0.62
1:E:330:HIS:CB	4:H:100(E):VAL:HG23	2.30	0.61
1:A:100:MET:N	1:A:100:MET:SD	2.73	0.61
1:I:100:MET:SD	1:I:100:MET:N	2.73	0.61
1:E:226:LEU:HD11	1:E:487:LYS:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:GLU:HG3	1:I:84:ILE:H	1.65	0.61
1:E:358:ILE:HG13	1:E:397:SER:H	1.66	0.61
1:A:332:ASN:HB3	5:A:1295:NAG:H82	1.82	0.61
1:E:330:HIS:CE1	1:E:415:THR:CG2	2.84	0.61
1:E:363:ASN:O	1:E:469:ARG:NH1	2.33	0.61
1:I:226:LEU:HD11	1:I:487:LYS:HB3	1.83	0.60
1:A:177:TYR:HE2	1:A:422:GLN:HE21	1.49	0.60
1:E:332:ASN:HB3	5:E:1295:NAG:H82	1.83	0.60
1:A:330:HIS:ND1	4:D:100(E):VAL:HG23	2.16	0.60
1:I:358:ILE:HG13	1:I:397:SER:H	1.66	0.60
4:H:37:ILE:HG13	4:H:47:TRP:HD1	1.67	0.60
4:L:34:TRP:CZ3	4:L:94:THR:HG22	2.37	0.60
1:E:83:GLU:HG3	1:E:84:ILE:H	1.65	0.60
1:I:177:TYR:HE2	1:I:422:GLN:HE21	1.49	0.60
7:I:1332:NAG:H4	4:L:100(C):GLY:CA	2.31	0.60
1:E:226:LEU:HD11	1:E:487:LYS:HD3	1.82	0.60
3:G:37:GLN:O	3:G:45:SER:O	2.20	0.60
1:E:100:MET:SD	1:E:100:MET:N	2.73	0.59
1:I:226:LEU:HD11	1:I:487:LYS:HD3	1.82	0.59
1:A:226:LEU:HD11	1:A:487:LYS:HD3	1.82	0.59
1:A:358:ILE:HG13	1:A:397:SER:H	1.66	0.59
1:E:52:LEU:HB3	1:E:217:TYR:HD2	1.67	0.59
1:A:226:LEU:HD11	1:A:487:LYS:HB3	1.83	0.59
1:I:52:LEU:HB3	1:I:217:TYR:HD2	1.68	0.59
3:K:37:GLN:O	3:K:45:SER:O	2.20	0.59
3:C:37:GLN:O	3:C:45:SER:O	2.20	0.59
6:I:1137:MAN:O4	4:L:54:SER:HB2	2.03	0.59
3:K:31:ARG:O	4:L:100:ARG:NH1	2.34	0.59
4:L:37:ILE:HG13	4:L:47:TRP:HD1	1.66	0.59
1:E:256:SER:HB2	1:E:374:HIS:HE1	1.68	0.59
1:I:226:LEU:CD1	1:I:487:LYS:HB3	2.33	0.59
1:I:258:GLN:O	1:I:452:LEU:HA	2.03	0.59
1:I:476:ARG:HA	1:I:479:TRP:CD1	2.38	0.59
1:E:177:TYR:HE2	1:E:422:GLN:HE21	1.49	0.59
4:D:37:ILE:HG13	4:D:47:TRP:HD1	1.67	0.58
1:E:258:GLN:O	1:E:452:LEU:HA	2.03	0.58
1:I:256:SER:HB2	1:I:374:HIS:HE1	1.68	0.58
1:E:226:LEU:CD1	1:E:487:LYS:HB3	2.33	0.58
1:E:476:ARG:HA	1:E:479:TRP:CD1	2.38	0.58
4:L:33:TYR:HB2	4:L:95:THR:O	2.03	0.58
1:A:256:SER:HB2	1:A:374:HIS:HE1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASP:O	4:D:100(I):GLU:OE2	2.22	0.58
3:K:36:TYR:HA	3:K:46:LEU:HA	1.85	0.58
1:A:258:GLN:O	1:A:452:LEU:HA	2.03	0.58
4:D:4:LEU:HD11	4:D:94:THR:HG23	1.85	0.58
1:A:476:ARG:HA	1:A:479:TRP:CD1	2.38	0.57
3:G:36:TYR:HA	3:G:46:LEU:HA	1.85	0.57
1:E:122:LEU:HA	1:E:201:ILE:HA	1.86	0.57
1:I:332:ASN:HB3	5:I:1295:NAG:H82	1.85	0.57
1:A:98:ASN:HB3	1:A:100:MET:HG2	1.87	0.57
3:C:36:TYR:HA	3:C:46:LEU:HA	1.85	0.57
1:A:226:LEU:CD1	1:A:487:LYS:HB3	2.33	0.57
1:A:422:GLN:O	1:A:434:MET:HA	2.05	0.57
1:I:98:ASN:HB3	1:I:100:MET:HG2	1.87	0.57
3:C:145:VAL:HG12	3:C:198:HIS:HB2	1.86	0.57
1:A:122:LEU:HA	1:A:201:ILE:HA	1.86	0.57
1:A:52:LEU:HB3	1:A:217:TYR:HD2	1.68	0.57
1:A:53:PHE:HB3	1:A:218:CYS:HB2	1.87	0.57
1:I:53:PHE:HB3	1:I:218:CYS:HB2	1.87	0.57
3:G:145:VAL:HG12	3:G:198:HIS:HB2	1.86	0.57
1:I:422:GLN:O	1:I:434:MET:HA	2.05	0.57
1:A:259:LEU:HB3	1:A:449:ILE:HG23	1.85	0.57
1:I:122:LEU:HA	1:I:201:ILE:HA	1.86	0.57
1:E:325:ASP:O	4:H:100(I):GLU:OE2	2.23	0.57
4:L:161:VAL:HG22	4:L:180:VAL:HG12	1.87	0.57
1:I:259:LEU:HB3	1:I:449:ILE:HG23	1.86	0.56
1:E:53:PHE:HB3	1:E:218:CYS:HB2	1.86	0.56
1:E:259:LEU:HB3	1:E:449:ILE:HG23	1.86	0.56
1:E:422:GLN:O	1:E:434:MET:HA	2.05	0.56
3:K:110:PRO:HB2	3:K:111:LYS:HB2	1.87	0.56
4:D:161:VAL:HG22	4:D:180:VAL:HG12	1.88	0.56
3:K:145:VAL:HG12	3:K:198:HIS:HB2	1.87	0.56
1:E:98:ASN:HB3	1:E:100:MET:HG2	1.86	0.56
1:E:330:HIS:HE1	1:E:415:THR:CG2	2.19	0.56
4:D:37:ILE:HG13	4:D:47:TRP:CD1	2.41	0.56
1:E:82:GLN:O	1:E:84:ILE:HG13	2.06	0.56
4:D:37:ILE:HA	4:D:47:TRP:HA	1.88	0.56
4:L:37:ILE:HG13	4:L:47:TRP:CD1	2.41	0.56
1:I:82:GLN:O	1:I:84:ILE:HG13	2.06	0.56
1:A:199:SER:HA	1:I:312:PRO:HB3	1.86	0.55
4:H:37:ILE:HA	4:H:47:TRP:HA	1.88	0.55
1:A:347:LYS:O	1:A:350:ARG:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:217:TYR:O	1:I:248:THR:HG23	2.07	0.55
4:H:37:ILE:HG13	4:H:47:TRP:CD1	2.41	0.55
1:I:347:LYS:O	1:I:350:ARG:HG2	2.06	0.55
3:C:50:ASN:OD1	4:D:100:ARG:NH2	2.36	0.55
1:E:217:TYR:O	1:E:248:THR:HG23	2.07	0.55
8:C:1340:MAN:H3	4:D:100(A):ILE:HB	1.88	0.55
1:E:347:LYS:O	1:E:350:ARG:HG2	2.06	0.55
4:H:161:VAL:HG22	4:H:180:VAL:HG12	1.88	0.55
1:I:93:PHE:CE1	1:I:226:LEU:HD13	2.42	0.54
1:E:451:GLY:O	1:E:452:LEU:HD23	2.08	0.54
1:A:82:GLN:O	1:A:84:ILE:HG13	2.06	0.54
1:E:93:PHE:CE1	1:E:226:LEU:HD13	2.42	0.54
1:A:93:PHE:CE1	1:A:226:LEU:HD13	2.42	0.54
3:C:39:ARG:NH1	3:C:81:GLY:O	2.40	0.54
1:E:478:ASN:O	1:E:481:SER:OG	2.20	0.54
3:K:39:ARG:NH1	3:K:81:GLY:O	2.40	0.54
1:A:217:TYR:O	1:A:248:THR:HG23	2.07	0.54
1:A:346:VAL:HG21	1:A:395:TRP:CD1	2.43	0.54
1:E:396:ILE:HG22	1:E:398:ASN:H	1.73	0.54
1:A:396:ILE:HG22	1:A:398:ASN:H	1.73	0.54
4:D:34:TRP:CZ3	4:D:94:THR:HG22	2.43	0.54
1:I:344:LYS:HA	1:I:347:LYS:HE2	1.90	0.54
1:E:344:LYS:HA	1:E:347:LYS:HE2	1.90	0.54
1:E:64:GLU:HB2	1:E:209:SER:HB3	1.90	0.54
1:I:63:THR:OG1	1:I:64:GLU:N	2.40	0.54
3:G:50:ASN:ND2	8:G:1341:MAN:O2	2.38	0.54
1:I:82:GLN:O	1:I:84:ILE:N	2.41	0.54
1:I:64:GLU:HB2	1:I:209:SER:HB3	1.90	0.54
1:E:346:VAL:HG21	1:E:395:TRP:CD1	2.43	0.54
4:L:37:ILE:HA	4:L:47:TRP:HA	1.89	0.54
4:H:4:LEU:HD11	4:H:94:THR:HG23	1.90	0.54
1:I:451:GLY:O	1:I:452:LEU:HD23	2.07	0.53
1:A:64:GLU:HB2	1:A:209:SER:HB3	1.90	0.53
1:E:55:ALA:O	1:E:216:HIS:ND1	2.42	0.53
1:A:451:GLY:O	1:A:452:LEU:HD23	2.07	0.53
1:E:63:THR:OG1	1:E:64:GLU:N	2.40	0.53
1:A:265:LEU:HD23	1:A:450:THR:HG23	1.91	0.53
1:I:55:ALA:O	1:I:216:HIS:ND1	2.42	0.53
3:K:37:GLN:HB2	3:K:47:ILE:HG12	1.91	0.53
3:G:37:GLN:HB2	3:G:47:ILE:HG12	1.90	0.53
3:K:109:GLN:HB3	3:K:141:TYR:HE2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:346:VAL:HG21	1:I:395:TRP:CD1	2.43	0.53
1:A:298:ARG:HG2	1:A:383:PHE:CZ	2.43	0.53
1:I:265:LEU:HD23	1:I:450:THR:HG23	1.90	0.53
1:A:82:GLN:O	1:A:84:ILE:N	2.41	0.53
1:A:344:LYS:HA	1:A:347:LYS:HE2	1.90	0.53
1:E:82:GLN:O	1:E:84:ILE:N	2.41	0.53
1:A:63:THR:OG1	1:A:64:GLU:N	2.40	0.53
1:I:46:LYS:HB3	1:I:490:LYS:HG3	1.90	0.53
3:C:37:GLN:HB2	3:C:47:ILE:HG12	1.91	0.53
1:A:378:CYS:HB2	1:A:383:PHE:CE1	2.44	0.53
1:I:252:LYS:HD3	6:I:1261:NAG:H81	1.89	0.53
1:A:299:PRO:HA	1:A:442:VAL:HA	1.91	0.53
1:E:46:LYS:HB3	1:E:490:LYS:HG3	1.91	0.53
4:L:35:SER:OG	4:L:95:THR:OG1	2.19	0.53
1:A:66:HIS:HB3	1:A:213:ILE:HG12	1.90	0.53
1:E:265:LEU:HD23	1:E:450:THR:HG23	1.91	0.53
7:A:1332:NAG:H4	4:D:100(C):GLY:CA	2.37	0.53
1:E:378:CYS:HB2	1:E:383:PHE:CE1	2.44	0.53
1:E:66:HIS:HB3	1:E:213:ILE:HG12	1.90	0.53
1:A:305:LYS:O	1:A:318:ALA:N	2.42	0.53
1:I:305:LYS:O	1:I:318:ALA:N	2.42	0.53
1:I:298:ARG:HG2	1:I:383:PHE:CZ	2.43	0.52
1:E:298:ARG:HG2	1:E:383:PHE:CZ	2.43	0.52
1:I:66:HIS:HB3	1:I:213:ILE:HG12	1.91	0.52
4:L:189:THR:OG1	4:L:190:GLN:N	2.42	0.52
1:E:305:LYS:O	1:E:318:ALA:N	2.42	0.52
3:K:133:LEU:HD12	3:K:179:LEU:HD23	1.92	0.52
1:I:299:PRO:HA	1:I:442:VAL:HA	1.91	0.52
1:E:93:PHE:HE1	1:E:226:LEU:HD13	1.75	0.52
1:A:55:ALA:O	1:A:216:HIS:ND1	2.42	0.52
1:I:396:ILE:HG22	1:I:398:ASN:H	1.73	0.52
1:A:93:PHE:HE1	1:A:226:LEU:HD13	1.75	0.52
3:K:109:GLN:HB3	3:K:141:TYR:CE2	2.45	0.52
1:I:346:VAL:HA	1:I:349:LEU:HD12	1.92	0.52
4:H:189:THR:OG1	4:H:190:GLN:N	2.42	0.52
3:C:133:LEU:HD12	3:C:179:LEU:HD23	1.92	0.52
1:I:378:CYS:HB2	1:I:383:PHE:CE1	2.44	0.52
1:I:330:HIS:ND1	4:L:100(E):VAL:HA	2.25	0.52
4:H:185:SER:O	4:H:188:GLY:N	2.44	0.51
1:E:159:PHE:HB2	1:E:172:VAL:HG23	1.93	0.51
3:G:39:ARG:NH1	3:G:81:GLY:O	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:PRO:HA	1:E:442:VAL:HA	1.91	0.51
1:I:478:ASN:O	1:I:481:SER:OG	2.20	0.51
1:E:346:VAL:HA	1:E:349:LEU:HD12	1.92	0.51
3:C:50:ASN:ND2	8:C:1341:MAN:O2	2.38	0.51
1:E:252:LYS:HD3	6:E:1261:NAG:H81	1.93	0.51
4:D:185:SER:O	4:D:188:GLY:N	2.44	0.51
4:L:185:SER:O	4:L:188:GLY:N	2.44	0.51
1:A:334:SER:HB2	5:A:1295:NAG:H83	1.93	0.51
1:I:90:THR:HG22	1:I:91:GLU:H	1.76	0.51
1:E:90:THR:HG22	1:E:91:GLU:H	1.76	0.51
1:A:346:VAL:HA	1:A:349:LEU:HD12	1.92	0.51
1:I:64:GLU:HA	1:I:209:SER:N	2.26	0.51
4:H:35:SER:HB3	4:H:47:TRP:HE1	1.76	0.50
3:G:133:LEU:HD12	3:G:179:LEU:HD23	1.92	0.50
1:I:248:THR:HG22	1:I:486:TYR:CE1	2.46	0.50
1:A:335:LYS:HG3	1:A:339:ASN:OD1	2.11	0.50
1:A:64:GLU:HA	1:A:209:SER:N	2.26	0.50
1:I:286:VAL:HB	1:I:452:LEU:HB2	1.94	0.50
1:I:325:ASP:O	4:L:100(I):GLU:OE2	2.29	0.50
1:I:335:LYS:HG3	1:I:339:ASN:OD1	2.12	0.50
1:A:212:PRO:HB2	6:A:1261:NAG:C8	2.42	0.50
1:E:332:ASN:OD1	1:E:415:THR:HG23	2.11	0.50
1:A:248:THR:HG22	1:A:486:TYR:CE1	2.46	0.50
1:E:64:GLU:HA	1:E:209:SER:N	2.26	0.50
1:A:159:PHE:HB2	1:A:172:VAL:HG23	1.92	0.50
1:I:159:PHE:HB2	1:I:172:VAL:HG23	1.92	0.50
1:A:252:LYS:HD3	6:A:1261:NAG:H81	1.93	0.50
1:A:327:ARG:CA	4:D:100(H):LYS:HD2	2.41	0.50
4:D:189:THR:OG1	4:D:190:GLN:N	2.42	0.50
1:A:330:HIS:CE1	4:D:100(E):VAL:HA	2.46	0.49
1:I:93:PHE:HE1	1:I:226:LEU:HD13	1.75	0.49
1:A:158:SER:O	1:A:159:PHE:HD1	1.94	0.49
1:E:96:TRP:HZ2	1:E:273:ARG:HB3	1.77	0.49
1:A:226:LEU:HA	1:A:243:SER:O	2.12	0.49
1:A:90:THR:HG22	1:A:91:GLU:H	1.76	0.49
1:E:474:ASP:HB3	1:E:476:ARG:HG2	1.94	0.49
1:E:129:LEU:HA	1:E:159:PHE:CE1	2.47	0.49
3:G:37:GLN:HB2	3:G:47:ILE:CG1	2.42	0.49
1:E:212:PRO:HB2	6:E:1261:NAG:C8	2.42	0.49
1:E:335:LYS:HG3	1:E:339:ASN:OD1	2.12	0.49
1:A:96:TRP:HZ2	1:A:273:ARG:HB3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:LEU:HA	1:E:243:SER:O	2.12	0.49
3:K:37:GLN:HB2	3:K:47:ILE:CG1	2.42	0.49
1:E:248:THR:HG22	1:E:486:TYR:CE1	2.46	0.49
1:I:96:TRP:HZ2	1:I:273:ARG:HB3	1.77	0.49
1:I:226:LEU:HA	1:I:243:SER:O	2.12	0.49
1:E:202:THR:HA	1:E:434:MET:HB2	1.95	0.49
1:E:286:VAL:HB	1:E:452:LEU:HB2	1.94	0.49
1:A:474:ASP:HB3	1:A:476:ARG:HG2	1.94	0.49
1:E:158:SER:O	1:E:159:PHE:HD1	1.94	0.49
1:E:334:SER:HB2	5:E:1295:NAG:H83	1.94	0.48
1:I:202:THR:HA	1:I:434:MET:HB2	1.95	0.48
7:I:1332:NAG:H4	4:L:100(C):GLY:HA3	1.95	0.48
8:C:1340:MAN:C3	4:D:100(A):ILE:HB	2.42	0.48
4:L:35:SER:CB	4:L:95:THR:OG1	2.61	0.48
1:I:158:SER:O	1:I:159:PHE:HD1	1.95	0.48
1:I:129:LEU:HA	1:I:159:PHE:CE1	2.48	0.48
1:E:129:LEU:HG	1:E:159:PHE:CZ	2.48	0.48
1:A:455:THR:HG23	1:A:471:GLY:HA3	1.95	0.48
1:A:85:HIS:CE1	1:A:241:SER:HA	2.49	0.48
1:E:129:LEU:HA	1:E:159:PHE:HE1	1.79	0.48
1:A:46:LYS:HB3	1:A:490:LYS:HG3	1.94	0.48
1:I:474:ASP:HB3	1:I:476:ARG:HG2	1.94	0.48
1:A:129:LEU:HA	1:A:159:PHE:CE1	2.47	0.48
1:A:129:LEU:HA	1:A:159:PHE:HE1	1.79	0.48
1:A:478:ASN:O	1:A:481:SER:OG	2.20	0.48
3:C:37:GLN:HB2	3:C:47:ILE:CG1	2.42	0.48
3:C:37:GLN:O	3:C:45:SER:OG	2.21	0.48
1:A:212:PRO:HB2	6:A:1261:NAG:H83	1.96	0.48
3:C:36:TYR:HB3	3:C:45:SER:O	2.14	0.48
1:E:455:THR:HG23	1:E:471:GLY:HA3	1.95	0.48
1:I:455:THR:HG23	1:I:471:GLY:HA3	1.95	0.48
1:I:85:HIS:CE1	1:I:241:SER:HA	2.49	0.48
3:K:36:TYR:HB3	3:K:45:SER:O	2.14	0.47
1:I:375:SER:HA	1:I:383:PHE:O	2.14	0.47
1:I:365:SER:HB2	1:I:469:ARG:HD3	1.96	0.47
1:A:286:VAL:HB	1:A:452:LEU:HB2	1.94	0.47
1:A:375:SER:HA	1:A:383:PHE:O	2.14	0.47
1:A:365:SER:HB2	1:A:469:ARG:HD3	1.96	0.47
1:I:259:LEU:HD13	1:I:449:ILE:HD13	1.96	0.47
3:G:36:TYR:HB3	3:G:45:SER:O	2.14	0.47
3:K:30:SER:HB2	4:L:100(B):TYR:OH	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:OE2	1:A:211:GLU:N	2.48	0.47
3:K:17:GLN:CD	3:K:18:THR:H	2.18	0.47
1:I:55:ALA:HB3	1:I:216:HIS:CB	2.42	0.47
1:A:65:LYS:HG3	1:A:208:VAL:HB	1.96	0.47
1:E:85:HIS:ND1	1:E:242:VAL:O	2.36	0.47
1:E:85:HIS:CE1	1:E:241:SER:HA	2.49	0.47
1:I:330:HIS:CE1	1:I:415:THR:CG2	2.98	0.47
1:I:333:VAL:HG13	1:I:414:ILE:HD12	1.97	0.47
1:E:365:SER:HB2	1:E:469:ARG:HD3	1.97	0.47
1:I:64:GLU:OE2	1:I:211:GLU:N	2.48	0.47
1:E:212:PRO:HB2	6:E:1261:NAG:H83	1.96	0.47
1:I:129:LEU:HG	1:I:159:PHE:CZ	2.49	0.47
4:L:124:PRO:HG3	4:L:136:LEU:HG	1.97	0.47
4:D:43:LYS:HE3	4:D:43:LYS:HB3	1.65	0.47
1:E:354:GLY:O	1:E:357:THR:OG1	2.33	0.47
2:B:35:UNK:O	2:B:36:UNK:C	2.63	0.47
1:E:64:GLU:OE2	1:E:211:GLU:N	2.48	0.47
1:E:65:LYS:HG3	1:E:208:VAL:HB	1.96	0.47
1:E:375:SER:HA	1:E:383:PHE:O	2.15	0.47
1:E:175:LEU:HD21	1:E:320:GLY:HA3	1.97	0.47
1:A:416:LEU:HA	1:A:417:PRO:HD3	1.65	0.47
1:A:75:VAL:HG22	1:A:76:PRO:HD2	1.97	0.47
1:I:332:ASN:OD1	1:I:415:THR:HG23	2.15	0.47
4:L:35:SER:HG	4:L:95:THR:CB	2.25	0.47
3:G:37:GLN:O	3:G:45:SER:OG	2.20	0.47
1:I:65:LYS:HG3	1:I:208:VAL:HB	1.96	0.47
1:I:252:LYS:HD3	6:I:1261:NAG:C8	2.45	0.47
1:E:298:ARG:HB3	1:E:329:ALA:HB1	1.97	0.47
1:A:129:LEU:HG	1:A:159:PHE:CZ	2.49	0.47
1:I:75:VAL:HG22	1:I:76:PRO:HD2	1.97	0.47
3:G:17:GLN:CD	3:G:18:THR:H	2.18	0.47
1:I:330:HIS:CE1	4:L:100(E):VAL:HA	2.50	0.47
4:L:36:TRP:HE1	4:L:78:VAL:HG12	1.80	0.47
1:I:298:ARG:HG3	1:I:298:ARG:H	1.60	0.47
1:E:259:LEU:HD13	1:E:449:ILE:HD13	1.97	0.46
1:A:333:VAL:HG13	1:A:414:ILE:HD12	1.97	0.46
1:A:202:THR:HA	1:A:434:MET:HB2	1.96	0.46
1:E:64:GLU:HG2	1:E:67:ASN:H	1.80	0.46
4:H:36:TRP:HE1	4:H:78:VAL:HG12	1.80	0.46
1:A:64:GLU:HG2	1:A:67:ASN:H	1.80	0.46
1:A:85:HIS:CE1	1:A:242:VAL:H	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:413:SER:O	7:I:1331:NAG:O6	2.34	0.46
4:H:124:PRO:HG3	4:H:136:LEU:HG	1.98	0.46
1:A:324:GLY:HA2	3:C:67(C):PHE:CZ	2.50	0.46
1:E:55:ALA:HB3	1:E:216:HIS:CB	2.42	0.46
1:I:272:ILE:HG22	1:I:286:VAL:HG13	1.98	0.46
1:E:75:VAL:HG22	1:E:76:PRO:HD2	1.97	0.46
3:C:17:GLN:CD	3:C:18:THR:H	2.18	0.46
1:I:64:GLU:HG2	1:I:67:ASN:H	1.80	0.46
1:E:252:LYS:HD3	6:E:1261:NAG:C8	2.44	0.46
1:A:85:HIS:ND1	1:A:242:VAL:O	2.36	0.46
1:I:212:PRO:HB2	6:I:1261:NAG:C8	2.46	0.46
1:A:252:LYS:HD3	6:A:1261:NAG:C8	2.45	0.46
3:K:50:ASN:ND2	8:K:1341:MAN:H4	2.31	0.46
1:I:175:LEU:HD21	1:I:320:GLY:HA3	1.98	0.46
1:A:55:ALA:HB3	1:A:216:HIS:CB	2.42	0.46
1:A:259:LEU:HD13	1:A:449:ILE:HD13	1.97	0.46
1:I:129:LEU:HA	1:I:159:PHE:HE1	1.81	0.46
1:A:49:GLU:HG3	1:A:223:PHE:HE2	1.79	0.46
1:A:332:ASN:OD1	1:A:415:THR:HG23	2.16	0.46
1:I:330:HIS:CE1	1:I:415:THR:HG21	2.51	0.45
4:D:36:TRP:HE1	4:D:78:VAL:HG12	1.80	0.45
2:F:35:UNK:O	2:F:36:UNK:C	2.63	0.45
1:A:96:TRP:CH2	1:A:235:GLY:HA3	2.51	0.45
1:I:85:HIS:CE1	1:I:242:VAL:H	2.34	0.45
4:D:47:TRP:O	4:D:48:ILE:HG13	2.16	0.45
4:H:47:TRP:O	4:H:48:ILE:HG13	2.16	0.45
1:A:298:ARG:HB3	1:A:329:ALA:HB1	1.98	0.45
1:E:298:ARG:HG2	1:E:383:PHE:HZ	1.82	0.45
1:E:85:HIS:CE1	1:E:242:VAL:H	2.34	0.45
1:A:354:GLY:O	1:A:357:THR:OG1	2.34	0.45
3:G:31:ARG:O	4:H:100:ARG:NH1	2.45	0.45
1:A:57:ASP:OD1	1:A:58:ALA:N	2.49	0.45
1:A:272:ILE:HG22	1:A:286:VAL:HG13	1.98	0.45
1:E:223:PHE:CE2	1:E:490:LYS:HB3	2.52	0.45
1:E:49:GLU:HG3	1:E:223:PHE:HE2	1.81	0.45
1:E:96:TRP:CH2	1:E:235:GLY:HA3	2.51	0.45
1:E:57:ASP:OD1	1:E:58:ALA:N	2.48	0.45
1:A:175:LEU:HD21	1:A:320:GLY:HA3	1.97	0.45
2:J:35:UNK:O	2:J:36:UNK:C	2.63	0.45
1:A:298:ARG:HG2	1:A:383:PHE:HZ	1.82	0.45
1:I:298:ARG:HG2	1:I:383:PHE:HZ	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49:GLU:HG3	1:I:223:PHE:HE2	1.80	0.45
1:E:272:ILE:HG22	1:E:286:VAL:HG13	1.98	0.45
1:A:65:LYS:NZ	1:A:208:VAL:HG11	2.32	0.45
1:I:96:TRP:CH2	1:I:235:GLY:HA3	2.52	0.45
4:D:124:PRO:HG3	4:D:136:LEU:HG	1.97	0.45
1:I:65:LYS:NZ	1:I:208:VAL:HG11	2.32	0.45
1:E:44:VAL:HB	1:E:492:GLU:HB2	1.99	0.45
1:A:252:LYS:HB3	6:A:1261:NAG:H81	1.98	0.45
3:C:46:LEU:HD23	3:C:55:PRO:HG3	1.99	0.45
1:I:220:PRO:HG2	1:I:223:PHE:CD1	2.52	0.45
1:I:298:ARG:HB3	1:I:329:ALA:HB1	1.99	0.45
3:G:116:VAL:HG23	3:G:205:LYS:HD2	1.99	0.45
1:E:422:GLN:OE1	1:E:436:ALA:HA	2.17	0.44
4:L:66:ARG:HD2	4:L:82(A):THR:O	2.17	0.44
4:D:66:ARG:HD2	4:D:82(A):THR:O	2.17	0.44
1:I:354:GLY:O	1:I:357:THR:OG1	2.34	0.44
4:L:47:TRP:O	4:L:48:ILE:HG13	2.16	0.44
1:E:62:GLU:O	1:E:63:THR:OG1	2.35	0.44
1:E:220:PRO:HG2	1:E:223:PHE:CD1	2.52	0.44
1:E:161:MET:HE2	1:E:172:VAL:HG11	1.99	0.44
1:I:85:HIS:ND1	1:I:242:VAL:O	2.36	0.44
4:H:66:ARG:HD2	4:H:82(A):THR:O	2.17	0.44
1:E:219:ALA:HB2	1:E:225:ILE:HG13	2.00	0.44
3:K:37:GLN:O	3:K:45:SER:C	2.56	0.44
1:I:259:LEU:HA	1:I:451:GLY:O	2.18	0.44
1:I:327:ARG:CA	4:L:100(H):LYS:HD2	2.44	0.44
3:K:46:LEU:HD23	3:K:55:PRO:HG3	1.99	0.44
4:L:34:TRP:CZ3	4:L:94:THR:CG2	3.01	0.44
1:E:65:LYS:NZ	1:E:208:VAL:HG11	2.32	0.44
3:C:167:LYS:HE3	3:C:173:TYR:CE1	2.52	0.44
1:A:138:ILE:C	6:A:1131:NAG:HN2	2.21	0.44
1:A:260:LEU:HD21	1:A:481:SER:OG	2.18	0.44
1:I:260:LEU:HD21	1:I:481:SER:OG	2.17	0.44
3:G:37:GLN:O	3:G:45:SER:C	2.56	0.44
7:I:1332:NAG:H4	4:L:100(C):GLY:HA2	1.98	0.44
1:A:259:LEU:HA	1:A:451:GLY:O	2.18	0.44
1:I:440:GLN:HB3	1:I:441:GLY:H	1.53	0.44
1:A:369:LEU:HG	1:A:369:LEU:H	1.58	0.44
3:C:37:GLN:O	3:C:45:SER:C	2.56	0.44
1:I:223:PHE:CD2	1:I:490:LYS:HB3	2.51	0.44
1:E:255:VAL:HG13	1:E:475:MET:SD	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ALA:HB2	1:A:225:ILE:HG13	2.00	0.44
3:K:186:TRP:HH2	3:K:207:VAL:HG22	1.83	0.44
1:E:333:VAL:HG13	1:E:414:ILE:HD12	1.98	0.44
3:K:116:VAL:HG23	3:K:205:LYS:HD2	1.99	0.44
3:G:186:TRP:HH2	3:G:207:VAL:HG22	1.83	0.44
1:E:279:ASN:HB2	5:E:1276:NAG:O5	2.18	0.44
3:C:186:TRP:HH2	3:C:207:VAL:HG22	1.83	0.44
1:E:63:THR:O	1:E:208:VAL:HA	2.18	0.43
1:E:298:ARG:HG3	1:E:298:ARG:H	1.59	0.43
3:G:167:LYS:HE3	3:G:173:TYR:CE1	2.53	0.43
4:L:18:LEU:HD11	4:L:20:LEU:HD21	2.00	0.43
3:C:47:ILE:HD13	3:C:47:ILE:HA	1.87	0.43
4:L:93:ALA:HA	4:L:100(R):VAL:O	2.18	0.43
1:I:255:VAL:HG13	1:I:475:MET:SD	2.58	0.43
1:I:369:LEU:HG	1:I:369:LEU:H	1.58	0.43
1:A:54:CYS:SG	1:A:215:ILE:HG23	2.58	0.43
1:I:422:GLN:OE1	1:I:436:ALA:HA	2.17	0.43
1:I:57:ASP:OD1	1:I:58:ALA:N	2.52	0.43
1:A:422:GLN:OE1	1:A:436:ALA:HA	2.17	0.43
1:E:416:LEU:HA	1:E:417:PRO:HD3	1.65	0.43
4:H:43:LYS:HE3	4:H:43:LYS:HB3	1.65	0.43
4:L:38:ARG:O	4:L:46:GLU:C	2.57	0.43
1:E:259:LEU:HA	1:E:451:GLY:O	2.18	0.43
1:A:255:VAL:HG13	1:A:475:MET:SD	2.58	0.43
3:C:116:VAL:HG23	3:C:205:LYS:HD2	2.00	0.43
1:I:219:ALA:HB2	1:I:225:ILE:HG13	2.00	0.43
1:A:330:HIS:CE1	1:A:415:THR:HG21	2.54	0.43
1:I:54:CYS:SG	1:I:215:ILE:HG23	2.59	0.43
1:E:61:TYR:HB3	1:E:62:GLU:H	1.53	0.43
3:K:167:LYS:HE3	3:K:173:TYR:CE1	2.53	0.43
1:E:239:CYS:HA	1:E:240:PRO:HD3	1.46	0.43
1:A:63:THR:O	1:A:208:VAL:HA	2.18	0.43
1:E:129:LEU:HG	1:E:159:PHE:HZ	1.83	0.43
3:G:46:LEU:HD23	3:G:55:PRO:HG3	1.99	0.43
1:I:104:MET:HG3	1:I:217:TYR:OH	2.19	0.43
1:I:63:THR:O	1:I:208:VAL:HA	2.18	0.43
4:D:111:SER:OG	4:D:111:SER:O	2.32	0.43
3:K:47:ILE:HG23	3:K:47:ILE:HD12	1.80	0.43
1:E:252:LYS:HB3	6:E:1261:NAG:H81	2.01	0.43
1:A:220:PRO:HG2	1:A:223:PHE:CD1	2.53	0.43
1:E:93:PHE:HD2	1:E:239:CYS:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:212:PRO:HB2	6:I:1261:NAG:H83	2.00	0.43
4:L:43:LYS:HB3	4:L:43:LYS:HE3	1.65	0.43
1:E:260:LEU:HD21	1:E:481:SER:OG	2.18	0.42
1:E:54:CYS:SG	1:E:215:ILE:HG23	2.58	0.42
1:A:292:VAL:HB	1:A:449:ILE:HB	2.01	0.42
1:I:301:ASN:O	1:I:302:ASN:ND2	2.52	0.42
4:D:38:ARG:O	4:D:46:GLU:C	2.57	0.42
1:I:335:LYS:HA	1:I:338:TRP:HB3	2.02	0.42
1:A:298:ARG:HG3	1:A:298:ARG:H	1.58	0.42
1:A:453:ILE:O	1:A:454:LEU:HD23	2.19	0.42
1:A:93:PHE:HD2	1:A:239:CYS:HB3	1.84	0.42
1:I:44:VAL:HB	1:I:492:GLU:HB2	2.00	0.42
1:I:239:CYS:HA	1:I:240:PRO:HD3	1.46	0.42
1:I:359:ILE:HD13	1:I:466:GLU:HB2	2.02	0.42
1:A:104:MET:HG3	1:A:217:TYR:OH	2.19	0.42
1:A:129:LEU:HG	1:A:159:PHE:HZ	1.84	0.42
1:I:129:LEU:HG	1:I:159:PHE:HZ	1.85	0.42
1:E:292:VAL:HB	1:E:449:ILE:HB	2.01	0.42
1:A:223:PHE:CE2	1:A:490:LYS:HB3	2.54	0.42
1:E:453:ILE:O	1:E:454:LEU:HD23	2.19	0.42
1:E:223:PHE:CD2	1:E:490:LYS:HB3	2.55	0.42
1:I:161:MET:SD	1:I:172:VAL:HG21	2.60	0.42
1:I:453:ILE:O	1:I:454:LEU:HD23	2.19	0.42
1:I:161:MET:O	1:I:169:LYS:HA	2.20	0.42
1:E:104:MET:HG3	1:E:217:TYR:OH	2.19	0.42
4:H:18:LEU:HD11	4:H:20:LEU:HD21	2.01	0.42
1:E:54:CYS:HA	1:E:216:HIS:O	2.20	0.42
1:A:359:ILE:HD13	1:A:466:GLU:HB2	2.02	0.42
1:E:138:ILE:C	6:E:1131:NAG:HN2	2.23	0.42
1:I:45:TRP:HB3	1:I:489:VAL:HG21	2.02	0.42
1:A:330:HIS:CE1	1:A:415:THR:CG2	3.03	0.41
1:I:54:CYS:HA	1:I:216:HIS:O	2.20	0.41
4:D:18:LEU:HD11	4:D:20:LEU:HD21	2.01	0.41
1:E:335:LYS:O	1:E:339:ASN:N	2.48	0.41
1:E:335:LYS:HA	1:E:338:TRP:HB3	2.03	0.41
1:A:54:CYS:HA	1:A:216:HIS:O	2.20	0.41
1:E:436:ALA:CB	1:E:437:PRO:HD3	2.46	0.41
4:H:197:ASN:OD1	4:H:199:LYS:HG3	2.21	0.41
4:D:197:ASN:OD1	4:D:199:LYS:HG3	2.21	0.41
1:I:93:PHE:HD2	1:I:239:CYS:HB3	1.84	0.41
1:E:220:PRO:HB2	1:E:221:ALA:H	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:38:ARG:HB3	4:L:48:ILE:HD11	2.03	0.41
1:A:335:LYS:O	1:A:339:ASN:N	2.48	0.41
1:E:325:ASP:CB	3:G:94:ARG:HH11	2.33	0.41
1:A:385:CYS:O	1:A:387:THR:HG23	2.21	0.41
1:A:301:ASN:O	1:A:302:ASN:ND2	2.54	0.41
4:H:38:ARG:HB3	4:H:48:ILE:HD11	2.03	0.41
1:A:279:ASN:HB2	5:A:1276:NAG:O5	2.21	0.41
1:A:44:VAL:HB	1:A:492:GLU:HB2	2.01	0.41
1:A:231:LYS:HD3	1:A:231:LYS:H	1.85	0.41
1:E:231:LYS:HD3	1:E:231:LYS:H	1.85	0.41
1:I:334:SER:HB2	5:I:1295:NAG:H83	2.02	0.41
4:D:36:TRP:O	4:D:48:ILE:HB	2.21	0.41
4:H:46:GLU:O	4:H:47:TRP:O	2.39	0.41
4:H:36:TRP:O	4:H:48:ILE:HB	2.21	0.41
1:I:335:LYS:HE2	1:I:339:ASN:ND2	2.36	0.41
1:E:359:ILE:HD13	1:E:466:GLU:HB2	2.02	0.41
4:L:197:ASN:OD1	4:L:199:LYS:HG3	2.20	0.41
1:I:385:CYS:O	1:I:387:THR:HG23	2.21	0.41
1:A:83:GLU:HA	1:A:244:THR:O	2.21	0.41
1:I:62:GLU:HB3	1:I:63:THR:H	1.67	0.41
1:A:231:LYS:NZ	1:A:231:LYS:HB2	2.36	0.41
1:E:385:CYS:O	1:E:387:THR:HG23	2.21	0.41
1:I:231:LYS:H	1:I:231:LYS:HD3	1.85	0.41
1:I:231:LYS:NZ	1:I:231:LYS:HB2	2.36	0.41
1:E:292:VAL:HG11	1:E:338:TRP:HE3	1.86	0.41
1:I:83:GLU:HA	1:I:244:THR:O	2.21	0.41
1:I:292:VAL:HB	1:I:449:ILE:HB	2.02	0.40
1:I:330:HIS:HB3	4:L:100(E):VAL:HG23	2.03	0.40
4:D:46:GLU:O	4:D:47:TRP:O	2.39	0.40
1:E:335:LYS:HE2	1:E:339:ASN:ND2	2.36	0.40
1:A:220:PRO:HB2	1:A:221:ALA:H	1.76	0.40
1:E:45:TRP:HB3	1:E:489:VAL:HG21	2.02	0.40
1:E:331:CYS:SG	1:E:332:ASN:N	2.95	0.40
1:A:239:CYS:HA	1:A:240:PRO:HD3	1.46	0.40
4:L:36:TRP:O	4:L:48:ILE:HB	2.21	0.40
4:L:35:SER:HB2	4:L:95:THR:OG1	2.21	0.40
4:L:117:PRO:HB3	4:L:143:TYR:HB3	2.04	0.40
1:I:359:ILE:HD12	1:I:468:PHE:CE1	2.50	0.40
1:I:345:VAL:O	1:I:349:LEU:HG	2.22	0.40
1:I:223:PHE:CE2	1:I:490:LYS:HB3	2.57	0.40
4:H:30:ARG:HD3	4:H:73:LYS:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:9:UNK:O	2:J:10:UNK:C	2.69	0.40
1:I:292:VAL:HG11	1:I:338:TRP:HE3	1.86	0.40
1:A:335:LYS:HE2	1:A:339:ASN:ND2	2.36	0.40
1:A:335:LYS:HA	1:A:338:TRP:HB3	2.03	0.40
1:A:161:MET:SD	1:A:172:VAL:HG21	2.61	0.40
4:D:1:GLN:N	4:D:1:GLN:OE1	2.53	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	414/475 (87%)	349 (84%)	51 (12%)	14 (3%)	5 41
1	E	414/475 (87%)	348 (84%)	51 (12%)	15 (4%)	4 40
1	I	414/475 (87%)	348 (84%)	52 (13%)	14 (3%)	5 41
3	C	198/211 (94%)	191 (96%)	7 (4%)	0	100 100
3	G	198/211 (94%)	191 (96%)	7 (4%)	0	100 100
3	K	198/211 (94%)	192 (97%)	6 (3%)	0	100 100
4	D	220/235 (94%)	213 (97%)	6 (3%)	1 (0%)	34 77
4	H	220/235 (94%)	213 (97%)	6 (3%)	1 (0%)	34 77
4	L	220/235 (94%)	213 (97%)	6 (3%)	1 (0%)	34 77
All	All	2496/2763 (90%)	2258 (90%)	192 (8%)	46 (2%)	11 54

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	83	GLU

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Mol	Chain	Res	Type
1	A	323	ILE
1	A	429	ARG
1	E	57	ASP
1	E	83	GLU
1	E	323	ILE
1	E	429	ARG
1	I	57	ASP
1	I	83	GLU
1	I	323	ILE
1	I	429	ARG
1	A	195	ASN
1	A	322	ILE
4	D	189	THR
1	E	195	ASN
1	E	322	ILE
4	H	189	THR
1	I	195	ASN
1	I	322	ILE
4	L	189	THR
1	A	56	SER
1	E	56	SER
1	I	56	SER
1	A	63	THR
1	A	220	PRO
1	E	63	THR
1	E	220	PRO
1	I	63	THR
1	I	220	PRO
1	A	84	ILE
1	A	118	PRO
1	E	84	ILE
1	E	118	PRO
1	I	84	ILE
1	I	89	VAL
1	I	118	PRO
1	A	89	VAL
1	A	437	PRO
1	E	89	VAL
1	E	437	PRO
1	I	437	PRO
1	A	442	VAL
1	E	442	VAL

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Mol	Chain	Res	Type
1	I	442	VAL
1	E	194	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/422 (75%)	293 (92%)	24 (8%)	16	55
1	E	317/422 (75%)	293 (92%)	24 (8%)	16	55
1	I	317/422 (75%)	293 (92%)	24 (8%)	16	55
3	C	171/180 (95%)	164 (96%)	7 (4%)	37	72
3	G	171/180 (95%)	164 (96%)	7 (4%)	37	72
3	K	171/180 (95%)	163 (95%)	8 (5%)	32	69
4	D	196/205 (96%)	189 (96%)	7 (4%)	42	75
4	H	196/205 (96%)	189 (96%)	7 (4%)	42	75
4	L	196/205 (96%)	189 (96%)	7 (4%)	42	75
All	All	2052/2421 (85%)	1937 (94%)	115 (6%)	26	65

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	53	PHE
1	A	61	TYR
1	A	75	VAL
1	A	90	THR
1	A	100	MET
1	A	107	ASP
1	A	125	LEU
1	A	156	ASN
1	A	197	ASN
1	A	226	LEU
1	A	231	LYS

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Mol	Chain	Res	Type
1	A	277	ILE
1	A	298	ARG
1	A	330	HIS
1	A	357	THR
1	A	369	LEU
1	A	374	HIS
1	A	382	PHE
1	A	386	ASN
1	A	399	THR
1	A	412	ASP
1	A	414	ILE
1	A	467	THR
3	C	13	VAL
3	C	17	GLN
3	C	31	ARG
3	C	130	LYS
3	C	136	LEU
3	C	161	GLU
3	C	164	THR
4	D	1	GLN
4	D	16	GLU
4	D	69	LEU
4	D	70	SER
4	D	71	LEU
4	D	181	THR
4	D	191	THR
1	E	47	ASP
1	E	53	PHE
1	E	61	TYR
1	E	75	VAL
1	E	90	THR
1	E	100	MET
1	E	107	ASP
1	E	125	LEU
1	E	156	ASN
1	E	197	ASN
1	E	226	LEU
1	E	231	LYS
1	E	277	ILE
1	E	298	ARG
1	E	330	HIS
1	E	357	THR

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Mol	Chain	Res	Type
1	E	369	LEU
1	E	374	HIS
1	E	382	PHE
1	E	386	ASN
1	E	399	THR
1	E	412	ASP
1	E	414	ILE
1	E	467	THR
3	G	13	VAL
3	G	17	GLN
3	G	31	ARG
3	G	130	LYS
3	G	136	LEU
3	G	161	GLU
3	G	164	THR
4	H	1	GLN
4	H	16	GLU
4	H	69	LEU
4	H	70	SER
4	H	71	LEU
4	H	181	THR
4	H	191	THR
1	I	47	ASP
1	I	53	PHE
1	I	61	TYR
1	I	75	VAL
1	I	90	THR
1	I	100	MET
1	I	107	ASP
1	I	125	LEU
1	I	156	ASN
1	I	197	ASN
1	I	226	LEU
1	I	231	LYS
1	I	277	ILE
1	I	298	ARG
1	I	330	HIS
1	I	357	THR
1	I	369	LEU
1	I	374	HIS
1	I	382	PHE
1	I	386	ASN

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Mol	Chain	Res	Type
1	I	399	THR
1	I	412	ASP
1	I	414	ILE
1	I	467	THR
3	K	13	VAL
3	K	17	GLN
3	K	31	ARG
3	K	109	GLN
3	K	130	LYS
3	K	136	LEU
3	K	161	GLU
3	K	164	THR
4	L	1	GLN
4	L	16	GLU
4	L	69	LEU
4	L	70	SER
4	L	71	LEU
4	L	181	THR
4	L	191	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	374	HIS
1	E	289	ASN
1	E	330	HIS
1	E	374	HIS
1	I	289	ASN
1	I	374	HIS

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 (i)

117 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	A	1131	1,6	14,14,15	0.54	0	15,19,21	1.34	1 (6%)
6	NAG	A	1132	6	14,14,15	0.52	0	15,19,21	0.74	0
6	BMA	A	1133	6	11,11,12	0.66	0	14,15,17	0.91	1 (7%)
6	MAN	A	1134	6	11,11,12	0.57	0	14,15,17	0.67	0
6	MAN	A	1135	6	11,11,12	0.68	0	14,15,17	0.89	0
6	MAN	A	1136	6	11,11,12	0.60	0	14,15,17	0.65	0
6	MAN	A	1137	6	11,11,12	0.63	0	14,15,17	1.04	1 (7%)
6	NAG	A	1151	1,6	14,14,15	0.58	0	15,19,21	1.22	1 (6%)
6	NAG	A	1152	6	14,14,15	0.54	0	15,19,21	0.83	0
6	BMA	A	1153	6	11,11,12	0.73	0	14,15,17	0.87	1 (7%)
6	MAN	A	1154	6	11,11,12	0.56	0	14,15,17	0.70	0
6	MAN	A	1155	6	11,11,12	0.70	0	14,15,17	1.13	2 (14%)
6	MAN	A	1156	6	11,11,12	0.60	0	14,15,17	0.67	0
6	MAN	A	1157	6	11,11,12	0.68	0	14,15,17	0.88	1 (7%)
6	NAG	A	1261	1,6	14,14,15	0.72	0	15,19,21	1.44	2 (13%)
6	NAG	A	1262	6	14,14,15	0.53	0	15,19,21	0.77	0
6	BMA	A	1263	6	11,11,12	0.71	0	14,15,17	0.73	0
6	MAN	A	1264	6	11,11,12	0.57	0	14,15,17	0.68	0
6	MAN	A	1265	6	11,11,12	0.67	0	14,15,17	0.94	0
6	MAN	A	1266	6	11,11,12	0.61	0	14,15,17	0.64	0
6	MAN	A	1267	6	11,11,12	0.68	0	14,15,17	0.89	1 (7%)
6	NAG	A	1301	1,6	14,14,15	0.58	0	15,19,21	1.17	1 (6%)
6	NAG	A	1302	6	14,14,15	0.56	0	15,19,21	0.75	0
6	BMA	A	1303	6	11,11,12	0.70	0	14,15,17	0.82	1 (7%)
6	MAN	A	1304	6	11,11,12	0.56	0	14,15,17	0.67	0
6	MAN	A	1305	6	11,11,12	0.67	0	14,15,17	0.94	0
6	MAN	A	1306	6	11,11,12	0.60	0	14,15,17	0.64	0
6	MAN	A	1307	6	11,11,12	0.66	0	14,15,17	0.89	1 (7%)
7	NAG	A	1331	1,7	14,14,15	0.59	0	15,19,21	1.32	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	A	1332	7	14,14,15	0.50	0	15,19,21	1.15	1 (6%)
7	BMA	A	1333	7	11,11,12	0.67	0	14,15,17	1.46	1 (7%)
7	MAN	A	1334	7	11,11,12	0.51	0	14,15,17	0.84	0
7	MAN	A	1335	7	11,11,12	0.58	0	14,15,17	0.86	0
7	MAN	A	1336	7	11,11,12	0.63	0	14,15,17	0.71	0
7	MAN	A	1337	7	11,11,12	0.64	0	14,15,17	1.02	0
7	MAN	A	1338	7	11,11,12	0.59	0	14,15,17	0.66	0
7	MAN	A	1339	7	11,11,12	0.60	0	14,15,17	0.59	0
8	MAN	C	1340	8	11,11,12	0.69	0	14,15,17	1.29	1 (7%)
8	MAN	C	1341	8	11,11,12	0.67	0	14,15,17	0.71	0
6	NAG	E	1131	1,6	14,14,15	0.55	0	15,19,21	1.35	1 (6%)
6	NAG	E	1132	6	14,14,15	0.51	0	15,19,21	0.75	0
6	BMA	E	1133	6	11,11,12	0.67	0	14,15,17	0.91	1 (7%)
6	MAN	E	1134	6	11,11,12	0.58	0	14,15,17	0.66	0
6	MAN	E	1135	6	11,11,12	0.67	0	14,15,17	0.89	0
6	MAN	E	1136	6	11,11,12	0.59	0	14,15,17	0.65	0
6	MAN	E	1137	6	11,11,12	0.66	0	14,15,17	0.82	0
6	NAG	E	1151	1,6	14,14,15	0.58	0	15,19,21	1.19	1 (6%)
6	NAG	E	1152	6	14,14,15	0.53	0	15,19,21	0.85	0
6	BMA	E	1153	6	11,11,12	0.74	0	14,15,17	0.89	1 (7%)
6	MAN	E	1154	6	11,11,12	0.56	0	14,15,17	0.71	0
6	MAN	E	1155	6	11,11,12	0.71	0	14,15,17	1.12	1 (7%)
6	MAN	E	1156	6	11,11,12	0.60	0	14,15,17	0.66	0
6	MAN	E	1157	6	11,11,12	0.68	0	14,15,17	0.88	1 (7%)
6	NAG	E	1261	1,6	14,14,15	0.71	0	15,19,21	1.41	2 (13%)
6	NAG	E	1262	6	14,14,15	0.52	0	15,19,21	0.74	0
6	BMA	E	1263	6	11,11,12	0.71	0	14,15,17	0.73	0
6	MAN	E	1264	6	11,11,12	0.57	0	14,15,17	0.69	0
6	MAN	E	1265	6	11,11,12	0.67	0	14,15,17	0.93	0
6	MAN	E	1266	6	11,11,12	0.60	0	14,15,17	0.64	0
6	MAN	E	1267	6	11,11,12	0.67	0	14,15,17	0.89	1 (7%)
6	NAG	E	1301	1,6	14,14,15	0.58	0	15,19,21	1.10	1 (6%)
6	NAG	E	1302	6	14,14,15	0.54	0	15,19,21	0.74	0
6	BMA	E	1303	6	11,11,12	0.69	0	14,15,17	0.84	1 (7%)
6	MAN	E	1304	6	11,11,12	0.58	0	14,15,17	0.67	0
6	MAN	E	1305	6	11,11,12	0.68	0	14,15,17	0.94	0
6	MAN	E	1306	6	11,11,12	0.62	0	14,15,17	0.65	0
6	MAN	E	1307	6	11,11,12	0.67	0	14,15,17	0.88	1 (7%)
7	NAG	E	1331	1,7	14,14,15	0.61	0	15,19,21	1.35	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	E	1332	7	14,14,15	0.55	0	15,19,21	0.81	0
7	BMA	E	1333	7	11,11,12	0.72	0	14,15,17	1.01	1 (7%)
7	MAN	E	1334	7	11,11,12	0.51	0	14,15,17	0.82	0
7	MAN	E	1335	7	11,11,12	0.57	0	14,15,17	0.87	0
7	MAN	E	1336	7	11,11,12	0.63	0	14,15,17	0.71	0
7	MAN	E	1337	7	11,11,12	0.64	0	14,15,17	1.02	0
7	MAN	E	1338	7	11,11,12	0.60	0	14,15,17	0.65	0
7	MAN	E	1339	7	11,11,12	0.61	0	14,15,17	0.60	0
8	MAN	G	1340	8	11,11,12	0.63	0	14,15,17	1.19	1 (7%)
8	MAN	G	1341	8	11,11,12	0.63	0	14,15,17	0.87	0
6	NAG	I	1131	1,6	14,14,15	0.54	0	15,19,21	1.41	1 (6%)
6	NAG	I	1132	6	14,14,15	0.49	0	15,19,21	0.84	0
6	BMA	I	1133	6	11,11,12	0.65	0	14,15,17	0.99	1 (7%)
6	MAN	I	1134	6	11,11,12	0.57	0	14,15,17	0.66	0
6	MAN	I	1135	6	11,11,12	0.67	0	14,15,17	0.86	0
6	MAN	I	1136	6	11,11,12	0.61	0	14,15,17	0.63	0
6	MAN	I	1137	6	11,11,12	0.66	0	14,15,17	1.09	1 (7%)
6	NAG	I	1151	1,6	14,14,15	0.60	0	15,19,21	1.27	1 (6%)
6	NAG	I	1152	6	14,14,15	0.56	0	15,19,21	0.85	1 (6%)
6	BMA	I	1153	6	11,11,12	0.73	0	14,15,17	0.87	1 (7%)
6	MAN	I	1154	6	11,11,12	0.54	0	14,15,17	0.71	0
6	MAN	I	1155	6	11,11,12	0.71	0	14,15,17	1.14	2 (14%)
6	MAN	I	1156	6	11,11,12	0.60	0	14,15,17	0.66	0
6	MAN	I	1157	6	11,11,12	0.66	0	14,15,17	0.88	1 (7%)
6	NAG	I	1261	1,6	14,14,15	0.69	0	15,19,21	1.46	2 (13%)
6	NAG	I	1262	6	14,14,15	0.53	0	15,19,21	0.77	0
6	BMA	I	1263	6	11,11,12	0.71	0	14,15,17	0.73	0
6	MAN	I	1264	6	11,11,12	0.56	0	14,15,17	0.69	0
6	MAN	I	1265	6	11,11,12	0.67	0	14,15,17	0.95	0
6	MAN	I	1266	6	11,11,12	0.60	0	14,15,17	0.64	0
6	MAN	I	1267	6	11,11,12	0.68	0	14,15,17	0.89	1 (7%)
6	NAG	I	1301	1,6	14,14,15	0.65	0	15,19,21	1.15	1 (6%)
6	NAG	I	1302	6	14,14,15	0.56	0	15,19,21	0.77	0
6	BMA	I	1303	6	11,11,12	0.70	0	14,15,17	0.82	1 (7%)
6	MAN	I	1304	6	11,11,12	0.57	0	14,15,17	0.67	0
6	MAN	I	1305	6	11,11,12	0.68	0	14,15,17	0.94	0
6	MAN	I	1306	6	11,11,12	0.61	0	14,15,17	0.64	0
6	MAN	I	1307	6	11,11,12	0.68	0	14,15,17	0.88	1 (7%)
7	NAG	I	1331	1,7	14,14,15	0.55	0	15,19,21	1.34	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	I	1332	7	14,14,15	0.54	0	15,19,21	1.17	1 (6%)
7	BMA	I	1333	7	11,11,12	0.68	0	14,15,17	1.53	1 (7%)
7	MAN	I	1334	7	11,11,12	0.50	0	14,15,17	0.85	0
7	MAN	I	1335	7	11,11,12	0.57	0	14,15,17	0.87	0
7	MAN	I	1336	7	11,11,12	0.64	0	14,15,17	0.71	1 (7%)
7	MAN	I	1337	7	11,11,12	0.64	0	14,15,17	1.10	1 (7%)
7	MAN	I	1338	7	11,11,12	0.59	0	14,15,17	0.64	0
7	MAN	I	1339	7	11,11,12	0.60	0	14,15,17	0.60	0
8	MAN	K	1340	8	11,11,12	0.69	0	14,15,17	1.27	1 (7%)
8	MAN	K	1341	8	11,11,12	0.72	0	14,15,17	0.83	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	A	1131	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1132	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1133	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1134	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1135	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1136	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1137	6	-	0/2/19/22	0/1/1/1
6	NAG	A	1151	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1152	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1153	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1154	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1155	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1156	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1157	6	-	0/2/19/22	0/1/1/1
6	NAG	A	1261	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1262	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1263	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1264	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1265	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1266	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1267	6	-	0/2/19/22	0/1/1/1
6	NAG	A	1301	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1302	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1303	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	1304	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1305	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1306	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1307	6	-	0/2/19/22	0/1/1/1
7	NAG	A	1331	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1332	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1333	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1334	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1335	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1336	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1337	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1338	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1339	7	-	0/2/19/22	0/1/1/1
8	MAN	C	1340	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1341	8	-	0/2/19/22	0/1/1/1
6	NAG	E	1131	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1132	6	-	0/6/23/26	0/1/1/1
6	BMA	E	1133	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1134	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1135	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1136	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1137	6	-	0/2/19/22	0/1/1/1
6	NAG	E	1151	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1152	6	-	0/6/23/26	0/1/1/1
6	BMA	E	1153	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1154	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1155	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1156	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1157	6	-	0/2/19/22	0/1/1/1
6	NAG	E	1261	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1262	6	-	0/6/23/26	0/1/1/1
6	BMA	E	1263	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1264	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1265	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1266	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1267	6	-	0/2/19/22	0/1/1/1
6	NAG	E	1301	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1302	6	-	0/6/23/26	0/1/1/1
6	BMA	E	1303	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1304	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1305	6	-	0/2/19/22	0/1/1/1
6	MAN	E	1306	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	E	1307	6	-	0/2/19/22	0/1/1/1
7	NAG	E	1331	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	1332	7	-	0/6/23/26	0/1/1/1
7	BMA	E	1333	7	-	0/2/19/22	0/1/1/1
7	MAN	E	1334	7	-	0/2/19/22	0/1/1/1
7	MAN	E	1335	7	-	0/2/19/22	0/1/1/1
7	MAN	E	1336	7	-	0/2/19/22	0/1/1/1
7	MAN	E	1337	7	-	0/2/19/22	0/1/1/1
7	MAN	E	1338	7	-	0/2/19/22	0/1/1/1
7	MAN	E	1339	7	-	0/2/19/22	0/1/1/1
8	MAN	G	1340	8	-	0/2/19/22	1/1/1/1
8	MAN	G	1341	8	-	0/2/19/22	0/1/1/1
6	NAG	I	1131	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	1132	6	-	0/6/23/26	0/1/1/1
6	BMA	I	1133	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1134	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1135	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1136	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1137	6	-	0/2/19/22	0/1/1/1
6	NAG	I	1151	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	1152	6	-	0/6/23/26	0/1/1/1
6	BMA	I	1153	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1154	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1155	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1156	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1157	6	-	0/2/19/22	0/1/1/1
6	NAG	I	1261	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	1262	6	-	0/6/23/26	0/1/1/1
6	BMA	I	1263	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1264	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1265	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1266	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1267	6	-	0/2/19/22	0/1/1/1
6	NAG	I	1301	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	1302	6	-	0/6/23/26	0/1/1/1
6	BMA	I	1303	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1304	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1305	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1306	6	-	0/2/19/22	0/1/1/1
6	MAN	I	1307	6	-	0/2/19/22	0/1/1/1
7	NAG	I	1331	1,7	-	0/6/23/26	0/1/1/1
7	NAG	I	1332	7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	I	1333	7	-	0/2/19/22	0/1/1/1
7	MAN	I	1334	7	-	0/2/19/22	0/1/1/1
7	MAN	I	1335	7	-	0/2/19/22	0/1/1/1
7	MAN	I	1336	7	-	0/2/19/22	0/1/1/1
7	MAN	I	1337	7	-	0/2/19/22	0/1/1/1
7	MAN	I	1338	7	-	0/2/19/22	0/1/1/1
7	MAN	I	1339	7	-	0/2/19/22	0/1/1/1
8	MAN	K	1340	8	-	0/2/19/22	0/1/1/1
8	MAN	K	1341	8	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	1137	MAN	C2-C3-C4	-2.56	106.69	111.04
6	E	1157	MAN	O5-C1-C2	-2.40	106.96	110.86
6	I	1157	MAN	O5-C1-C2	-2.40	106.97	110.86
6	A	1157	MAN	O5-C1-C2	-2.40	106.97	110.86
6	A	1267	MAN	O5-C1-C2	-2.39	106.97	110.86
6	I	1267	MAN	O5-C1-C2	-2.38	106.99	110.86
6	E	1307	MAN	O5-C1-C2	-2.37	107.01	110.86
6	A	1307	MAN	O5-C1-C2	-2.36	107.03	110.86
6	E	1267	MAN	O5-C1-C2	-2.35	107.04	110.86
6	I	1307	MAN	O5-C1-C2	-2.34	107.06	110.86
6	A	1137	MAN	C2-C3-C4	-2.28	107.17	111.04
6	A	1155	MAN	C1-O5-C5	-2.15	109.52	112.25
6	I	1155	MAN	C1-O5-C5	-2.14	109.53	112.25
6	E	1155	MAN	C1-O5-C5	-2.08	109.61	112.25
6	I	1155	MAN	O6-C6-C5	-2.03	104.64	111.33
7	I	1336	MAN	O5-C1-C2	-2.00	107.61	110.86
6	A	1155	MAN	O6-C6-C5	-2.00	104.72	111.33
7	E	1331	NAG	C4-C3-C2	2.03	114.38	111.23
6	I	1152	NAG	C3-C4-C5	2.05	113.78	110.20
7	I	1337	MAN	O5-C5-C6	2.09	111.87	107.35
7	I	1331	NAG	C4-C3-C2	2.12	114.52	111.23
7	A	1331	NAG	C4-C3-C2	2.13	114.55	111.23
6	I	1303	BMA	C1-C2-C3	2.17	112.11	109.54
6	A	1303	BMA	C1-C2-C3	2.20	112.14	109.54
6	A	1301	NAG	C4-C3-C2	2.22	114.68	111.23
6	I	1153	BMA	C1-C2-C3	2.24	112.19	109.54
6	E	1301	NAG	C4-C3-C2	2.30	114.81	111.23
6	A	1153	BMA	C1-C2-C3	2.32	112.28	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	1301	NAG	C4-C3-C2	2.32	114.83	111.23
6	E	1303	BMA	C1-C2-C3	2.32	112.28	109.54
7	A	1332	NAG	C3-C4-C5	2.35	114.29	110.20
6	E	1153	BMA	C1-C2-C3	2.41	112.39	109.54
6	I	1261	NAG	C4-C3-C2	2.51	115.14	111.23
7	I	1332	NAG	C3-C4-C5	2.53	114.61	110.20
6	A	1261	NAG	C4-C3-C2	2.54	115.18	111.23
6	A	1133	BMA	C1-C2-C3	2.57	112.58	109.54
6	E	1261	NAG	C4-C3-C2	2.59	115.26	111.23
6	E	1133	BMA	C1-C2-C3	2.61	112.63	109.54
6	E	1151	NAG	C3-C4-C5	2.90	115.26	110.20
6	I	1133	BMA	C1-C2-C3	2.96	113.05	109.54
7	E	1333	BMA	C1-C2-C3	2.99	113.08	109.54
6	A	1151	NAG	C3-C4-C5	3.06	115.53	110.20
8	C	1340	MAN	O5-C1-C2	3.23	116.10	110.86
8	G	1340	MAN	O5-C1-C2	3.40	116.37	110.86
8	K	1340	MAN	O5-C1-C2	3.42	116.40	110.86
6	I	1151	NAG	C3-C4-C5	3.48	116.27	110.20
6	A	1131	NAG	C4-C3-C2	3.49	116.65	111.23
6	E	1261	NAG	C3-C4-C5	3.49	116.28	110.20
6	E	1131	NAG	C4-C3-C2	3.51	116.69	111.23
7	A	1331	NAG	C3-C4-C5	3.54	116.36	110.20
6	I	1261	NAG	C3-C4-C5	3.60	116.47	110.20
6	A	1261	NAG	C3-C4-C5	3.60	116.47	110.20
7	I	1331	NAG	C3-C4-C5	3.63	116.52	110.20
7	E	1331	NAG	C3-C4-C5	3.64	116.53	110.20
6	I	1131	NAG	C4-C3-C2	3.74	117.05	111.23
7	A	1333	BMA	C1-C2-C3	4.40	114.75	109.54
7	I	1333	BMA	C1-C2-C3	4.63	115.01	109.54

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	G	1340	MAN	C1-C2-C3-C4-C5-O5

14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1131	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1261	NAG	5	0
7	A	1332	NAG	2	0
8	C	1340	MAN	2	0
8	C	1341	MAN	1	0
6	E	1131	NAG	1	0
6	E	1261	NAG	5	0
8	G	1341	MAN	1	0
6	I	1137	MAN	1	0
6	I	1261	NAG	4	0
7	I	1331	NAG	1	0
7	I	1332	NAG	3	0
8	K	1340	MAN	1	0
8	K	1341	MAN	1	0

5.6 Ligand geometry (i)

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	1088	1	14,14,15	0.47	0	15,19,21	0.96	1 (6%)
5	NAG	A	1160	1	14,14,15	0.47	0	15,19,21	0.82	0
5	NAG	A	1197	1	14,14,15	0.44	0	15,19,21	0.93	1 (6%)
5	NAG	A	1234	1	14,14,15	0.42	0	15,19,21	1.15	2 (13%)
5	NAG	A	1276	1	14,14,15	0.39	0	15,19,21	1.21	2 (13%)
5	NAG	A	1295	1	14,14,15	0.52	0	15,19,21	0.78	0
5	NAG	A	1355	1	14,14,15	0.48	0	15,19,21	0.82	0
5	NAG	A	1386	1	14,14,15	0.55	0	15,19,21	0.82	1 (6%)
5	NAG	A	1392	1	14,14,15	0.44	0	15,19,21	0.73	0
5	NAG	A	1448	1	14,14,15	0.48	0	15,19,21	1.39	2 (13%)
5	NAG	E	1088	1	14,14,15	0.53	0	15,19,21	0.81	0
5	NAG	E	1160	1	14,14,15	0.47	0	15,19,21	0.76	0
5	NAG	E	1197	1	14,14,15	0.44	0	15,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	E	1234	1	14,14,15	0.41	0	15,19,21	1.08	2 (13%)
5	NAG	E	1276	1	14,14,15	0.43	0	15,19,21	1.23	2 (13%)
5	NAG	E	1295	1	14,14,15	0.48	0	15,19,21	0.82	0
5	NAG	E	1355	1	14,14,15	0.48	0	15,19,21	0.78	0
5	NAG	E	1386	1	14,14,15	0.56	0	15,19,21	0.79	0
5	NAG	E	1392	1	14,14,15	0.46	0	15,19,21	0.66	0
5	NAG	E	1448	1	14,14,15	0.47	0	15,19,21	1.44	2 (13%)
5	NAG	I	1088	1	14,14,15	0.48	0	15,19,21	0.96	1 (6%)
5	NAG	I	1160	1	14,14,15	0.40	0	15,19,21	0.96	1 (6%)
5	NAG	I	1197	1	14,14,15	0.47	0	15,19,21	0.84	1 (6%)
5	NAG	I	1234	1	14,14,15	0.45	0	15,19,21	1.10	2 (13%)
5	NAG	I	1276	1	14,14,15	0.44	0	15,19,21	1.05	1 (6%)
5	NAG	I	1295	1	14,14,15	0.49	0	15,19,21	0.87	1 (6%)
5	NAG	I	1355	1	14,14,15	0.45	0	15,19,21	0.92	1 (6%)
5	NAG	I	1386	1	14,14,15	0.52	0	15,19,21	0.84	1 (6%)
5	NAG	I	1392	1	14,14,15	0.41	0	15,19,21	0.72	0
5	NAG	I	1448	1	14,14,15	0.44	0	15,19,21	1.46	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
5	NAG	A	1088	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1160	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1197	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1234	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1276	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1295	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1355	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1386	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1392	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1448	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1088	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1160	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1197	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1234	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1276	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1295	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1355	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1386	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1392	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1448	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1088	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1160	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1197	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1234	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1276	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1295	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1355	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1386	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1392	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1448	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	1448	NAG	C2-N2-C7	-2.75	119.50	123.04
5	E	1448	NAG	C2-N2-C7	-2.65	119.64	123.04
5	A	1448	NAG	C2-N2-C7	-2.59	119.71	123.04
5	E	1276	NAG	C2-N2-C7	-2.29	120.09	123.04
5	A	1276	NAG	C2-N2-C7	-2.20	120.22	123.04
5	E	1234	NAG	C2-N2-C7	-2.12	120.32	123.04
5	I	1234	NAG	C2-N2-C7	-2.09	120.36	123.04
5	A	1234	NAG	C2-N2-C7	-2.05	120.41	123.04
5	I	1197	NAG	C1-O5-C5	2.05	114.85	112.25
5	I	1295	NAG	C1-O5-C5	2.11	114.93	112.25
5	I	1386	NAG	C1-O5-C5	2.13	114.95	112.25
5	I	1355	NAG	C1-O5-C5	2.13	114.95	112.25
5	A	1386	NAG	C1-O5-C5	2.16	114.99	112.25
5	E	1234	NAG	C1-O5-C5	2.17	115.00	112.25
5	I	1234	NAG	C1-O5-C5	2.22	115.06	112.25
5	I	1160	NAG	C1-O5-C5	2.33	115.21	112.25
5	A	1197	NAG	C1-O5-C5	2.36	115.25	112.25
5	I	1088	NAG	C1-O5-C5	2.53	115.46	112.25
5	A	1088	NAG	C1-O5-C5	2.54	115.47	112.25
5	I	1276	NAG	C1-O5-C5	2.66	115.62	112.25
5	A	1234	NAG	C1-O5-C5	2.75	115.73	112.25
5	E	1276	NAG	C1-O5-C5	3.12	116.21	112.25
5	A	1276	NAG	C1-O5-C5	3.15	116.25	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1448	NAG	C1-O5-C5	3.26	116.38	112.25
5	E	1448	NAG	C1-O5-C5	3.49	116.68	112.25
5	I	1448	NAG	C1-O5-C5	3.51	116.71	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1276	NAG	1	0
5	A	1295	NAG	2	0
5	E	1276	NAG	1	0
5	E	1295	NAG	2	0
5	I	1295	NAG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	420/475 (88%)	0.06	11 (2%) 59 50	7, 227, 434, 596	0
1	E	420/475 (88%)	0.10	19 (4%) 37 30	16, 221, 423, 559	0
1	I	420/475 (88%)	0.12	17 (4%) 42 34	25, 216, 434, 550	0
2	B	0/78	-	-	-	-
2	F	0/78	-	-	-	-
2	J	0/78	-	-	-	-
3	C	202/211 (95%)	0.46	19 (9%) 11 9	74, 234, 422, 563	0
3	G	202/211 (95%)	0.56	26 (12%) 5 6	43, 229, 392, 572	0
3	K	202/211 (95%)	0.87	37 (18%) 2 3	47, 291, 454, 533	0
4	D	226/235 (96%)	0.50	24 (10%) 8 8	67, 232, 488, 582	0
4	H	226/235 (96%)	0.34	16 (7%) 19 15	56, 232, 421, 563	0
4	L	226/235 (96%)	0.66	27 (11%) 6 7	71, 287, 466, 582	0
All	All	2544/2997 (84%)	0.33	196 (7%) 16 13	7, 236, 440, 596	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	204	GLU	7.5
4	D	100(A)	ILE	7.4
4	L	111	SER	6.9
3	G	204	GLU	6.1
3	K	147	VAL	5.9
4	L	112	ALA	5.8
4	D	29	VAL	5.6
3	K	175	ALA	5.6
4	L	188	GLY	5.4
4	D	112	ALA	5.4
3	K	108	SER	5.1
3	G	133	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
4	H	112	ALA	5.0
4	H	71	LEU	4.9
3	K	179	LEU	4.9
3	K	145	VAL	4.8
3	K	159	GLY	4.8
4	L	177	SER	4.7
4	H	100(A)	ILE	4.7
3	K	193	SER	4.7
3	K	133	LEU	4.6
3	C	111	LYS	4.5
3	K	174	ALA	4.4
4	L	185	SER	4.3
3	G	190	LYS	4.3
4	D	105	THR	4.3
4	L	71	LEU	4.3
3	G	71	ALA	4.3
4	D	71	LEU	4.2
4	D	109	VAL	4.2
4	H	102	GLY	4.2
4	L	92	CYS	4.1
4	D	102	GLY	4.1
4	L	102	GLY	4.1
4	L	100(A)	ILE	4.1
3	K	47	ILE	4.0
4	L	184	SER	3.9
3	C	13	VAL	3.9
3	K	192	TYR	3.8
3	G	132	THR	3.7
3	G	192	TYR	3.7
3	K	162	THR	3.7
3	G	70	THR	3.7
3	K	82	ASP	3.7
4	L	156	ALA	3.7
3	G	203	VAL	3.6
4	D	104	GLY	3.6
1	E	357	THR	3.6
3	K	113	ALA	3.6
3	K	190	LYS	3.5
4	D	90	TYR	3.5
3	C	47	ILE	3.5
3	C	204	GLU	3.5
4	L	29	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	207	VAL	3.4
3	K	132	THR	3.4
4	L	176	LEU	3.4
3	K	50	ASN	3.4
1	E	262	ASN	3.4
1	I	357	THR	3.4
3	G	189	HIS	3.3
3	G	72	THR	3.3
1	E	236	THR	3.2
1	I	63	THR	3.2
3	C	151	ALA	3.2
4	H	73	LYS	3.2
4	D	100	ARG	3.2
1	E	237	GLY	3.1
3	K	164	THR	3.1
1	E	94	ASN	3.1
1	E	59	LYS	3.1
3	K	146	THR	3.1
3	C	181	LEU	3.0
4	H	72	ASP	3.0
1	I	309	ILE	3.0
1	A	59	LYS	3.0
4	H	111	SER	3.0
4	L	73	LYS	3.0
4	L	157	LEU	3.0
1	I	262	ASN	3.0
4	H	175	SER	2.9
3	C	62	PHE	2.9
3	G	131	ALA	2.9
4	L	183	PRO	2.9
1	E	137	ASN	2.9
4	D	8	GLY	2.9
3	C	158	ALA	2.9
3	G	82	ASP	2.9
1	A	63	THR	2.9
4	L	110	SER	2.9
4	H	109	VAL	2.8
4	L	72	ASP	2.8
1	I	59	LYS	2.8
4	L	160	GLY	2.8
3	K	114	PRO	2.8
3	G	180	SER	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	157	LEU	2.8
1	E	309	ILE	2.8
3	G	179	LEU	2.8
1	A	137	ASN	2.8
1	E	78	ASP	2.7
3	C	190	LYS	2.7
1	I	78	ASP	2.7
1	E	238	PRO	2.7
3	C	110	PRO	2.7
3	K	141	TYR	2.7
3	C	208	ALA	2.7
1	I	491	ILE	2.7
3	K	111	LYS	2.6
4	H	166	ALA	2.6
3	C	192	TYR	2.6
1	A	256	SER	2.6
3	G	62	PHE	2.6
3	K	194	CYS	2.6
3	K	119	PHE	2.6
3	G	205	LYS	2.6
3	G	195	GLN	2.6
4	H	113	SER	2.6
1	E	70	ALA	2.6
3	C	179	LEU	2.6
3	G	193	SER	2.6
3	K	62	PHE	2.5
3	G	50	ASN	2.5
4	H	30	ARG	2.5
4	H	69	LEU	2.5
3	K	109	GLN	2.5
4	D	18	LEU	2.5
1	E	45	TRP	2.5
1	A	392	ASN	2.5
4	L	8	GLY	2.5
3	G	32	SER	2.5
3	C	152	ASP	2.5
1	I	238	PRO	2.4
4	H	4	LEU	2.4
4	L	90	TYR	2.4
4	D	70	SER	2.4
4	D	72	ASP	2.4
3	G	20	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	242	VAL	2.4
4	H	157	LEU	2.4
3	G	24	GLY	2.4
1	I	379	GLY	2.4
1	E	264	SER	2.4
1	A	70	ALA	2.4
1	I	71	THR	2.4
3	K	163	THR	2.4
1	I	174	SER	2.4
1	E	330	HIS	2.4
3	G	181	LEU	2.3
1	I	263	GLY	2.3
4	D	78	VAL	2.3
3	K	195	GLN	2.3
1	A	291	PRO	2.3
3	C	195	GLN	2.3
4	L	175	SER	2.3
1	A	57	ASP	2.3
3	G	194	CYS	2.3
3	K	196	VAL	2.3
1	A	357	THR	2.3
3	C	131	ALA	2.2
4	L	150	VAL	2.2
3	K	95(C)	ASN	2.2
3	K	112	ALA	2.2
1	I	236	THR	2.2
3	K	110	PRO	2.2
3	K	165	PRO	2.2
1	I	264	SER	2.2
3	K	48	ILE	2.2
4	L	194	CYS	2.2
4	D	110	SER	2.2
4	D	4	LEU	2.2
4	H	29	VAL	2.2
1	A	262	ASN	2.1
1	E	356	ASN	2.1
3	K	150	LYS	2.1
1	I	330	HIS	2.1
3	G	65	SER	2.1
4	D	7	SER	2.1
1	I	94	ASN	2.1
4	L	113	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	85	HIS	2.1
3	C	196	VAL	2.1
4	L	17	THR	2.1
1	E	191	TYR	2.1
4	D	69	LEU	2.1
3	C	147	VAL	2.0
4	D	124	PRO	2.0
4	L	81	ARG	2.0
4	D	166	ALA	2.0
1	I	378	CYS	2.0
4	D	77	LEU	2.0
1	E	171	LYS	2.0
3	G	207	VAL	2.0
4	D	91	TYR	2.0
1	E	219	ALA	2.0
3	K	134	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)

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
6	NAG	E	1131	14/15	-0.17	1.43	6.76	550,550,550,550	0
7	NAG	A	1331	14/15	0.69	0.54	2.79	366,366,366,366	0
6	NAG	I	1131	14/15	0.26	0.79	2.40	530,530,530,530	0
6	NAG	A	1261	14/15	0.53	0.66	2.06	423,423,423,423	0
6	NAG	I	1261	14/15	0.54	0.70	2.05	437,437,437,437	0
6	NAG	E	1261	14/15	0.38	0.69	1.72	408,408,408,408	0
6	NAG	I	1301	14/15	0.79	0.36	1.11	276,276,276,276	0
7	NAG	E	1331	14/15	0.76	0.36	1.08	302,302,302,302	0
6	NAG	A	1131	14/15	0.37	0.59	0.98	439,439,439,439	0
6	NAG	A	1151	14/15	0.86	0.33	0.90	356,356,356,356	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	NAG	E	1301	14/15	0.84	0.30	0.77	242,242,242,242	0
6	NAG	A	1301	14/15	0.81	0.30	0.32	202,202,202,202	0
6	NAG	E	1151	14/15	0.84	0.30	0.22	186,186,186,186	0
6	NAG	I	1151	14/15	0.77	0.34	0.21	337,337,337,337	0
7	NAG	I	1331	14/15	0.77	0.34	-0.15	292,292,292,292	0
6	BMA	E	1153	11/12	0.56	0.28	-	466,466,466,466	0
6	MAN	A	1264	11/12	0.82	0.17	-	229,229,229,229	0
6	NAG	A	1302	14/15	0.78	0.24	-	307,307,307,307	0
7	MAN	I	1335	11/12	0.73	0.27	-	277,277,277,277	0
6	MAN	A	1134	11/12	0.47	0.58	-	451,451,451,451	0
8	MAN	G	1341	11/12	-0.05	1.32	-	545,545,545,545	0
6	MAN	A	1306	11/12	0.40	0.88	-	418,418,418,418	0
8	MAN	G	1340	11/12	-0.05	1.03	-	427,427,427,427	0
6	MAN	I	1306	11/12	0.62	1.03	-	482,482,482,482	0
6	MAN	I	1154	11/12	-0.23	1.92	-	550,550,550,550	0
6	BMA	I	1263	11/12	0.82	0.16	-	297,297,297,297	0
8	MAN	K	1340	11/12	0.30	1.04	-	408,408,408,408	0
6	MAN	E	1136	11/12	-0.18	1.91	-	550,550,550,550	0
6	NAG	A	1132	14/15	0.63	0.99	-	519,519,519,519	0
6	MAN	I	1304	11/12	0.67	0.36	-	330,330,330,330	0
7	BMA	E	1333	11/12	0.57	0.29	-	400,400,400,400	0
6	MAN	A	1157	11/12	0.16	0.69	-	464,464,464,464	0
6	NAG	E	1132	14/15	0.65	1.11	-	488,488,488,488	0
8	MAN	C	1341	11/12	-0.27	2.20	-	489,489,489,489	0
6	MAN	A	1305	11/12	0.64	0.56	-	483,483,483,483	0
7	MAN	E	1335	11/12	0.55	0.36	-	330,330,330,330	0
6	MAN	E	1157	11/12	0.44	0.51	-	446,446,446,446	0
6	BMA	E	1133	11/12	0.29	1.06	-	500,500,500,500	0
7	MAN	A	1338	11/12	0.90	0.76	-	500,500,500,500	0
7	MAN	A	1339	11/12	0.60	0.34	-	303,303,303,303	0
6	MAN	E	1154	11/12	0.58	1.36	-	542,542,542,542	0
7	BMA	I	1333	11/12	0.91	0.23	-	345,345,345,345	0
7	MAN	A	1336	11/12	0.54	0.47	-	422,422,422,422	0
7	NAG	I	1332	14/15	0.96	0.22	-	213,213,213,213	0
6	NAG	A	1262	14/15	0.88	0.33	-	410,410,410,410	0
6	NAG	E	1262	14/15	0.72	0.41	-	310,310,310,310	0
6	MAN	I	1155	11/12	0.51	0.50	-	550,550,550,550	0
7	MAN	A	1334	11/12	0.85	0.36	-	550,550,550,550	0
7	MAN	I	1338	11/12	0.83	0.78	-	507,507,507,507	0
7	MAN	I	1336	11/12	0.59	0.49	-	436,436,436,436	0
6	MAN	I	1137	11/12	0.21	1.66	-	494,494,494,494	0
7	MAN	I	1337	11/12	0.71	0.41	-	382,382,382,382	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	MAN	C	1340	11/12	-0.04	1.95	-	550,550,550,550	0
6	MAN	A	1135	11/12	0.41	0.81	-	517,517,517,517	0
6	NAG	I	1262	14/15	0.83	0.31	-	231,231,231,231	0
6	MAN	A	1155	11/12	0.53	0.80	-	550,550,550,550	0
7	BMA	A	1333	11/12	0.83	0.35	-	292,292,292,292	0
6	MAN	I	1134	11/12	0.38	0.84	-	520,520,520,520	0
6	MAN	A	1137	11/12	0.51	1.02	-	434,434,434,434	0
6	MAN	A	1304	11/12	0.15	1.22	-	447,447,447,447	0
6	MAN	E	1264	11/12	0.83	0.28	-	195,195,195,195	0
6	NAG	E	1302	14/15	0.77	0.32	-	335,335,335,335	0
6	MAN	A	1136	11/12	0.07	1.57	-	481,481,481,481	0
6	MAN	E	1307	11/12	0.09	0.82	-	454,454,454,454	0
6	MAN	E	1155	11/12	0.57	0.52	-	550,550,550,550	0
6	MAN	I	1265	11/12	0.37	0.70	-	545,545,545,545	0
7	MAN	E	1336	11/12	0.38	0.61	-	452,452,452,452	0
6	BMA	A	1133	11/12	0.67	0.49	-	356,356,356,356	0
6	BMA	I	1303	11/12	0.61	0.27	-	474,474,474,474	0
6	MAN	A	1265	11/12	0.47	0.58	-	550,550,550,550	0
6	BMA	I	1133	11/12	0.39	0.45	-	402,402,402,402	0
6	MAN	I	1266	11/12	0.33	0.95	-	507,507,507,507	0
6	MAN	E	1266	11/12	-0.08	1.39	-	550,550,550,550	0
6	MAN	I	1267	11/12	-0.46	1.78	-	532,532,532,532	0
6	MAN	A	1156	11/12	0.55	0.49	-	329,329,329,329	0
6	NAG	I	1152	14/15	0.79	0.37	-	375,375,375,375	0
6	MAN	E	1265	11/12	0.12	0.72	-	550,550,550,550	0
7	MAN	E	1338	11/12	0.77	0.78	-	491,491,491,491	0
6	BMA	A	1303	11/12	0.61	0.48	-	455,455,455,455	0
6	MAN	I	1305	11/12	0.12	0.35	-	467,467,467,467	0
6	MAN	A	1266	11/12	0.37	0.91	-	468,468,468,468	0
6	MAN	I	1156	11/12	0.71	0.43	-	410,410,410,410	0
6	MAN	E	1267	11/12	-0.00	0.91	-	515,515,515,515	0
7	NAG	A	1332	14/15	0.85	0.37	-	258,258,258,258	0
6	MAN	I	1157	11/12	0.40	0.27	-	428,428,428,428	0
6	MAN	E	1134	11/12	0.16	1.21	-	518,518,518,518	0
6	NAG	I	1302	14/15	0.68	0.42	-	382,382,382,382	0
6	MAN	I	1135	11/12	-0.26	1.13	-	550,550,550,550	0
8	MAN	K	1341	11/12	-0.05	1.89	-	550,550,550,550	0
6	MAN	I	1136	11/12	0.02	1.72	-	477,477,477,477	0
6	MAN	A	1307	11/12	0.23	0.69	-	470,470,470,470	0
7	NAG	E	1332	14/15	0.76	0.41	-	388,388,388,388	0
7	MAN	E	1339	11/12	0.83	0.53	-	335,335,335,335	0
6	MAN	E	1306	11/12	0.32	1.18	-	495,495,495,495	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MAN	E	1135	11/12	-0.13	1.30	-	550,550,550,550	0
7	MAN	E	1337	11/12	0.54	0.53	-	418,418,418,418	0
6	NAG	E	1152	14/15	0.93	0.27	-	301,301,301,301	0
6	MAN	E	1305	11/12	0.37	0.55	-	471,471,471,471	0
6	MAN	E	1304	11/12	0.76	0.42	-	377,377,377,377	0
6	BMA	A	1153	11/12	0.42	0.46	-	483,483,483,483	0
6	MAN	E	1137	11/12	-0.16	1.53	-	497,497,497,497	0
6	MAN	I	1307	11/12	0.53	0.75	-	474,474,474,474	0
6	MAN	E	1156	11/12	0.63	0.58	-	422,422,422,422	0
6	NAG	I	1132	14/15	0.55	0.57	-	460,460,460,460	0
7	MAN	E	1334	11/12	0.63	0.56	-	550,550,550,550	0
6	MAN	I	1264	11/12	0.84	0.25	-	197,197,197,197	0
7	MAN	I	1339	11/12	0.70	0.49	-	362,362,362,362	0
6	MAN	A	1154	11/12	0.39	1.59	-	498,498,498,498	0
6	MAN	A	1267	11/12	-0.17	0.82	-	455,455,455,455	0
6	BMA	I	1153	11/12	0.42	0.52	-	491,491,491,491	0
6	NAG	A	1152	14/15	0.89	0.28	-	310,310,310,310	0
6	BMA	E	1263	11/12	0.57	0.26	-	340,340,340,340	0
6	BMA	A	1263	11/12	0.53	0.23	-	506,506,506,506	0
7	MAN	A	1337	11/12	0.69	0.32	-	309,309,309,309	0
7	MAN	I	1334	11/12	0.78	0.66	-	550,550,550,550	0
6	BMA	E	1303	11/12	0.36	0.26	-	492,492,492,492	0
7	MAN	A	1335	11/12	0.48	0.34	-	302,302,302,302	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, 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
5	NAG	E	1386	14/15	0.66	0.65	5.53	427,427,427,427	0
5	NAG	E	1295	14/15	0.25	0.73	4.98	356,356,356,356	0
5	NAG	I	1386	14/15	0.74	0.46	3.12	331,331,331,331	0
5	NAG	A	1386	14/15	0.70	0.55	3.09	356,356,356,356	0
5	NAG	A	1295	14/15	0.39	0.61	2.85	330,330,330,330	0
5	NAG	I	1295	14/15	0.61	0.44	0.85	323,323,323,323	0
5	NAG	I	1448	14/15	0.61	0.48	-	287,287,287,287	0
5	NAG	I	1197	14/15	0.84	0.21	-	304,304,304,304	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	E	1276	14/15	0.79	0.43	-	313,313,313,313	0
5	NAG	E	1355	14/15	0.70	0.39	-	411,411,411,411	0
5	NAG	A	1448	14/15	0.51	0.61	-	279,279,279,279	0
5	NAG	E	1392	14/15	0.39	0.84	-	305,305,305,305	0
5	NAG	E	1088	14/15	0.63	0.62	-	486,486,486,486	0
5	NAG	A	1234	14/15	0.88	0.29	-	431,431,431,431	0
5	NAG	A	1392	14/15	0.16	0.98	-	386,386,386,386	0
5	NAG	E	1234	14/15	0.71	0.49	-	405,405,405,405	0
5	NAG	A	1197	14/15	0.86	0.23	-	302,302,302,302	0
5	NAG	I	1392	14/15	0.43	0.71	-	345,345,345,345	0
5	NAG	I	1276	14/15	0.92	0.37	-	281,281,281,281	0
5	NAG	E	1448	14/15	0.55	0.55	-	361,361,361,361	0
5	NAG	E	1197	14/15	0.84	0.32	-	288,288,288,288	0
5	NAG	I	1234	14/15	0.69	0.41	-	345,345,345,345	0
5	NAG	I	1355	14/15	0.51	0.44	-	266,266,266,266	0
5	NAG	I	1088	14/15	0.43	0.68	-	503,503,503,503	0
5	NAG	E	1160	14/15	0.55	0.62	-	245,245,245,245	0
5	NAG	A	1088	14/15	0.43	0.61	-	474,474,474,474	0
5	NAG	A	1160	14/15	0.76	0.51	-	267,267,267,267	0
5	NAG	A	1276	14/15	0.89	0.34	-	288,288,288,288	0
5	NAG	A	1355	14/15	0.71	0.48	-	238,238,238,238	0
5	NAG	I	1160	14/15	0.33	1.08	-	362,362,362,362	0

6.5 Other polymers (i)

There are no such residues in this entry.