



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 01:56 AM EDT

PDB ID : 1RVZ
Title : 1934 H1 Hemagglutinin in complex with LSTC
Authors : Gamblin, S.J.; Haire, L.F.; Russell, R.J.; Stevens, D.J.; Xiao, B.; Ha, Y.; Vasisht, N.; Steinhauer, D.A.; Daniels, R.S.; Elliot, A.; Wiley, D.C.; Skehel, J.J.
Deposited on : 2003-12-15
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

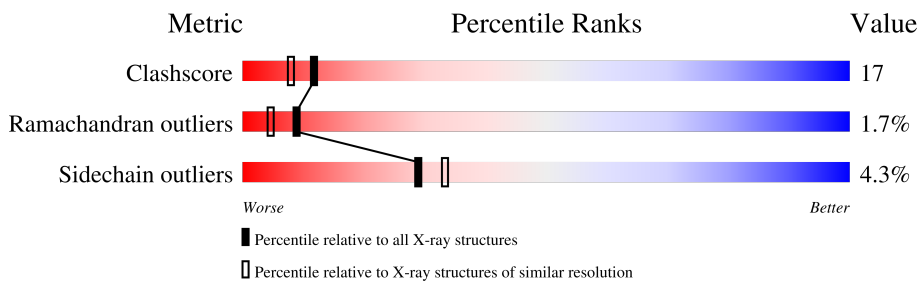
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)





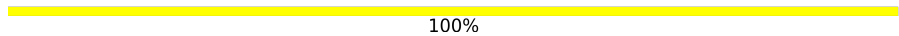
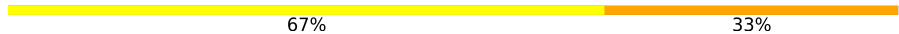
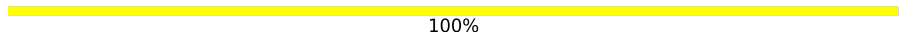

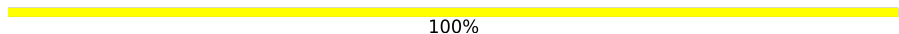
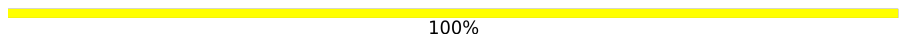
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	327	75% 21% ..
1	C	327	74% 22% ..
1	E	327	73% 22% ..
1	G	327	76% 20% ..
1	I	327	77% 20% ..
1	K	327	71% 25% ..
2	B	160	62% 33% 5%
2	D	160	70% 24% 5%

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Mol	Chain	Length	Quality of chain
2	F	160	 61% 32% 7% .
2	H	160	 69% 26% . .
2	J	160	 70% 23% 7%
2	L	160	 68% 29% .
3	M	3	 100%
3	N	3	 67% 33%
3	O	3	 100%
3	P	3	 33% 67%
3	Q	3	 100%
3	R	3	 100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25452 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.

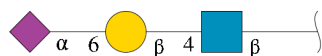
- Molecule 1 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	323	2556	1611	450	482	13	0	0	0
1	C	323	2557	1612	450	482	13	0	0	0
1	E	323	2557	1612	450	482	13	0	0	0
1	G	323	2557	1612	450	482	13	0	0	0
1	I	323	2557	1612	450	482	13	0	0	0
1	K	323	2557	1612	450	482	13	0	0	0

- Molecule 2 is a protein called hemagglutinin.

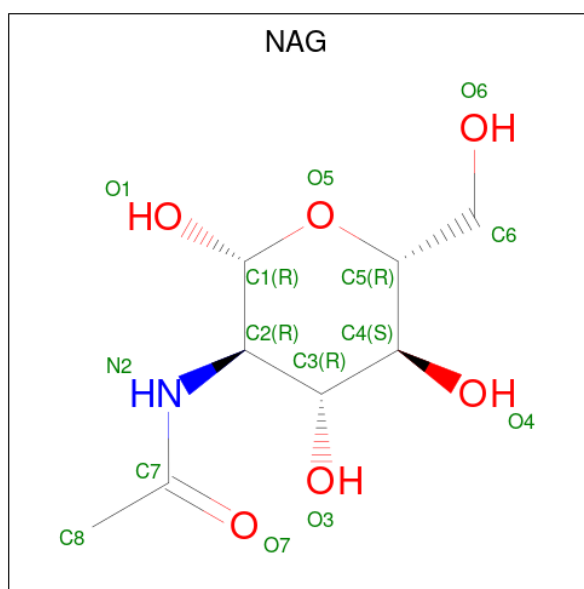
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	160	1283	805	218	253	7	0	0	0
2	D	160	1283	805	218	253	7	0	0	0
2	F	160	1283	805	218	253	7	0	0	0
2	H	160	1283	805	218	253	7	0	0	0
2	J	160	1283	805	218	253	7	0	0	0
2	L	160	1283	805	218	253	7	0	0	0

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	3	Total	C	N	O	0	0	0
			45	25	2	18			
3	N	3	Total	C	N	O	0	0	0
			45	25	2	18			
3	O	3	Total	C	N	O	0	0	0
			45	25	2	18			
3	P	3	Total	C	N	O	0	0	0
			45	25	2	18			
3	Q	3	Total	C	N	O	0	0	0
			45	25	2	18			
3	R	3	Total	C	N	O	0	0	0
			45	25	2	18			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	E	1	Total	C	N	O	0	0
			15	8	1	6		
4	F	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is water.

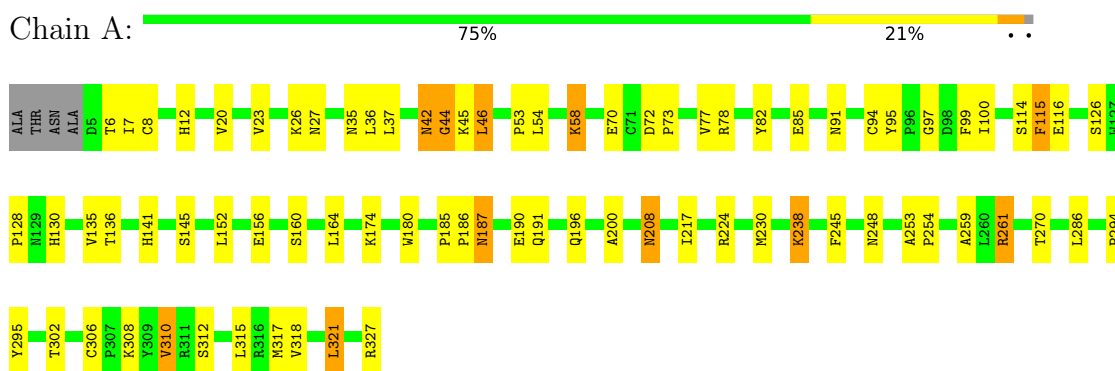
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	254	Total O 254 254	0	0
5	B	69	Total O 69 69	0	0
5	C	254	Total O 254 254	0	0
5	D	97	Total O 97 97	0	0
5	E	250	Total O 250 250	0	0
5	F	81	Total O 81 81	0	0
5	G	300	Total O 300 300	0	0
5	H	76	Total O 76 76	0	0
5	I	290	Total O 290 290	0	0
5	J	76	Total O 76 76	0	0
5	K	274	Total O 274 274	0	0
5	L	77	Total O 77 77	0	0

3 Residue-property plots [i](#)

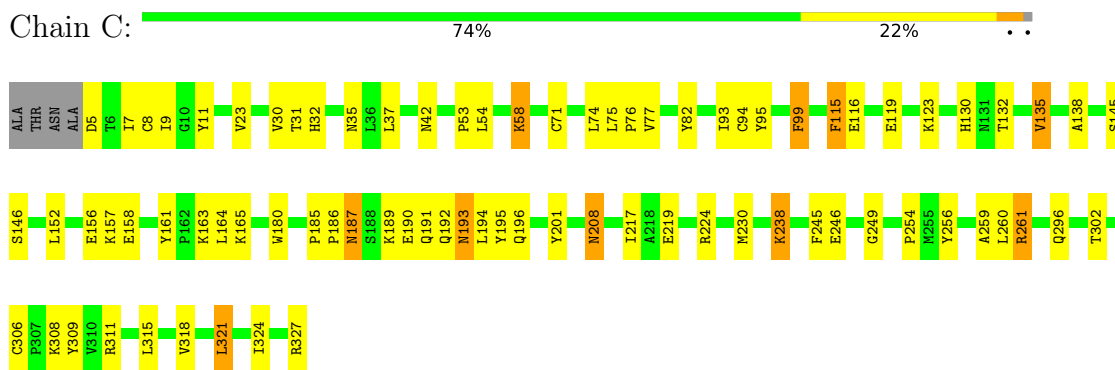
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

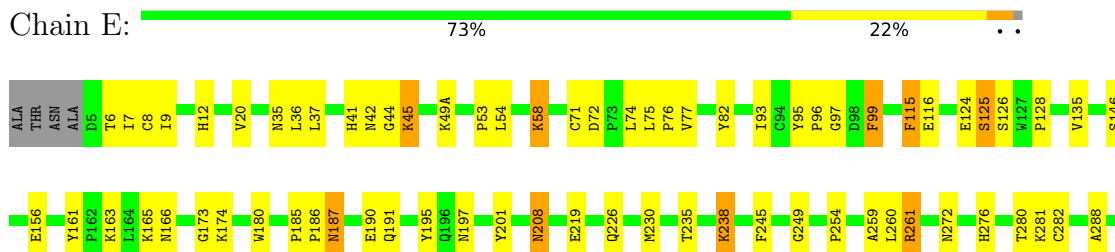
- Molecule 1: hemagglutinin



- Molecule 1: hemagglutinin

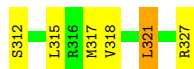
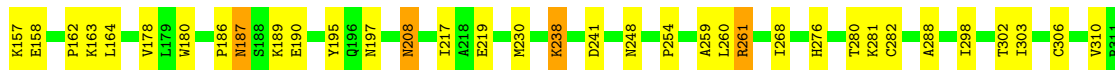
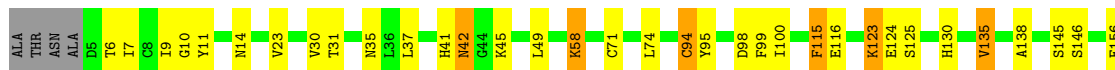
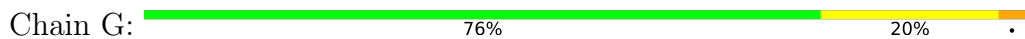


- Molecule 1: hemagglutinin





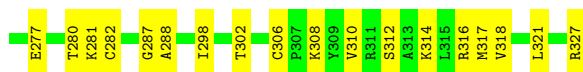
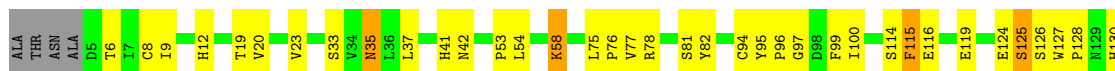
• Molecule 1: hemagglutinin



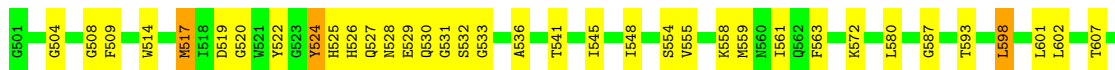
• Molecule 1: hemagglutinin



• Molecule 1: hemagglutinin



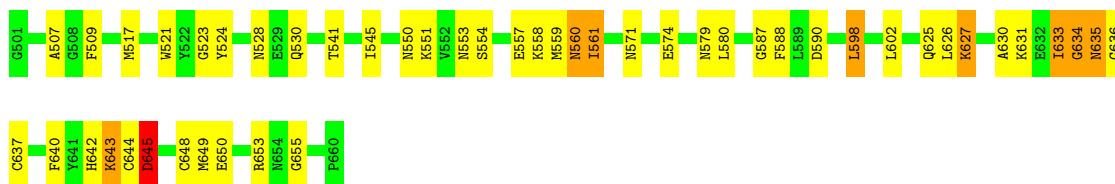
• Molecule 2: hemagglutinin





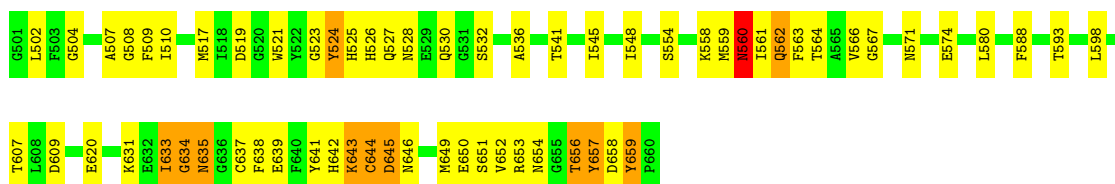
- Molecule 2: hemagglutinin

Chain D: 70% 24% 5%



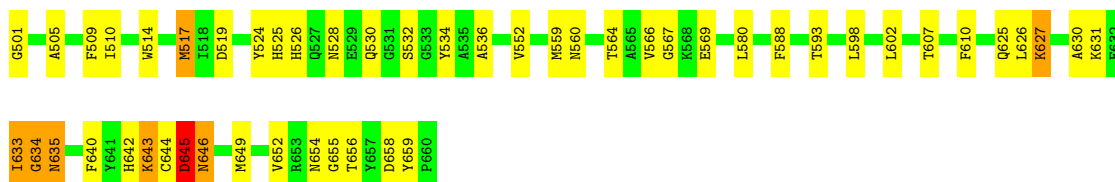
- Molecule 2: hemagglutinin

Chain F: 61% 32% 7%



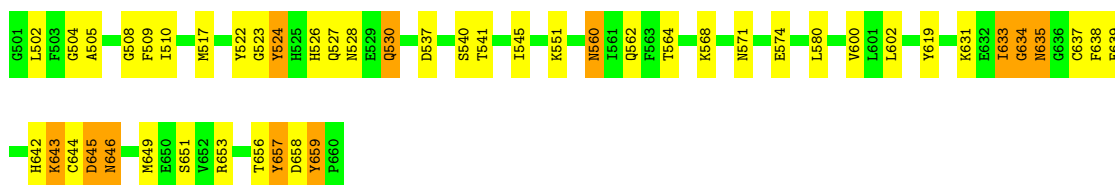
- Molecule 2: hemagglutinin

Chain H: 69% 26%



- Molecule 2: hemagglutinin

Chain J: 70% 23% 7%



- Molecule 2: hemagglutinin

Chain L: 68% 29%





- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 100%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 67% 33%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 100%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 33% 67%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 100%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 100%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	227.58Å 131.52Å 175.02Å 90.00° 110.07° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.25)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	25452	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	0/2620	0.62	0/3561
1	C	0.34	0/2621	0.63	0/3563
1	E	0.35	0/2620	0.63	0/3560
1	G	0.36	0/2621	0.64	0/3563
1	I	0.34	0/2621	0.61	0/3563
1	K	0.34	0/2621	0.62	0/3563
2	B	0.32	0/1309	0.52	0/1761
2	D	0.34	0/1309	0.56	0/1761
2	F	0.34	0/1309	0.57	0/1761
2	H	0.33	0/1309	0.56	0/1761
2	J	0.34	0/1309	0.56	0/1761
2	L	0.32	0/1309	0.52	0/1761
All	All	0.34	0/23578	0.60	0/31939

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 [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	2556	0	2491	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2557	0	2495	85	0
1	E	2557	0	2494	98	0
1	G	2557	0	2495	89	1
1	I	2557	0	2495	66	0
1	K	2557	0	2495	93	0
2	B	1283	0	1205	64	0
2	D	1283	0	1205	45	0
2	F	1283	0	1205	82	0
2	H	1283	0	1205	57	0
2	J	1283	0	1205	51	0
2	L	1283	0	1205	53	0
3	M	45	0	37	0	0
3	N	45	0	37	1	0
3	O	45	0	37	0	0
3	P	45	0	37	1	0
3	Q	45	0	37	0	0
3	R	45	0	37	0	0
4	A	15	0	15	4	0
4	E	15	0	15	4	0
4	F	15	0	15	4	0
5	A	254	0	0	5	1
5	B	69	0	0	2	0
5	C	254	0	0	3	0
5	D	97	0	0	3	0
5	E	250	0	0	4	0
5	F	81	0	0	4	0
5	G	300	0	0	9	0
5	H	76	0	0	2	0
5	I	290	0	0	2	0
5	J	76	0	0	4	0
5	K	274	0	0	5	1
5	L	77	0	0	1	0
All	All	25452	0	22462	795	2

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 17.

All (795) 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:238:LYS:H	1:G:238:LYS:CE	1.65	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:LYS:H	1:G:58:LYS:HD3	1.14	1.07
1:G:238:LYS:H	1:G:238:LYS:HE3	0.94	1.06
1:G:280:THR:HG22	1:G:282:CYS:H	1.19	1.03
1:E:280:THR:HG22	1:E:282:CYS:H	1.23	1.02
1:G:238:LYS:HE3	1:G:238:LYS:N	1.76	1.01
1:E:58:LYS:H	1:E:58:LYS:HD3	1.25	1.00
1:C:58:LYS:H	1:C:58:LYS:HD3	1.23	0.99
1:A:238:LYS:H	1:A:238:LYS:HZ2	1.15	0.95
1:G:10:GLY:HA2	2:H:510:ILE:HD11	1.48	0.94
1:K:280:THR:HG22	1:K:282:CYS:H	1.33	0.92
1:I:6:THR:H	2:J:527:GLN:HB3	1.35	0.90
1:G:310:VAL:HG12	1:G:312:SER:H	1.37	0.90
1:E:42:ASN:HD22	1:E:288:ALA:HB3	1.36	0.90
1:A:238:LYS:H	1:A:238:LYS:NZ	1.70	0.89
1:I:58:LYS:H	1:I:58:LYS:HD3	1.39	0.87
1:E:310:VAL:HG12	1:E:312:SER:H	1.38	0.87
2:B:650:GLU:HA	2:B:653:ARG:NH1	1.90	0.86
2:F:560:ASN:HB3	5:F:3351:HOH:O	1.76	0.85
2:H:517:MET:HE1	2:H:536:ALA:HB2	1.60	0.83
1:G:58:LYS:HD3	1:G:58:LYS:N	1.93	0.83
1:E:42:ASN:HB3	1:E:44:GLY:O	1.79	0.82
1:A:208:ASN:HD21	1:A:238:LYS:HE2	1.44	0.81
2:J:509:PHE:O	2:J:635:ASN:HB3	1.81	0.81
1:K:208:ASN:HD21	1:K:238:LYS:HE2	1.45	0.81
1:E:6:THR:H	2:F:527:GLN:HB3	1.46	0.81
2:B:528:ASN:HD21	2:B:646:ASN:ND2	1.79	0.81
1:G:58:LYS:H	1:G:58:LYS:CD	1.91	0.80
1:C:58:LYS:HD3	1:C:58:LYS:N	1.96	0.80
2:F:509:PHE:O	2:F:635:ASN:HB3	1.82	0.80
2:F:527:GLN:O	2:F:527:GLN:HG2	1.83	0.79
1:C:208:ASN:HD21	1:C:238:LYS:HE2	1.46	0.79
1:C:58:LYS:H	1:C:58:LYS:CD	1.97	0.78
2:B:528:ASN:HD21	2:B:646:ASN:HD22	1.27	0.78
1:C:193:ASN:C	1:C:193:ASN:HD22	1.85	0.77
1:E:238:LYS:H	1:E:238:LYS:HZ2	1.32	0.77
1:K:208:ASN:ND2	1:K:238:LYS:HE2	1.98	0.77
1:C:238:LYS:NZ	1:C:238:LYS:H	1.83	0.77
2:J:527:GLN:O	2:J:527:GLN:HG2	1.82	0.77
1:A:208:ASN:ND2	1:A:238:LYS:HE2	1.97	0.77
1:K:238:LYS:H	1:K:238:LYS:HZ2	1.30	0.77
2:H:566:VAL:HG12	2:H:567:GLY:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:GLU:HG2	5:E:3438:HOH:O	1.85	0.75
1:G:219:GLU:HG3	5:I:3315:HOH:O	1.86	0.75
1:E:58:LYS:HD3	1:E:58:LYS:N	1.98	0.75
2:J:633:ILE:HG22	2:J:634:GLY:H	1.51	0.75
2:F:528:ASN:HD21	2:F:649:MET:CG	1.99	0.75
1:E:272:ASN:ND2	4:E:3311:NAG:H1	2.02	0.75
2:H:566:VAL:HG12	2:H:567:GLY:H	1.53	0.74
1:E:58:LYS:H	1:E:58:LYS:CD	1.98	0.74
1:E:208:ASN:HD21	1:E:238:LYS:HE2	1.53	0.74
2:F:633:ILE:H	2:F:633:ILE:HD12	1.53	0.73
2:J:633:ILE:HG22	2:J:634:GLY:N	2.03	0.72
2:D:633:ILE:HG22	2:D:634:GLY:N	2.04	0.72
1:A:78:ARG:HH21	1:A:261:ARG:HH22	1.36	0.72
1:E:41:HIS:HB3	1:E:298:ILE:HD13	1.70	0.72
1:C:189:LYS:HB3	5:C:3350:HOH:O	1.90	0.71
1:C:238:LYS:H	1:C:238:LYS:HZ2	1.33	0.71
1:E:238:LYS:H	1:E:238:LYS:NZ	1.87	0.71
2:L:528:ASN:HD21	2:L:649:MET:HG2	1.55	0.71
1:C:238:LYS:H	1:C:238:LYS:CE	2.04	0.71
2:D:553:ASN:O	2:D:557:GLU:HG3	1.91	0.71
1:A:187:ASN:ND2	1:A:190:GLU:H	1.89	0.70
1:K:238:LYS:H	1:K:238:LYS:NZ	1.88	0.70
1:G:23:VAL:HG22	2:H:602:LEU:HD12	1.72	0.70
2:H:631:LYS:HG3	2:H:633:ILE:HD11	1.72	0.70
2:L:633:ILE:HD12	2:L:633:ILE:N	2.07	0.70
1:I:58:LYS:HD3	1:I:58:LYS:N	2.07	0.70
1:K:135:VAL:HG13	1:K:145:SER:HB3	1.72	0.70
2:B:650:GLU:OE2	2:B:653:ARG:NH1	2.25	0.69
1:E:45:LYS:HG2	1:E:276:HIS:CD2	2.26	0.69
1:G:268:ILE:O	2:H:566:VAL:HG11	1.92	0.69
1:C:208:ASN:ND2	1:C:238:LYS:HE2	2.08	0.69
1:C:157:LYS:HG2	1:C:158:GLU:HG3	1.74	0.69
1:E:208:ASN:ND2	1:E:238:LYS:HE2	2.08	0.68
2:J:633:ILE:N	2:J:633:ILE:HD12	2.07	0.68
2:L:509:PHE:O	2:L:635:ASN:HB3	1.94	0.68
1:K:187:ASN:ND2	1:K:190:GLU:H	1.91	0.68
1:G:317:MET:HE3	2:H:552:VAL:HG22	1.75	0.68
2:F:633:ILE:HD12	2:F:633:ILE:N	2.09	0.68
1:I:58:LYS:H	1:I:58:LYS:CD	2.05	0.67
1:K:58:LYS:HD3	1:K:58:LYS:H	1.58	0.67
2:B:633:ILE:HD12	2:B:633:ILE:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:642:HIS:CE1	2:B:644:CYS:HB3	2.30	0.67
1:A:238:LYS:HZ2	1:A:238:LYS:N	1.91	0.67
1:A:42:ASN:O	1:A:45:LYS:N	2.26	0.67
2:H:514:TRP:HE3	2:H:517:MET:HG3	1.60	0.67
1:A:6:THR:O	2:B:527:GLN:HB2	1.94	0.66
1:I:327:ARG:C	1:I:327:ARG:HD2	2.15	0.66
2:B:631:LYS:HG3	2:B:633:ILE:HD11	1.78	0.66
1:G:42:ASN:C	1:G:42:ASN:HD22	1.96	0.66
1:C:208:ASN:H	1:C:208:ASN:HD22	1.43	0.66
1:K:6:THR:H	2:L:527:GLN:HB3	1.61	0.66
2:L:631:LYS:HE3	2:L:633:ILE:HG13	1.77	0.66
2:B:650:GLU:CA	2:B:653:ARG:NH1	2.58	0.66
1:C:187:ASN:ND2	1:C:190:GLU:H	1.94	0.66
1:E:42:ASN:OD1	1:E:45:LYS:HE3	1.95	0.66
1:G:208:ASN:ND2	1:G:238:LYS:HZ3	1.94	0.66
1:K:35:ASN:ND2	1:K:37:LEU:H	1.93	0.66
2:L:633:ILE:HD11	2:L:639:GLU:HB2	1.77	0.66
1:G:98:ASP:HB3	5:G:3294:HOH:O	1.95	0.66
1:A:35:ASN:ND2	1:A:37:LEU:H	1.93	0.66
2:B:642:HIS:HE1	2:B:644:CYS:HB3	1.59	0.66
1:C:193:ASN:C	1:C:193:ASN:ND2	2.49	0.65
1:I:42:ASN:ND2	1:I:288:ALA:H	1.94	0.65
1:I:97:GLY:HA3	1:I:230:MET:O	1.95	0.65
2:J:528:ASN:HD21	2:J:646:ASN:ND2	1.94	0.65
1:I:42:ASN:ND2	1:I:45:LYS:H	1.95	0.65
1:I:116:GLU:HG2	1:I:259:ALA:HB3	1.77	0.65
2:L:527:GLN:O	2:L:527:GLN:HG3	1.97	0.65
2:L:593:THR:O	2:L:597:GLU:HG3	1.97	0.65
2:F:633:ILE:HD11	2:F:639:GLU:N	2.11	0.65
2:J:571:ASN:OD1	2:J:574:GLU:HG3	1.96	0.65
2:H:528:ASN:HD21	2:H:530:GLN:NE2	1.95	0.65
1:C:193:ASN:HD22	1:C:194:LEU:N	1.93	0.64
2:F:651:SER:HA	2:F:654:ASN:HD21	1.62	0.64
2:L:504:GLY:O	2:L:508:GLY:HA3	1.96	0.64
2:B:631:LYS:HE3	2:B:633:ILE:HG13	1.79	0.64
1:G:10:GLY:HA2	2:H:510:ILE:CD1	2.26	0.64
2:L:631:LYS:HG3	2:L:633:ILE:HD11	1.79	0.64
1:K:19:THR:HG23	1:K:314:LYS:NZ	2.12	0.64
1:E:260:LEU:C	1:E:261:ARG:HD2	2.18	0.64
1:K:42:ASN:O	1:K:42:ASN:OD1	2.16	0.64
1:G:187:ASN:ND2	1:G:190:GLU:H	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:579:ASN:HB3	5:F:3407:HOH:O	1.98	0.63
1:G:135:VAL:HG13	1:G:145:SER:HB3	1.81	0.63
2:F:528:ASN:HD21	2:F:649:MET:HG3	1.62	0.63
1:G:280:THR:HG22	1:G:282:CYS:N	2.04	0.63
1:A:186:PRO:HD2	1:A:190:GLU:OE2	1.99	0.62
1:E:71:CYS:HB3	1:E:74:LEU:HD12	1.80	0.62
1:K:280:THR:HG22	1:K:281:LYS:N	2.15	0.62
1:K:54:LEU:HD13	1:K:77:VAL:HG11	1.82	0.62
1:E:280:THR:HG22	1:E:281:LYS:N	2.14	0.62
1:G:189:LYS:HG3	5:G:3373:HOH:O	2.00	0.62
2:H:528:ASN:HD21	2:H:530:GLN:HE21	1.48	0.62
1:K:186:PRO:HD2	1:K:190:GLU:OE2	1.99	0.62
1:E:124:GLU:O	1:E:125:SER:CB	2.47	0.62
1:I:186:PRO:HD2	1:I:190:GLU:OE2	1.99	0.62
2:D:625:GLN:HE22	2:D:655:GLY:C	2.03	0.62
2:B:558:LYS:HG3	2:F:598:LEU:CD2	2.30	0.61
1:G:321:LEU:H	1:G:321:LEU:HD23	1.65	0.61
2:D:509:PHE:O	2:D:635:ASN:HB3	2.00	0.61
1:C:135:VAL:HG13	1:C:145:SER:HB3	1.82	0.61
5:G:3437:HOH:O	1:K:219:GLU:HG3	1.99	0.61
1:C:35:ASN:ND2	1:C:37:LEU:H	1.98	0.61
1:E:238:LYS:H	1:E:238:LYS:CE	2.13	0.61
1:E:305:GLU:C	2:F:561:ILE:HD11	2.20	0.61
2:H:526:HIS:HB2	2:H:649:MET:CE	2.30	0.61
1:G:280:THR:HG22	1:G:281:LYS:N	2.16	0.61
2:B:558:LYS:HG3	2:F:598:LEU:HD21	1.83	0.61
1:E:185:PRO:HG2	1:E:191:GLN:HE21	1.66	0.61
1:G:116:GLU:O	1:G:116:GLU:HG3	2.00	0.60
2:L:528:ASN:ND2	2:L:649:MET:HG2	2.15	0.60
1:A:116:GLU:HG2	1:A:259:ALA:HB3	1.83	0.60
2:B:650:GLU:HB2	2:B:653:ARG:HH12	1.66	0.60
1:C:135:VAL:HG22	1:C:146:SER:CA	2.31	0.60
1:E:306:CYS:N	2:F:561:ILE:HD11	2.15	0.60
1:G:208:ASN:HD21	1:G:238:LYS:NZ	1.99	0.60
1:A:27:ASN:HD21	4:A:3321:NAG:H1	1.66	0.60
1:C:93:ILE:HD11	1:C:99:PHE:HB2	1.84	0.60
1:A:327:ARG:HD2	1:A:327:ARG:O	2.01	0.60
1:E:97:GLY:HA3	1:E:230:MET:O	2.02	0.60
1:I:23:VAL:HG22	2:J:602:LEU:HD12	1.82	0.60
1:A:78:ARG:HH21	1:A:261:ARG:NH2	1.99	0.60
1:K:23:VAL:HG22	2:L:602:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:321:LEU:HD23	1:G:321:LEU:N	2.15	0.60
1:G:186:PRO:HD2	1:G:190:GLU:OE2	2.02	0.60
2:H:526:HIS:HB2	2:H:649:MET:HE2	1.82	0.59
1:I:42:ASN:C	1:I:42:ASN:HD22	2.05	0.59
1:A:238:LYS:H	1:A:238:LYS:CE	2.14	0.59
1:G:208:ASN:OD1	1:G:238:LYS:HD3	2.02	0.59
1:A:208:ASN:HD22	1:A:208:ASN:H	1.49	0.59
1:G:42:ASN:ND2	1:G:45:LYS:H	1.99	0.59
1:A:97:GLY:HA3	1:A:230:MET:O	2.03	0.59
1:A:310:VAL:HG13	1:A:312:SER:H	1.66	0.59
1:E:261:ARG:HD2	1:E:261:ARG:N	2.18	0.59
1:I:6:THR:HB	2:J:527:GLN:OE1	2.02	0.59
2:D:645:ASP:O	2:D:649:MET:HG2	2.03	0.59
2:J:642:HIS:O	2:J:643:LYS:O	2.21	0.59
1:G:208:ASN:ND2	1:G:238:LYS:NZ	2.51	0.59
2:H:566:VAL:CG1	2:H:567:GLY:H	2.16	0.59
1:K:95:TYR:CD2	1:K:230:MET:HB2	2.38	0.59
1:A:116:GLU:HG3	1:A:116:GLU:O	2.01	0.58
1:G:116:GLU:HG2	1:G:259:ALA:HB3	1.85	0.58
2:F:528:ASN:HD21	2:F:649:MET:HG2	1.68	0.58
1:I:180:TRP:HB3	1:I:254:PRO:HG3	1.84	0.58
1:K:58:LYS:H	1:K:58:LYS:CD	2.16	0.58
2:D:560:ASN:N	2:D:560:ASN:HD22	2.01	0.58
1:I:94:CYS:O	1:I:224:ARG:HD3	2.04	0.58
1:K:238:LYS:H	1:K:238:LYS:CE	2.16	0.58
2:B:630:ALA:HB2	2:B:640:PHE:HA	1.85	0.58
2:B:530:GLN:NE2	2:B:646:ASN:H	2.01	0.58
1:I:185:PRO:HG2	1:I:191:GLN:HE21	1.67	0.58
5:G:3291:HOH:O	2:H:569:GLU:HG3	2.02	0.58
2:H:644:CYS:O	2:H:649:MET:HG2	2.04	0.58
2:D:631:LYS:HG3	2:D:633:ILE:HD11	1.85	0.57
1:G:317:MET:HE3	2:H:552:VAL:HA	1.86	0.57
1:K:97:GLY:HA3	1:K:230:MET:O	2.04	0.57
1:E:280:THR:HG22	1:E:281:LYS:H	1.70	0.57
2:H:528:ASN:HD22	2:H:646:ASN:ND2	2.03	0.57
2:L:528:ASN:HD21	2:L:649:MET:CG	2.16	0.57
1:C:186:PRO:HD2	1:C:190:GLU:OE2	2.04	0.57
2:F:654:ASN:CB	4:F:3331:NAG:O1	2.53	0.57
1:G:310:VAL:HG13	2:H:593:THR:HA	1.86	0.57
1:E:6:THR:HB	2:F:527:GLN:OE1	2.04	0.57
1:G:35:ASN:ND2	1:G:37:LEU:H	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:ASN:HD21	1:I:288:ALA:H	1.53	0.57
1:K:280:THR:HG22	1:K:282:CYS:N	2.14	0.57
1:A:27:ASN:ND2	4:A:3321:NAG:O1	2.38	0.57
2:D:633:ILE:HD12	2:D:633:ILE:N	2.19	0.57
2:H:566:VAL:CG1	2:H:567:GLY:N	2.68	0.57
2:F:571:ASN:OD1	2:F:574:GLU:HG3	2.05	0.57
2:H:633:ILE:HG22	2:H:634:GLY:N	2.20	0.57
1:I:6:THR:HG23	2:J:638:PHE:O	2.05	0.57
1:I:327:ARG:HD2	1:I:327:ARG:O	2.05	0.57
2:F:633:ILE:HD11	2:F:639:GLU:H	1.70	0.56
1:A:53:PRO:HB3	1:A:82:TYR:CE2	2.41	0.56
1:G:238:LYS:CE	1:G:238:LYS:N	2.50	0.56
1:K:41:HIS:HB3	1:K:298:ILE:HD13	1.88	0.56
1:G:58:LYS:HG3	5:G:3386:HOH:O	2.05	0.56
1:C:135:VAL:HG22	1:C:146:SER:HA	1.87	0.56
1:K:280:THR:HG21	1:K:288:ALA:HB1	1.86	0.56
1:C:115:PHE:C	1:C:115:PHE:HD1	2.09	0.56
2:F:528:ASN:ND2	2:F:649:MET:HG3	2.20	0.56
1:G:208:ASN:H	1:G:208:ASN:HD22	1.52	0.56
1:E:208:ASN:H	1:E:208:ASN:HD22	1.53	0.56
1:C:115:PHE:C	1:C:115:PHE:CD1	2.79	0.56
2:D:630:ALA:HB2	2:D:640:PHE:HA	1.88	0.56
2:H:630:ALA:HB2	2:H:640:PHE:HA	1.87	0.56
2:J:509:PHE:O	2:J:635:ASN:CB	2.52	0.56
1:C:217:ILE:N	1:C:217:ILE:HD12	2.21	0.56
2:D:560:ASN:N	2:D:560:ASN:ND2	2.52	0.56
2:F:502:LEU:HB2	2:F:609:ASP:OD1	2.06	0.55
2:H:625:GLN:HE22	2:H:655:GLY:C	2.10	0.55
2:J:541:THR:O	2:J:545:ILE:HG13	2.06	0.55
2:L:631:LYS:HE3	2:L:633:ILE:CG1	2.36	0.55
1:C:164:LEU:C	1:C:164:LEU:HD12	2.27	0.55
1:G:9:ILE:N	1:G:9:ILE:HD12	2.21	0.55
2:D:633:ILE:HG22	2:D:634:GLY:H	1.71	0.55
2:H:625:GLN:C	2:H:627:LYS:H	2.08	0.55
1:C:23:VAL:HG22	2:D:602:LEU:HD12	1.88	0.55
2:H:509:PHE:O	2:H:635:ASN:HB3	2.05	0.55
2:J:528:ASN:HD21	2:J:646:ASN:HD22	1.53	0.55
1:K:116:GLU:O	1:K:116:GLU:HG3	2.07	0.55
1:A:95:TYR:CD2	1:A:230:MET:HB2	2.41	0.55
1:E:180:TRP:HB3	1:E:254:PRO:HG3	1.88	0.55
1:A:114:SER:O	1:A:261:ARG:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:VAL:HG22	2:B:593:THR:HA	1.87	0.55
1:E:185:PRO:HG2	1:E:191:GLN:NE2	2.21	0.55
1:K:135:VAL:HG22	1:K:146:SER:HA	1.87	0.55
1:K:310:VAL:HG13	1:K:312:SER:H	1.71	0.55
2:L:519:ASP:HB2	2:L:536:ALA:CB	2.37	0.55
1:C:261:ARG:HD2	1:C:261:ARG:N	2.22	0.55
1:K:53:PRO:HB3	1:K:82:TYR:CE2	2.42	0.55
1:I:9:ILE:HD12	1:I:9:ILE:O	2.07	0.54
2:B:509:PHE:O	2:B:635:ASN:HB3	2.07	0.54
2:B:601:LEU:HG	5:B:702:HOH:O	2.07	0.54
1:C:32:HIS:ND1	5:D:701:HOH:O	2.33	0.54
1:K:124:GLU:O	1:K:125:SER:HB3	2.07	0.54
1:E:124:GLU:O	1:E:125:SER:HB3	2.07	0.54
2:B:504:GLY:O	2:B:508:GLY:HA3	2.08	0.54
1:E:6:THR:N	2:F:527:GLN:HB3	2.19	0.54
1:G:163:LYS:HG2	1:G:248:ASN:HB3	1.89	0.54
2:H:633:ILE:N	2:H:633:ILE:HD12	2.22	0.54
2:J:562:GLN:HG3	5:J:722:HOH:O	2.07	0.54
1:C:135:VAL:CG2	1:C:146:SER:HA	2.38	0.54
1:G:23:VAL:CG2	2:H:602:LEU:HD12	2.36	0.54
2:B:633:ILE:HD11	2:B:639:GLU:HB2	1.89	0.54
1:I:95:TYR:CD2	1:I:230:MET:HB2	2.42	0.54
1:K:280:THR:HG22	1:K:281:LYS:H	1.73	0.54
1:E:186:PRO:HD2	1:E:190:GLU:OE2	2.07	0.54
2:F:566:VAL:CG1	2:F:567:GLY:N	2.71	0.54
1:G:115:PHE:C	1:G:115:PHE:HD1	2.11	0.54
1:I:126:SER:C	1:I:128:PRO:HD3	2.28	0.54
1:E:42:ASN:C	1:E:44:GLY:N	2.61	0.54
1:I:208:ASN:HD22	1:I:208:ASN:H	1.55	0.54
1:K:100:ILE:N	1:K:100:ILE:HD12	2.22	0.54
1:K:58:LYS:HD3	1:K:58:LYS:N	2.23	0.54
2:D:517:MET:SD	2:D:523:GLY:HA3	2.49	0.53
2:L:642:HIS:HE1	2:L:644:CYS:HB3	1.72	0.53
1:C:321:LEU:N	1:C:321:LEU:HD23	2.23	0.53
2:D:650:GLU:HA	2:D:653:ARG:HH11	1.72	0.53
1:G:115:PHE:C	1:G:115:PHE:CD1	2.82	0.53
1:G:123:LYS:HG3	1:G:124:GLU:N	2.23	0.53
2:D:528:ASN:C	2:D:530:GLN:H	2.11	0.53
1:E:186:PRO:HD2	1:E:190:GLU:CD	2.29	0.53
1:E:20:VAL:HG21	1:E:318:VAL:HB	1.91	0.53
1:E:95:TYR:CD2	1:E:230:MET:HB2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:142:GLU:HG2	5:K:3340:HOH:O	2.08	0.53
2:L:633:ILE:CD1	2:L:639:GLU:H	2.21	0.53
1:G:302:THR:HB	1:G:306:CYS:SG	2.49	0.53
1:I:187:ASN:ND2	1:I:190:GLU:H	2.06	0.53
2:H:526:HIS:O	2:H:532:SER:HA	2.08	0.53
1:K:302:THR:HB	1:K:306:CYS:SG	2.49	0.53
1:A:126:SER:C	1:A:128:PRO:HD3	2.29	0.53
2:F:530:GLN:HE22	2:F:646:ASN:H	1.57	0.53
2:F:541:THR:O	2:F:545:ILE:HG13	2.09	0.53
2:B:650:GLU:HG3	2:B:654:ASN:ND2	2.24	0.53
1:C:163:LYS:HE3	1:C:201:TYR:OH	2.08	0.53
2:D:643:LYS:HD3	5:D:727:HOH:O	2.08	0.53
1:I:302:THR:HB	1:I:306:CYS:SG	2.49	0.53
1:I:321:LEU:N	1:I:321:LEU:HD23	2.23	0.53
1:A:302:THR:HB	1:A:306:CYS:SG	2.49	0.53
2:D:541:THR:O	2:D:545:ILE:HG13	2.09	0.53
2:L:642:HIS:CE1	2:L:644:CYS:HB3	2.44	0.53
1:A:6:THR:HG23	2:B:638:PHE:O	2.09	0.52
1:A:135:VAL:CG1	1:A:145:SER:HB3	2.39	0.52
1:A:58:LYS:HD3	1:A:58:LYS:H	1.74	0.52
1:A:78:ARG:NH2	1:A:261:ARG:HH22	2.07	0.52
2:D:571:ASN:OD1	2:D:574:GLU:HG3	2.09	0.52
3:P:1:NAG:H61	3:P:2:GAL:O5	2.09	0.52
1:I:54:LEU:HD13	1:I:77:VAL:HG11	1.91	0.52
1:K:94:CYS:O	1:K:224:ARG:HD3	2.10	0.52
1:K:116:GLU:HG2	1:K:259:ALA:HB3	1.91	0.52
2:B:647:GLU:O	2:B:650:GLU:HB3	2.09	0.52
2:J:560:ASN:HB3	5:J:686:HOH:O	2.09	0.52
2:B:631:LYS:HE3	2:B:633:ILE:CG1	2.39	0.52
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.45	0.52
2:B:519:ASP:HB2	2:B:536:ALA:CB	2.40	0.52
1:G:219:GLU:OE2	1:I:165:LYS:HD2	2.10	0.52
1:C:260:LEU:C	1:C:261:ARG:HD2	2.30	0.52
2:J:645:ASP:O	2:J:649:MET:HG2	2.10	0.52
1:A:217:ILE:HD12	1:A:217:ILE:N	2.25	0.51
2:B:525:HIS:HA	2:B:533:GLY:O	2.09	0.51
1:C:164:LEU:HD12	1:C:164:LEU:O	2.10	0.51
1:C:185:PRO:HG2	1:C:191:GLN:HE21	1.75	0.51
1:G:115:PHE:HD1	1:G:115:PHE:O	1.94	0.51
1:E:35:ASN:ND2	1:E:37:LEU:H	2.08	0.51
2:L:528:ASN:ND2	2:L:649:MET:CG	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:HIS:HD2	5:A:3400:HOH:O	1.93	0.51
1:C:311:ARG:NH1	2:D:590:ASP:OD1	2.41	0.51
1:C:115:PHE:HD1	1:C:115:PHE:O	1.94	0.51
2:D:631:LYS:HE3	2:D:633:ILE:HG13	1.92	0.51
2:H:631:LYS:O	2:H:633:ILE:HD12	2.10	0.51
2:B:528:ASN:ND2	2:B:646:ASN:ND2	2.55	0.51
1:C:180:TRP:HB3	1:C:254:PRO:HG3	1.92	0.51
2:H:631:LYS:HG3	2:H:633:ILE:CD1	2.39	0.51
1:I:185:PRO:HG2	1:I:191:GLN:NE2	2.25	0.51
1:G:7:ILE:HG23	1:G:7:ILE:O	2.10	0.51
1:A:115:PHE:HD1	1:A:115:PHE:C	2.15	0.51
1:A:208:ASN:OD1	1:A:238:LYS:HD3	2.11	0.51
1:C:327:ARG:HD2	1:C:327:ARG:O	2.11	0.51
1:E:327:ARG:HD2	1:E:327:ARG:C	2.31	0.51
1:I:116:GLU:O	1:I:116:GLU:HG3	2.08	0.51
1:A:27:ASN:ND2	4:A:3321:NAG:C1	2.74	0.51
1:A:58:LYS:H	1:A:58:LYS:CD	2.24	0.51
2:B:624:SER:O	2:B:627:LYS:HE3	2.10	0.51
2:F:651:SER:HA	2:F:654:ASN:ND2	2.26	0.51
1:K:317:MET:HE3	2:L:555:VAL:HG11	1.93	0.51
1:E:261:ARG:N	1:E:261:ARG:CD	2.74	0.50
1:A:35:ASN:ND2	5:A:3505:HOH:O	2.45	0.50
1:C:238:LYS:H	1:C:238:LYS:HE3	1.74	0.50
1:K:135:VAL:HG22	1:K:146:SER:CA	2.42	0.50
1:K:190:GLU:HA	1:K:193:ASN:HD21	1.74	0.50
1:K:277:GLU:HB3	5:K:3383:HOH:O	2.10	0.50
2:F:633:ILE:HG22	2:F:634:GLY:N	2.27	0.50
2:H:644:CYS:O	2:H:645:ASP:O	2.30	0.50
1:K:164:LEU:C	1:K:164:LEU:HD12	2.32	0.50
1:A:115:PHE:C	1:A:115:PHE:CD1	2.85	0.50
2:L:650:GLU:HA	2:L:653:ARG:HH11	1.76	0.50
1:A:160:SER:HA	1:A:196:GLN:OE1	2.11	0.50
1:A:186:PRO:HD2	1:A:190:GLU:CD	2.32	0.50
1:C:187:ASN:HD22	1:C:190:GLU:H	1.58	0.50
1:E:8:CYS:HA	2:F:637:CYS:HA	1.93	0.50
5:E:3521:HOH:O	2:F:559:MET:HG2	2.11	0.50
1:I:71:CYS:HB3	1:I:74:LEU:HD12	1.92	0.50
1:C:30:VAL:HG11	1:C:318:VAL:HG21	1.93	0.50
2:D:598:LEU:CD2	2:F:558:LYS:HG3	2.42	0.50
1:K:193:ASN:HD22	1:K:194:LEU:N	2.10	0.50
2:L:519:ASP:HB2	2:L:536:ALA:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:566:VAL:HG12	2:F:567:GLY:O	2.12	0.50
2:J:528:ASN:HD21	2:J:646:ASN:HA	1.77	0.50
2:B:658:ASP:C	2:B:659:TYR:HD2	2.16	0.50
1:C:308:LYS:HD2	2:D:559:MET:HE1	1.93	0.50
2:D:626:LEU:O	2:D:627:LYS:C	2.50	0.50
2:F:526:HIS:HB2	2:F:649:MET:HE2	1.93	0.50
1:K:95:TYR:HD2	1:K:230:MET:HB2	1.75	0.50
1:E:115:PHE:CD1	1:E:115:PHE:C	2.85	0.49
1:E:115:PHE:C	1:E:115:PHE:HD1	2.15	0.49
1:C:302:THR:HB	1:C:306:CYS:SG	2.51	0.49
1:E:116:GLU:O	1:E:116:GLU:HG3	2.11	0.49
2:J:517:MET:CE	2:J:523:GLY:HA3	2.41	0.49
2:J:651:SER:HB2	2:J:657:TYR:H	1.78	0.49
2:J:658:ASP:O	2:J:659:TYR:CG	2.65	0.49
1:G:124:GLU:HA	5:G:3316:HOH:O	2.11	0.49
2:B:659:TYR:N	2:B:659:TYR:CD2	2.76	0.49
1:E:7:ILE:HD13	2:F:652:VAL:HG11	1.94	0.49
1:E:36:LEU:CD1	1:E:317:MET:HE3	2.42	0.49
1:E:116:GLU:HG2	1:E:259:ALA:HB3	1.94	0.49
1:E:306:CYS:O	2:F:562:GLN:HB3	2.13	0.49
1:C:164:LEU:O	1:C:246:GLU:HA	2.12	0.49
2:D:631:LYS:HG3	2:D:633:ILE:CD1	2.43	0.49
1:E:302:THR:HB	1:E:306:CYS:SG	2.53	0.49
1:E:321:LEU:HD23	1:E:321:LEU:N	2.27	0.49
1:A:174:LYS:NZ	1:A:261:ARG:HG3	2.27	0.49
2:B:517:MET:HE2	2:B:536:ALA:HB2	1.93	0.49
2:F:519:ASP:HB2	2:F:536:ALA:CB	2.42	0.49
1:C:116:GLU:HG3	1:C:116:GLU:O	2.11	0.49
1:E:163:LYS:HE3	1:E:201:TYR:OH	2.13	0.49
2:F:631:LYS:HB3	2:F:641:TYR:OH	2.13	0.49
1:I:37:LEU:HB2	1:I:315:LEU:HB2	1.94	0.49
1:K:53:PRO:HB3	1:K:82:TYR:CZ	2.47	0.49
1:C:186:PRO:HD2	1:C:190:GLU:CD	2.33	0.49
1:I:6:THR:N	2:J:527:GLN:HB3	2.16	0.49
2:D:631:LYS:O	2:D:633:ILE:HD12	2.13	0.49
1:I:41:HIS:HB3	1:I:298:ILE:HD13	1.95	0.49
1:I:100:ILE:N	1:I:100:ILE:HD12	2.28	0.49
1:K:12:HIS:HB2	2:L:520:GLY:O	2.11	0.49
1:K:115:PHE:CD1	1:K:115:PHE:C	2.87	0.48
1:K:115:PHE:C	1:K:115:PHE:HD1	2.17	0.48
1:E:327:ARG:HD2	1:E:327:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:642:HIS:O	2:F:643:LYS:O	2.30	0.48
1:G:71:CYS:HB3	1:G:74:LEU:HD12	1.95	0.48
2:H:517:MET:HE1	2:H:536:ALA:CB	2.39	0.48
2:J:522:TYR:HD1	2:J:540:SER:HB3	1.78	0.48
1:A:27:ASN:ND2	4:A:3321:NAG:H1	2.29	0.48
1:A:94:CYS:O	1:A:224:ARG:HD3	2.14	0.48
2:H:505:ALA:O	2:H:510:ILE:HG23	2.13	0.48
1:I:35:ASN:ND2	5:I:3358:HOH:O	2.46	0.48
1:K:156:GLU:HG2	1:K:160:SER:H	1.78	0.48
1:A:164:LEU:C	1:A:164:LEU:HD12	2.33	0.48
1:A:174:LYS:HE2	5:A:3456:HOH:O	2.13	0.48
2:F:566:VAL:HG12	2:F:567:GLY:N	2.28	0.48
2:F:654:ASN:OD1	2:F:656:THR:HG23	2.13	0.48
1:K:260:LEU:C	1:K:261:ARG:HD2	2.33	0.48
2:B:626:LEU:HD12	2:B:638:PHE:CD2	2.48	0.48
1:C:132:THR:HB	1:C:152:LEU:HD13	1.95	0.48
2:F:560:ASN:ND2	5:F:3387:HOH:O	2.35	0.48
1:G:317:MET:CE	2:H:552:VAL:HG22	2.40	0.48
2:H:525:HIS:HD2	2:H:534:TYR:CE2	2.31	0.48
1:K:19:THR:HG23	1:K:314:LYS:HZ1	1.77	0.48
2:L:631:LYS:HG3	2:L:633:ILE:CD1	2.43	0.48
1:E:135:VAL:CG2	1:E:146:SER:HA	2.43	0.48
1:G:187:ASN:HD22	1:G:190:GLU:H	1.61	0.48
1:G:260:LEU:C	1:G:261:ARG:HD2	2.34	0.48
1:K:135:VAL:CG1	1:K:145:SER:HB3	2.42	0.48
1:A:26:LYS:HE3	2:D:550:ASN:OD1	2.13	0.48
1:E:126:SER:C	1:E:128:PRO:HD3	2.34	0.48
1:G:42:ASN:C	1:G:42:ASN:ND2	2.64	0.48
1:G:95:TYR:CD2	1:G:230:MET:HB2	2.47	0.48
1:G:157:LYS:HG2	1:G:158:GLU:HG3	1.96	0.48
1:A:185:PRO:HG2	1:A:191:GLN:HE21	1.79	0.48
1:C:130:HIS:HD2	5:C:3269:HOH:O	1.96	0.48
1:C:296:GLN:O	1:C:309:TYR:HA	2.14	0.48
1:C:71:CYS:HB3	1:C:74:LEU:HD12	1.96	0.48
1:A:58:LYS:HE2	1:A:70:GLU:O	2.14	0.47
1:A:141:HIS:NE2	5:A:3354:HOH:O	2.10	0.47
2:F:649:MET:O	2:F:653:ARG:HG3	2.14	0.47
2:F:651:SER:HB2	2:F:657:TYR:H	1.79	0.47
1:C:185:PRO:HG2	1:C:191:GLN:NE2	2.29	0.47
2:J:530:GLN:HE22	2:J:646:ASN:H	1.62	0.47
1:K:78:ARG:O	1:K:114:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PHE:HD1	1:A:115:PHE:O	1.97	0.47
1:C:238:LYS:HZ2	1:C:238:LYS:N	2.05	0.47
1:I:35:ASN:ND2	1:I:37:LEU:H	2.12	0.47
2:J:504:GLY:O	2:J:508:GLY:HA3	2.14	0.47
1:A:310:VAL:CG1	1:A:312:SER:H	2.26	0.47
5:G:3370:HOH:O	2:H:559:MET:HG2	2.14	0.47
1:C:208:ASN:HD22	1:C:208:ASN:N	2.05	0.47
2:F:504:GLY:O	2:F:508:GLY:HA3	2.14	0.47
2:F:658:ASP:O	2:F:659:TYR:CG	2.68	0.47
2:H:519:ASP:HB2	2:H:536:ALA:HB3	1.96	0.47
2:J:631:LYS:HE3	2:J:633:ILE:HG13	1.97	0.47
1:K:130:HIS:CE1	1:K:162:PRO:HD2	2.49	0.47
2:L:541:THR:O	2:L:545:ILE:HG13	2.15	0.47
1:A:7:ILE:HG23	1:A:7:ILE:O	2.15	0.47
1:A:208:ASN:HD22	1:A:208:ASN:N	2.09	0.47
1:A:208:ASN:CG	1:A:238:LYS:HE2	2.35	0.47
2:B:526:HIS:HD2	2:B:533:GLY:HA3	1.79	0.47
2:F:658:ASP:O	2:F:659:TYR:CD1	2.67	0.47
1:G:14:ASN:ND2	1:G:31:THR:HB	2.30	0.47
1:I:115:PHE:CD1	1:I:115:PHE:C	2.88	0.47
1:K:6:THR:OG1	2:L:639:GLU:HG2	2.14	0.47
1:K:119:GLU:HG3	1:K:256:TYR:CE2	2.50	0.47
1:A:180:TRP:HB3	1:A:254:PRO:HG3	1.97	0.47
1:C:7:ILE:O	1:C:7:ILE:HG23	2.14	0.47
1:K:189:LYS:HG3	5:K:3307:HOH:O	2.13	0.47
1:K:195:TYR:O	1:K:196:GLN:HB3	2.14	0.47
1:E:54:LEU:HD13	1:E:77:VAL:HG11	1.96	0.47
1:E:238:LYS:HZ2	1:E:238:LYS:N	2.06	0.47
1:K:208:ASN:OD1	1:K:238:LYS:HD3	2.14	0.47
1:C:135:VAL:HG22	1:C:146:SER:C	2.35	0.47
1:G:261:ARG:HD2	1:G:261:ARG:N	2.30	0.47
1:I:115:PHE:C	1:I:115:PHE:HD1	2.18	0.47
2:B:541:THR:O	2:B:545:ILE:HG13	2.15	0.46
1:G:11:TYR:HB2	1:G:321:LEU:HD11	1.96	0.46
1:G:164:LEU:HD12	1:G:164:LEU:C	2.35	0.46
2:F:527:GLN:O	2:F:527:GLN:CG	2.56	0.46
1:K:238:LYS:HZ2	1:K:238:LYS:N	2.07	0.46
1:K:310:VAL:CG1	1:K:312:SER:H	2.27	0.46
2:L:509:PHE:O	2:L:635:ASN:CB	2.62	0.46
1:G:180:TRP:HB3	1:G:254:PRO:HG3	1.96	0.46
2:H:501:GLY:HA3	5:H:672:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:519:ASP:HB2	2:H:536:ALA:CB	2.44	0.46
2:J:502:LEU:HG	2:L:503:PHE:CZ	2.49	0.46
1:A:327:ARG:HD2	1:A:327:ARG:C	2.36	0.46
2:F:508:GLY:C	2:F:510:ILE:H	2.18	0.46
2:H:607:THR:O	2:H:610:PHE:HB3	2.15	0.46
2:J:524:TYR:CE1	2:J:537:ASP:HB2	2.49	0.46
2:F:633:ILE:HD11	2:F:639:GLU:HB2	1.96	0.46
1:C:31:THR:C	1:C:32:HIS:ND1	2.69	0.46
1:G:217:ILE:N	1:G:217:ILE:HD12	2.31	0.46
1:I:68:ASN:HB3	1:I:71:CYS:SG	2.56	0.46
1:I:208:ASN:HD22	1:I:208:ASN:N	2.12	0.46
1:K:180:TRP:HB3	1:K:254:PRO:HG3	1.96	0.46
1:I:317:MET:HE2	2:J:600:VAL:HG22	1.98	0.46
1:C:208:ASN:OD1	1:C:238:LYS:HD3	2.15	0.46
2:D:521:TRP:NE1	5:D:701:HOH:O	2.30	0.46
1:E:93:ILE:HD11	1:E:99:PHE:HB2	1.97	0.46
1:G:130:HIS:HD2	5:G:3247:HOH:O	1.98	0.46
1:K:127:TRP:CZ3	1:K:166:ASN:ND2	2.83	0.46
1:A:135:VAL:CG1	1:A:136:THR:N	2.79	0.46
1:A:317:MET:HE3	2:B:555:VAL:HG11	1.98	0.46
1:K:190:GLU:O	1:K:193:ASN:ND2	2.49	0.46
1:K:217:ILE:HD12	1:K:217:ILE:N	2.31	0.46
1:A:44:GLY:HA2	1:A:286:LEU:O	2.15	0.46
1:E:72:ASP:HA	1:E:75:LEU:HG	1.98	0.46
2:F:645:ASP:O	2:F:649:MET:HG2	2.16	0.46
1:G:280:THR:HG21	1:G:288:ALA:HB1	1.97	0.46
2:B:598:LEU:O	2:B:602:LEU:HD13	2.16	0.45
1:E:6:THR:HG23	2:F:638:PHE:O	2.16	0.45
1:E:49(A):LYS:HE3	5:E:3466:HOH:O	2.16	0.45
1:E:208:ASN:HD22	1:E:208:ASN:N	2.11	0.45
2:H:625:GLN:NE2	2:H:656:THR:O	2.49	0.45
2:L:631:LYS:HB3	2:L:641:TYR:OH	2.15	0.45
1:A:294:PRO:HG2	1:A:295:TYR:CD1	2.52	0.45
1:E:245:PHE:CZ	1:E:254:PRO:HG2	2.51	0.45
2:F:642:HIS:CE1	2:F:644:CYS:HB3	2.51	0.45
1:I:78:ARG:O	1:I:114:SER:HB2	2.16	0.45
1:A:72:ASP:N	1:A:73:PRO:CD	2.79	0.45
1:E:9:ILE:N	1:E:9:ILE:HD12	2.31	0.45
2:F:654:ASN:HB3	4:F:3331:NAG:O1	2.16	0.45
1:G:317:MET:CE	2:H:552:VAL:HA	2.46	0.45
2:B:623:LYS:HG3	2:B:632:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:CYS:HB2	1:C:138:ALA:O	2.17	0.45
1:E:163:LYS:CE	1:E:201:TYR:OH	2.64	0.45
1:E:173:GLY:O	1:E:174:LYS:HG3	2.16	0.45
2:F:658:ASP:O	2:F:659:TYR:CB	2.64	0.45
1:G:100:ILE:N	1:G:100:ILE:HD12	2.32	0.45
2:H:626:LEU:O	2:H:627:LYS:C	2.54	0.45
1:I:261:ARG:N	1:I:261:ARG:CD	2.80	0.45
1:A:23:VAL:CG1	2:D:551:LYS:HG3	2.46	0.45
1:C:95:TYR:CD2	1:C:230:MET:HB2	2.51	0.45
2:D:633:ILE:C	2:D:635:ASN:H	2.20	0.45
1:G:280:THR:HG21	1:G:282:CYS:O	2.16	0.45
1:I:296:GLN:O	1:I:309:TYR:HA	2.15	0.45
2:J:526:HIS:HB2	2:J:649:MET:CE	2.47	0.45
2:J:658:ASP:O	2:J:659:TYR:CB	2.64	0.45
1:K:9:ILE:HD11	2:L:622:VAL:HG21	1.98	0.45
1:K:327:ARG:HB3	5:K:3416:HOH:O	2.17	0.45
2:L:633:ILE:HG22	2:L:634:GLY:N	2.31	0.45
1:A:23:VAL:HG22	2:B:602:LEU:HD12	1.99	0.45
2:F:519:ASP:HB2	2:F:536:ALA:HB2	1.99	0.45
2:L:525:HIS:CE1	2:L:532:SER:HB3	2.52	0.45
1:A:6:THR:HB	2:B:527:GLN:OE1	2.17	0.45
1:C:94:CYS:O	1:C:224:ARG:HD2	2.17	0.45
1:C:116:GLU:HG2	1:C:259:ALA:HB3	1.98	0.45
2:B:631:LYS:HG3	2:B:633:ILE:CD1	2.45	0.45
1:G:37:LEU:HB2	1:G:315:LEU:HB2	1.98	0.45
2:H:634:GLY:O	2:H:635:ASN:O	2.34	0.45
1:I:124:GLU:O	1:I:125:SER:HB3	2.17	0.45
2:L:526:HIS:O	2:L:532:SER:HA	2.17	0.45
1:E:7:ILE:HA	2:F:525:HIS:O	2.17	0.45
1:G:195:TYR:O	1:G:197:ASN:N	2.43	0.45
1:C:5:ASP:N	2:D:643:LYS:HZ3	2.15	0.45
1:C:187:ASN:ND2	1:C:189:LYS:HB2	2.32	0.45
1:C:195:TYR:O	1:C:196:GLN:HB3	2.17	0.45
1:C:261:ARG:N	1:C:261:ARG:CD	2.80	0.44
1:I:36:LEU:HD11	1:I:317:MET:HE3	1.99	0.44
1:K:208:ASN:CG	1:K:238:LYS:HE2	2.38	0.44
2:L:654:ASN:OD1	2:L:656:THR:HG23	2.17	0.44
1:A:53:PRO:HB3	1:A:82:TYR:CZ	2.51	0.44
1:A:261:ARG:N	1:A:261:ARG:CD	2.81	0.44
1:E:75:LEU:N	1:E:76:PRO:HD2	2.32	0.44
1:A:114:SER:OG	1:A:261:ARG:NH1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:561:ILE:HG13	2:B:563:PHE:CE1	2.53	0.44
1:E:36:LEU:HD11	1:E:317:MET:HE3	1.99	0.44
2:F:548:ILE:HD12	2:F:607:THR:HG23	1.99	0.44
2:H:633:ILE:C	2:H:635:ASN:H	2.21	0.44
2:D:633:ILE:CG2	2:D:634:GLY:H	2.30	0.44
2:J:522:TYR:CD1	2:J:540:SER:HB3	2.52	0.44
1:A:185:PRO:HG2	1:A:191:GLN:NE2	2.32	0.44
1:E:238:LYS:H	1:E:238:LYS:HE3	1.82	0.44
2:J:526:HIS:HB2	2:J:649:MET:HE2	1.99	0.44
2:B:572:LYS:HE2	5:B:680:HOH:O	2.18	0.44
2:D:625:GLN:C	2:D:627:LYS:H	2.21	0.44
2:F:525:HIS:HE1	2:F:532:SER:HB3	1.83	0.44
1:I:44:GLY:HA2	1:I:286:LEU:O	2.17	0.44
2:J:560:ASN:N	2:J:560:ASN:ND2	2.63	0.44
1:K:222:LYS:HA	1:K:226:GLN:O	2.18	0.44
2:L:501:GLY:HA3	5:L:691:HOH:O	2.16	0.44
1:I:7:ILE:HG23	1:I:7:ILE:O	2.16	0.44
2:J:633:ILE:HD11	2:J:639:GLU:HB2	1.99	0.44
1:K:81:SER:HG	1:K:82:TYR:HD2	1.63	0.44
1:K:327:ARG:C	1:K:327:ARG:HD2	2.38	0.44
1:E:187:ASN:ND2	1:E:190:GLU:H	2.16	0.44
1:I:217:ILE:HD12	1:I:217:ILE:N	2.33	0.44
2:J:562:GLN:CG	5:J:722:HOH:O	2.66	0.44
2:L:528:ASN:CG	2:L:644:CYS:O	2.56	0.44
2:L:633:ILE:CD1	2:L:639:GLU:HB2	2.47	0.44
1:G:7:ILE:HD13	2:H:652:VAL:HG11	2.00	0.44
1:G:208:ASN:HD22	1:G:208:ASN:N	2.10	0.44
2:H:633:ILE:O	2:H:635:ASN:N	2.50	0.44
1:A:37:LEU:HB2	1:A:315:LEU:HB2	1.99	0.43
1:C:324:ILE:HD11	2:D:507:ALA:HB2	2.00	0.43
1:E:281:LYS:HB2	1:E:281:LYS:HE3	1.85	0.43
1:K:308:LYS:HD2	2:L:559:MET:HE1	2.00	0.43
1:A:85:GLU:O	1:A:270:THR:HA	2.19	0.43
2:F:526:HIS:HB2	2:F:649:MET:CE	2.48	0.43
1:K:261:ARG:N	1:K:261:ARG:CD	2.81	0.43
2:L:526:HIS:HB2	2:L:649:MET:HE2	2.00	0.43
1:A:100:ILE:HD12	1:A:100:ILE:N	2.33	0.43
2:J:649:MET:O	2:J:653:ARG:HG3	2.19	0.43
1:K:218:ALA:O	1:K:220:ARG:HG3	2.19	0.43
1:C:165:LYS:HA	1:C:245:PHE:O	2.18	0.43
2:F:561:ILE:HG23	2:F:563:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:ASN:ND2	1:I:42:ASN:C	2.70	0.43
2:B:514:TRP:HE3	2:B:517:MET:HG3	1.84	0.43
2:B:529:GLU:C	2:B:531:GLY:H	2.22	0.43
1:E:272:ASN:HD21	4:E:3311:NAG:H1	1.79	0.43
1:G:42:ASN:HD22	1:G:45:LYS:H	1.63	0.43
1:G:135:VAL:HG22	1:G:146:SER:HA	2.00	0.43
2:H:646:ASN:HD22	2:H:646:ASN:HA	1.59	0.43
1:K:20:VAL:HG21	1:K:318:VAL:HB	2.00	0.43
2:L:530:GLN:HE22	2:L:646:ASN:H	1.66	0.43
2:B:517:MET:HE1	2:B:536:ALA:N	2.32	0.43
1:I:187:ASN:HD22	1:I:190:GLU:H	1.66	0.43
1:K:96:PRO:HG3	1:K:226:GLN:HB2	2.01	0.43
1:K:185:PRO:HG2	1:K:191:GLN:HE21	1.84	0.43
1:K:193:ASN:HD22	1:K:193:ASN:C	2.22	0.43
1:K:208:ASN:HD22	1:K:208:ASN:H	1.65	0.43
2:B:554:SER:O	2:B:558:LYS:HG2	2.18	0.43
1:C:194:LEU:HD21	3:N:3:SIA:C11	2.48	0.43
2:F:517:MET:CE	2:F:523:GLY:HA3	2.48	0.43
1:I:42:ASN:HD22	1:I:45:LYS:H	1.65	0.43
2:B:642:HIS:O	2:B:643:LYS:O	2.37	0.43
1:I:53:PRO:HB3	1:I:82:TYR:CE2	2.53	0.43
1:A:78:ARG:O	1:A:114:SER:HB2	2.19	0.43
1:G:30:VAL:HG11	1:G:318:VAL:HG21	2.01	0.43
1:G:280:THR:HG22	1:G:281:LYS:H	1.83	0.43
1:I:8:CYS:O	2:J:524:TYR:HA	2.19	0.43
1:I:9:ILE:HG12	2:J:619:TYR:HD1	1.84	0.43
1:I:72:ASP:HA	1:I:75:LEU:HG	2.01	0.43
1:I:132:THR:HG22	1:I:154:LEU:CD2	2.48	0.43
1:K:185:PRO:HG2	1:K:191:GLN:NE2	2.34	0.43
1:A:308:LYS:HD2	2:B:559:MET:HE1	2.01	0.43
2:B:519:ASP:HB2	2:B:536:ALA:HB2	2.01	0.43
1:G:130:HIS:CE1	1:G:162:PRO:HD2	2.54	0.43
2:B:519:ASP:HB2	2:B:536:ALA:HB3	1.99	0.42
2:F:525:HIS:CE1	2:F:532:SER:HB3	2.54	0.42
2:F:658:ASP:OD1	2:F:658:ASP:C	2.57	0.42
1:G:208:ASN:ND2	1:G:208:ASN:H	2.17	0.42
1:K:8:CYS:O	2:L:524:TYR:HA	2.19	0.42
2:L:528:ASN:ND2	2:L:644:CYS:O	2.52	0.42
1:A:321:LEU:N	1:A:321:LEU:HD23	2.33	0.42
1:C:9:ILE:N	2:D:636:GLY:O	2.46	0.42
1:C:321:LEU:HD23	1:C:321:LEU:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:253:ALA:HA	1:K:254:PRO:HD3	1.88	0.42
1:C:54:LEU:HD13	1:C:77:VAL:HG11	2.00	0.42
1:C:219:GLU:OE1	1:E:165:LYS:HE2	2.19	0.42
1:C:324:ILE:CD1	2:D:507:ALA:HB2	2.49	0.42
1:E:96:PRO:HG3	1:E:226:GLN:HB2	2.00	0.42
1:K:115:PHE:HD1	1:K:115:PHE:O	2.02	0.42
2:L:525:HIS:HE1	2:L:532:SER:HB3	1.84	0.42
2:B:526:HIS:HD2	2:B:533:GLY:CA	2.33	0.42
2:B:650:GLU:CB	2:B:653:ARG:HH12	2.32	0.42
1:C:123:LYS:HG3	1:C:152:LEU:HD11	2.01	0.42
2:J:509:PHE:CD1	2:J:510:ILE:HG13	2.55	0.42
2:L:530:GLN:NE2	2:L:646:ASN:H	2.16	0.42
1:A:6:THR:OG1	2:B:639:GLU:HG2	2.20	0.42
1:C:189:LYS:H	1:C:189:LYS:HG3	1.54	0.42
1:E:53:PRO:HB3	1:E:82:TYR:CE2	2.54	0.42
2:F:654:ASN:ND2	4:F:3331:NAG:O5	2.52	0.42
1:I:195:TYR:O	1:I:196:GLN:HB3	2.20	0.42
2:J:656:THR:O	2:J:657:TYR:O	2.38	0.42
1:A:152:LEU:HD12	5:A:3474:HOH:O	2.20	0.42
1:A:174:LYS:CE	1:A:261:ARG:HG3	2.50	0.42
1:A:200:ALA:HA	1:A:248:ASN:OD1	2.19	0.42
1:C:161:TYR:CZ	1:C:249:GLY:HA2	2.54	0.42
1:E:208:ASN:OD1	1:E:238:LYS:HE2	2.20	0.42
4:F:3331:NAG:O1	4:F:3331:NAG:C7	2.67	0.42
2:J:560:ASN:N	2:J:560:ASN:HD22	2.16	0.42
2:J:633:ILE:CG2	2:J:634:GLY:N	2.69	0.42
2:L:633:ILE:N	2:L:633:ILE:CD1	2.78	0.42
1:A:12:HIS:HB2	2:B:520:GLY:O	2.20	0.42
2:B:525:HIS:NE2	2:B:532:SER:HB3	2.35	0.42
1:E:195:TYR:O	1:E:197:ASN:N	2.47	0.42
2:L:502:LEU:HB2	2:L:609:ASP:OD1	2.20	0.42
2:L:630:ALA:HB2	2:L:640:PHE:HA	2.02	0.42
1:G:23:VAL:CG1	2:J:551:LYS:HG3	2.50	0.42
1:G:280:THR:CG2	1:G:281:LYS:N	2.82	0.42
2:H:588:PHE:CZ	2:L:587:GLY:HA3	2.55	0.42
2:H:658:ASP:C	2:H:659:TYR:HD2	2.23	0.42
2:L:519:ASP:HB2	2:L:536:ALA:HB2	2.01	0.42
2:B:658:ASP:C	2:B:659:TYR:CD2	2.93	0.42
1:C:217:ILE:N	1:C:217:ILE:CD1	2.83	0.42
1:E:324:ILE:HD11	2:F:507:ALA:HB2	2.01	0.42
1:A:54:LEU:HD13	1:A:77:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3385:HOH:O	2:F:566:VAL:HG13	2.19	0.41
1:K:75:LEU:N	1:K:76:PRO:HD2	2.35	0.41
1:K:100:ILE:N	1:K:100:ILE:CD1	2.83	0.41
2:B:587:GLY:HA3	2:D:588:PHE:CZ	2.55	0.41
2:D:642:HIS:O	2:D:643:LYS:HB2	2.21	0.41
1:E:208:ASN:CG	1:E:238:LYS:HE2	2.39	0.41
1:E:280:THR:HG21	1:E:282:CYS:O	2.20	0.41
1:G:6:THR:HG22	1:G:7:ILE:N	2.34	0.41
1:I:260:LEU:C	1:I:261:ARG:HD2	2.40	0.41
1:A:78:ARG:NH2	1:A:261:ARG:NH2	2.68	0.41
1:C:119:GLU:HG3	1:C:256:TYR:CE2	2.55	0.41
2:H:643:LYS:HD3	5:H:696:HOH:O	2.20	0.41
1:K:126:SER:C	1:K:128:PRO:HD3	2.41	0.41
1:A:8:CYS:HA	2:B:636:GLY:O	2.21	0.41
1:A:20:VAL:HG21	1:A:318:VAL:HB	2.02	0.41
1:C:8:CYS:HA	2:D:637:CYS:HA	2.01	0.41
1:C:75:LEU:N	1:C:76:PRO:HD2	2.35	0.41
2:D:633:ILE:O	2:D:635:ASN:N	2.48	0.41
1:E:115:PHE:HD1	1:E:115:PHE:O	2.03	0.41
2:F:650:GLU:O	2:F:654:ASN:ND2	2.54	0.41
1:G:94:CYS:HB2	1:G:138:ALA:O	2.20	0.41
2:H:654:ASN:OD1	2:H:656:THR:HG23	2.20	0.41
1:K:306:CYS:O	2:L:562:GLN:HB3	2.21	0.41
1:C:11:TYR:HB2	1:C:321:LEU:HD11	2.02	0.41
1:C:37:LEU:HB2	1:C:315:LEU:HB2	2.01	0.41
1:E:208:ASN:OD1	1:E:238:LYS:HD3	2.19	0.41
1:E:280:THR:CG2	1:E:281:LYS:N	2.81	0.41
1:E:303:ILE:HD13	2:F:564:THR:HG23	2.03	0.41
1:G:41:HIS:HB3	1:G:298:ILE:HD13	2.02	0.41
1:G:238:LYS:NZ	1:G:241:ASP:OD1	2.51	0.41
1:I:107:GLU:O	1:I:110:SER:HB2	2.20	0.41
1:I:164:LEU:HD12	1:I:164:LEU:C	2.40	0.41
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.94	0.41
1:C:192:GLN:O	1:C:196:GLN:HA	2.20	0.41
1:E:8:CYS:O	2:F:524:TYR:HA	2.21	0.41
2:F:633:ILE:HG22	2:F:634:GLY:H	1.85	0.41
2:H:642:HIS:O	2:H:643:LYS:HB2	2.21	0.41
1:K:94:CYS:HB2	1:K:138:ALA:O	2.21	0.41
2:L:528:ASN:O	2:L:529:GLU:C	2.59	0.41
2:D:587:GLY:HA3	2:F:588:PHE:CZ	2.56	0.41
1:E:185:PRO:HA	1:E:190:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:620:GLU:HB2	5:F:3363:HOH:O	2.21	0.41
1:A:135:VAL:HG12	1:A:145:SER:HB3	2.02	0.41
2:B:525:HIS:CE1	2:B:533:GLY:H	2.39	0.41
2:D:642:HIS:O	2:D:643:LYS:O	2.39	0.41
1:E:6:THR:HA	2:F:638:PHE:O	2.21	0.41
1:E:95:TYR:HD2	1:E:230:MET:HB2	1.85	0.41
2:F:658:ASP:O	2:F:659:TYR:HB2	2.21	0.41
1:G:208:ASN:HD21	1:G:238:LYS:HZ1	1.69	0.41
1:G:303:ILE:HD13	2:H:564:THR:HG23	2.02	0.41
1:G:327:ARG:C	1:G:327:ARG:HD2	2.42	0.41
2:H:526:HIS:HB2	2:H:649:MET:HE3	2.01	0.41
1:I:303:ILE:HD13	2:J:564:THR:HG23	2.03	0.41
2:J:524:TYR:CD1	2:J:524:TYR:N	2.89	0.41
2:J:568:LYS:HG2	5:J:662:HOH:O	2.20	0.41
1:K:23:VAL:CG2	2:L:602:LEU:HD12	2.50	0.41
1:K:33:SER:OG	1:K:316:ARG:HD3	2.21	0.41
1:A:208:ASN:ND2	1:A:208:ASN:H	2.18	0.41
1:E:126:SER:O	1:E:128:PRO:HD3	2.21	0.41
1:E:272:ASN:ND2	4:E:3311:NAG:N2	2.69	0.41
2:F:554:SER:O	2:F:558:LYS:HG2	2.21	0.41
1:C:53:PRO:HB3	1:C:82:TYR:CE2	2.56	0.40
1:E:12:HIS:HB2	2:F:521:TRP:HA	2.03	0.40
1:E:272:ASN:CG	4:E:3311:NAG:H1	2.41	0.40
2:F:517:MET:CE	2:F:536:ALA:HA	2.52	0.40
2:F:656:THR:O	2:F:657:TYR:O	2.39	0.40
1:G:35:ASN:ND2	5:G:3449:HOH:O	2.55	0.40
1:I:8:CYS:HA	2:J:637:CYS:HA	2.03	0.40
1:K:42:ASN:O	1:K:287:GLY:HA3	2.21	0.40
1:K:317:MET:HE2	2:L:600:VAL:HG22	2.03	0.40
1:C:5:ASP:N	5:C:3378:HOH:O	2.53	0.40
2:F:560:ASN:ND2	2:F:560:ASN:N	2.67	0.40
2:F:633:ILE:CD1	2:F:639:GLU:N	2.82	0.40
1:G:9:ILE:O	2:H:510:ILE:HD12	2.21	0.40
2:J:633:ILE:HD12	2:J:633:ILE:H	1.86	0.40
1:K:280:THR:HG23	5:K:3375:HOH:O	2.22	0.40
1:K:280:THR:CG2	1:K:281:LYS:N	2.82	0.40
1:A:8:CYS:O	2:B:524:TYR:HA	2.21	0.40
1:A:36:LEU:HD11	1:A:317:MET:HE3	2.02	0.40
1:A:253:ALA:HA	1:A:254:PRO:HD3	1.90	0.40
2:D:528:ASN:HD21	2:D:649:MET:HG3	1.87	0.40
2:D:554:SER:O	2:D:558:LYS:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:ILE:HG23	1:E:7:ILE:O	2.20	0.40
1:E:44:GLY:O	1:E:45:LYS:HB2	2.20	0.40
2:F:524:TYR:CD1	2:F:524:TYR:N	2.89	0.40
1:G:23:VAL:HG12	2:J:551:LYS:HG3	2.02	0.40
1:A:8:CYS:HA	2:B:637:CYS:HA	2.04	0.40
1:A:245:PHE:CZ	1:A:254:PRO:HG2	2.55	0.40
2:B:631:LYS:O	2:B:638:PHE:HA	2.21	0.40
2:F:634:GLY:O	2:F:635:ASN:O	2.40	0.40
1:I:42:ASN:HD22	1:I:44:GLY:N	2.20	0.40
1:A:187:ASN:HD22	1:A:190:GLU:H	1.67	0.40
2:B:548:ILE:HD12	2:B:607:THR:HG23	2.04	0.40
2:D:634:GLY:O	2:D:635:ASN:O	2.39	0.40
1:E:310:VAL:HG13	2:F:593:THR:HA	2.04	0.40
1:G:14:ASN:HD21	1:G:31:THR:HB	1.85	0.40
1:I:253:ALA:HA	1:I:254:PRO:HD3	1.91	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:3421:HOH:O	5:K:3421:HOH:O[2_555]	2.14	0.06
1:G:276:HIS:ND1	5:A:3354:HOH:O[2_555]	2.15	0.05

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	321/327 (98%)	310 (97%)	9 (3%)	2 (1%)	25 25
1	C	321/327 (98%)	311 (97%)	10 (3%)	0	100 100
1	E	319/327 (98%)	308 (97%)	9 (3%)	2 (1%)	25 25
1	G	321/327 (98%)	309 (96%)	10 (3%)	2 (1%)	25 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	321/327 (98%)	312 (97%)	7 (2%)	2 (1%)	25	25
1	K	321/327 (98%)	307 (96%)	13 (4%)	1 (0%)	41	46
2	B	158/160 (99%)	137 (87%)	17 (11%)	4 (2%)	5	3
2	D	158/160 (99%)	138 (87%)	13 (8%)	7 (4%)	2	0
2	F	158/160 (99%)	139 (88%)	10 (6%)	9 (6%)	1	0
2	H	158/160 (99%)	136 (86%)	16 (10%)	6 (4%)	3	1
2	J	158/160 (99%)	139 (88%)	10 (6%)	9 (6%)	1	0
2	L	158/160 (99%)	141 (89%)	11 (7%)	6 (4%)	3	1
All	All	2872/2922 (98%)	2687 (94%)	135 (5%)	50 (2%)	9	4

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	627	LYS
2	D	635	ASN
2	D	645	ASP
2	F	635	ASN
2	F	645	ASP
2	F	659	TYR
1	G	123	LYS
2	H	627	LYS
2	H	645	ASP
1	I	125	SER
2	J	643	LYS
2	J	659	TYR
1	K	125	SER
1	A	44	GLY
1	A	91	ASN
2	B	635	ASN
2	B	643	LYS
1	E	125	SER
2	F	633	ILE
2	F	643	LYS
1	G	125	SER
2	H	635	ASN
2	J	633	ILE
2	J	635	ASN
2	J	645	ASP
2	D	643	LYS

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Mol	Chain	Res	Type
1	E	45	LYS
2	F	560	ASN
2	F	657	TYR
2	H	643	LYS
1	I	91	ASN
2	J	657	TYR
2	L	635	ASN
2	L	643	LYS
2	L	657	TYR
2	B	627	LYS
2	B	656	THR
2	D	633	ILE
2	F	656	THR
2	J	505	ALA
2	J	530	GLN
2	L	529	GLU
2	D	634	GLY
2	F	634	GLY
2	H	634	GLY
2	H	633	ILE
2	D	561	ILE
2	J	634	GLY
2	L	633	ILE
2	L	518	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	285/287 (99%)	273 (96%)	12 (4%)	30	34
1	C	285/287 (99%)	273 (96%)	12 (4%)	30	34
1	E	285/287 (99%)	274 (96%)	11 (4%)	32	38
1	G	285/287 (99%)	271 (95%)	14 (5%)	25	27
1	I	285/287 (99%)	276 (97%)	9 (3%)	39	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	285/287 (99%)	273 (96%)	12 (4%)	30	34
2	B	136/136 (100%)	129 (95%)	7 (5%)	24	25
2	D	136/136 (100%)	128 (94%)	8 (6%)	19	19
2	F	136/136 (100%)	131 (96%)	5 (4%)	34	40
2	H	136/136 (100%)	129 (95%)	7 (5%)	24	25
2	J	136/136 (100%)	131 (96%)	5 (4%)	34	40
2	L	136/136 (100%)	130 (96%)	6 (4%)	28	32
All	All	2526/2538 (100%)	2418 (96%)	108 (4%)	29	33

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	46	LEU
1	A	58	LYS
1	A	99	PHE
1	A	115	PHE
1	A	156	GLU
1	A	187	ASN
1	A	208	ASN
1	A	238	LYS
1	A	261	ARG
1	A	310	VAL
1	A	321	LEU
2	B	517	MET
2	B	522	TYR
2	B	524	TYR
2	B	580	LEU
2	B	598	LEU
2	B	644	CYS
2	B	646	ASN
1	C	42	ASN
1	C	58	LYS
1	C	99	PHE
1	C	115	PHE
1	C	135	VAL
1	C	156	GLU
1	C	187	ASN
1	C	193	ASN
1	C	208	ASN

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Mol	Chain	Res	Type
1	C	238	LYS
1	C	261	ARG
1	C	321	LEU
2	D	524	TYR
2	D	560	ASN
2	D	561	ILE
2	D	580	LEU
2	D	598	LEU
2	D	644	CYS
2	D	645	ASP
2	D	648	CYS
1	E	58	LYS
1	E	99	PHE
1	E	115	PHE
1	E	156	GLU
1	E	166	ASN
1	E	187	ASN
1	E	208	ASN
1	E	235	THR
1	E	238	LYS
1	E	261	ARG
1	E	321	LEU
2	F	524	TYR
2	F	560	ASN
2	F	562	GLN
2	F	580	LEU
2	F	644	CYS
1	G	42	ASN
1	G	49	LEU
1	G	58	LYS
1	G	94	CYS
1	G	99	PHE
1	G	115	PHE
1	G	135	VAL
1	G	156	GLU
1	G	178	VAL
1	G	187	ASN
1	G	208	ASN
1	G	238	LYS
1	G	261	ARG
1	G	321	LEU
2	H	517	MET

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Mol	Chain	Res	Type
2	H	524	TYR
2	H	560	ASN
2	H	580	LEU
2	H	598	LEU
2	H	645	ASP
2	H	646	ASN
1	I	42	ASN
1	I	58	LYS
1	I	99	PHE
1	I	115	PHE
1	I	156	GLU
1	I	187	ASN
1	I	208	ASN
1	I	261	ARG
1	I	321	LEU
2	J	524	TYR
2	J	560	ASN
2	J	580	LEU
2	J	644	CYS
2	J	646	ASN
1	K	35	ASN
1	K	58	LYS
1	K	99	PHE
1	K	115	PHE
1	K	135	VAL
1	K	156	GLU
1	K	187	ASN
1	K	193	ASN
1	K	208	ASN
1	K	238	LYS
1	K	261	ARG
1	K	321	LEU
2	L	522	TYR
2	L	524	TYR
2	L	580	LEU
2	L	598	LEU
2	L	644	CYS
2	L	659	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	35	ASN
1	A	55	GLN
1	A	130	HIS
1	A	187	ASN
1	A	191	GLN
1	A	208	ASN
1	A	250	ASN
1	A	276	HIS
2	B	526	HIS
2	B	530	GLN
2	B	625	GLN
2	B	629	ASN
2	B	635	ASN
2	B	646	ASN
1	C	35	ASN
1	C	55	GLN
1	C	91	ASN
1	C	130	HIS
1	C	187	ASN
1	C	191	GLN
1	C	193	ASN
1	C	208	ASN
1	C	250	ASN
2	D	528	ASN
2	D	530	GLN
2	D	560	ASN
2	D	625	GLN
2	D	635	ASN
2	D	646	ASN
1	E	35	ASN
1	E	42	ASN
1	E	55	GLN
1	E	91	ASN
1	E	130	HIS
1	E	187	ASN
1	E	191	GLN
1	E	208	ASN
1	E	250	ASN
1	E	272	ASN
1	E	276	HIS
2	F	525	HIS
2	F	528	ASN

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Mol	Chain	Res	Type
2	F	530	GLN
2	F	560	ASN
2	F	614	ASN
2	F	629	ASN
2	F	635	ASN
2	F	646	ASN
2	F	654	ASN
1	G	35	ASN
1	G	42	ASN
1	G	55	GLN
1	G	91	ASN
1	G	130	HIS
1	G	187	ASN
1	G	191	GLN
1	G	197	ASN
1	G	208	ASN
1	G	250	ASN
1	G	276	HIS
2	H	525	HIS
2	H	530	GLN
2	H	560	ASN
2	H	625	GLN
2	H	635	ASN
2	H	646	ASN
1	I	35	ASN
1	I	42	ASN
1	I	55	GLN
1	I	91	ASN
1	I	130	HIS
1	I	187	ASN
1	I	191	GLN
1	I	208	ASN
1	I	250	ASN
2	J	525	HIS
2	J	528	ASN
2	J	530	GLN
2	J	560	ASN
2	J	625	GLN
2	J	629	ASN
2	J	635	ASN
2	J	646	ASN
1	K	35	ASN

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Mol	Chain	Res	Type
1	K	55	GLN
1	K	130	HIS
1	K	187	ASN
1	K	191	GLN
1	K	193	ASN
1	K	208	ASN
1	K	250	ASN
1	K	276	HIS
2	L	528	ASN
2	L	530	GLN
2	L	542	GLN
2	L	546	ASN
2	L	625	GLN
2	L	635	ASN
2	L	646	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

18 monosaccharides 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
3	NAG	M	1	3	14,14,15	2.05	5 (35%)	17,19,21	0.72	0
3	GAL	M	2	3	11,11,12	2.33	4 (36%)	15,15,17	1.20	1 (6%)
3	SIA	M	3	3	20,20,21	3.89	9 (45%)	24,28,31	3.13	9 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	N	1	3	14,14,15	2.10	5 (35%)	17,19,21	0.85	0
3	GAL	N	2	3	11,11,12	2.27	5 (45%)	15,15,17	1.01	1 (6%)
3	SIA	N	3	3	20,20,21	3.96	9 (45%)	24,28,31	3.16	6 (25%)
3	NAG	O	1	3	14,14,15	1.87	4 (28%)	17,19,21	1.09	1 (5%)
3	GAL	O	2	3	11,11,12	2.79	4 (36%)	15,15,17	1.62	3 (20%)
3	SIA	O	3	3	20,20,21	4.12	8 (40%)	24,28,31	3.11	6 (25%)
3	NAG	P	1	3	14,14,15	2.31	7 (50%)	17,19,21	1.14	1 (5%)
3	GAL	P	2	3	11,11,12	2.45	4 (36%)	15,15,17	1.62	3 (20%)
3	SIA	P	3	3	20,20,21	4.03	7 (35%)	24,28,31	3.15	6 (25%)
3	NAG	Q	1	3	14,14,15	2.09	5 (35%)	17,19,21	0.82	0
3	GAL	Q	2	3	11,11,12	2.19	4 (36%)	15,15,17	0.96	0
3	SIA	Q	3	3	20,20,21	3.93	9 (45%)	24,28,31	3.19	8 (33%)
3	NAG	R	1	3	14,14,15	2.13	6 (42%)	17,19,21	0.86	0
3	GAL	R	2	3	11,11,12	2.26	5 (45%)	15,15,17	1.00	1 (6%)
3	SIA	R	3	3	20,20,21	3.90	8 (40%)	24,28,31	3.13	6 (25%)

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
3	NAG	M	1	3	-	0/6/23/26	0/1/1/1
3	GAL	M	2	3	-	0/2/19/22	0/1/1/1
3	SIA	M	3	3	-	3/18/34/38	0/1/1/1
3	NAG	N	1	3	-	0/6/23/26	0/1/1/1
3	GAL	N	2	3	-	0/2/19/22	0/1/1/1
3	SIA	N	3	3	-	3/18/34/38	0/1/1/1
3	NAG	O	1	3	-	0/6/23/26	0/1/1/1
3	GAL	O	2	3	-	0/2/19/22	0/1/1/1
3	SIA	O	3	3	-	4/18/34/38	0/1/1/1
3	NAG	P	1	3	-	0/6/23/26	0/1/1/1
3	GAL	P	2	3	-	0/2/19/22	0/1/1/1
3	SIA	P	3	3	-	4/18/34/38	0/1/1/1
3	NAG	Q	1	3	-	0/6/23/26	0/1/1/1
3	GAL	Q	2	3	-	0/2/19/22	0/1/1/1
3	SIA	Q	3	3	-	3/18/34/38	0/1/1/1
3	NAG	R	1	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	R	2	3	-	0/2/19/22	0/1/1/1
3	SIA	R	3	3	-	3/18/34/38	0/1/1/1

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	3	SIA	C2-C1	12.62	1.63	1.52
3	P	3	SIA	C2-C1	12.11	1.63	1.52
3	N	3	SIA	C2-C1	11.58	1.62	1.52
3	M	3	SIA	C2-C1	11.38	1.62	1.52
3	Q	3	SIA	C2-C1	11.24	1.62	1.52
3	R	3	SIA	C2-C1	10.95	1.62	1.52
3	M	3	SIA	O4-C4	-8.11	1.26	1.43
3	Q	3	SIA	O4-C4	-8.09	1.26	1.43
3	R	3	SIA	O4-C4	-8.05	1.26	1.43
3	N	3	SIA	O4-C4	-7.94	1.26	1.43
3	O	3	SIA	O4-C4	-7.87	1.26	1.43
3	P	3	SIA	O4-C4	-7.86	1.26	1.43
3	O	2	GAL	O5-C5	6.37	1.56	1.43
3	R	3	SIA	C4-C5	6.31	1.58	1.53
3	N	3	SIA	C4-C5	6.30	1.58	1.53
3	Q	3	SIA	C4-C5	6.24	1.58	1.53
3	P	3	SIA	C4-C5	6.17	1.58	1.53
3	O	3	SIA	C4-C5	6.07	1.58	1.53
3	P	2	GAL	O5-C5	5.94	1.55	1.43
3	M	3	SIA	C4-C5	5.90	1.58	1.53
3	O	2	GAL	O5-C1	5.13	1.51	1.43
3	P	1	NAG	C4-C5	4.92	1.63	1.53
3	Q	3	SIA	C6-C5	4.86	1.61	1.53
3	O	3	SIA	C6-C5	4.79	1.60	1.53
3	N	3	SIA	C6-C5	4.78	1.60	1.53
3	M	2	GAL	O5-C5	4.72	1.53	1.43
3	M	3	SIA	C6-C5	4.71	1.60	1.53
3	R	3	SIA	C6-C5	4.67	1.60	1.53
3	N	2	GAL	O5-C5	4.66	1.52	1.43
3	P	3	SIA	C6-C5	4.53	1.60	1.53
3	Q	2	GAL	O5-C5	4.51	1.52	1.43
3	R	2	GAL	O5-C5	4.50	1.52	1.43
3	N	1	NAG	C4-C5	4.32	1.62	1.53
3	P	1	NAG	O4-C4	4.29	1.53	1.43
3	R	1	NAG	C4-C5	4.20	1.61	1.53
3	P	3	SIA	C3-C2	-4.13	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	2	GAL	O5-C1	4.13	1.50	1.43
3	P	3	SIA	O6-C6	-4.11	1.37	1.44
3	O	1	NAG	O4-C4	4.10	1.52	1.43
3	Q	1	NAG	C4-C5	4.02	1.61	1.53
3	M	3	SIA	C3-C4	3.96	1.59	1.52
3	O	3	SIA	C3-C2	-3.92	1.45	1.52
3	N	3	SIA	C3-C4	3.86	1.59	1.52
3	Q	1	NAG	O4-C4	3.84	1.52	1.43
3	R	3	SIA	C3-C4	3.80	1.59	1.52
3	R	1	NAG	O4-C4	3.77	1.51	1.43
3	P	2	GAL	O5-C1	3.76	1.49	1.43
3	M	1	NAG	C4-C5	3.74	1.60	1.53
3	Q	3	SIA	O6-C6	-3.73	1.38	1.44
3	Q	3	SIA	C3-C4	3.72	1.59	1.52
3	N	1	NAG	O4-C4	3.72	1.51	1.43
3	N	3	SIA	O6-C6	-3.67	1.38	1.44
3	R	3	SIA	C3-C2	-3.63	1.46	1.52
3	O	3	SIA	O6-C6	-3.63	1.38	1.44
3	R	3	SIA	O6-C6	-3.60	1.38	1.44
3	N	2	GAL	O5-C1	3.57	1.49	1.43
3	R	2	GAL	O5-C1	3.57	1.49	1.43
3	Q	3	SIA	C3-C2	-3.54	1.46	1.52
3	O	3	SIA	C3-C4	3.50	1.58	1.52
3	N	3	SIA	C3-C2	-3.49	1.46	1.52
3	M	1	NAG	O4-C4	3.47	1.51	1.43
3	P	3	SIA	C3-C4	3.45	1.58	1.52
3	O	1	NAG	C4-C5	3.38	1.60	1.53
3	Q	2	GAL	O5-C1	3.37	1.49	1.43
3	M	3	SIA	C3-C2	-3.17	1.47	1.52
3	M	2	GAL	C2-C3	3.13	1.57	1.52
3	M	3	SIA	O6-C2	3.00	1.47	1.43
3	R	2	GAL	C1-C2	2.94	1.58	1.52
3	O	3	SIA	O6-C2	2.89	1.47	1.43
3	R	3	SIA	O6-C2	2.88	1.47	1.43
3	M	1	NAG	O5-C5	2.87	1.49	1.43
3	M	1	NAG	C1-C2	2.85	1.56	1.52
3	R	2	GAL	C2-C3	2.82	1.56	1.52
3	N	2	GAL	C1-C2	2.79	1.58	1.52
3	O	2	GAL	C2-C3	2.76	1.56	1.52
3	O	2	GAL	C1-C2	2.75	1.58	1.52
3	Q	2	GAL	C2-C3	2.74	1.56	1.52
3	N	2	GAL	C2-C3	2.73	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1	NAG	O5-C1	2.71	1.48	1.43
3	N	1	NAG	O5-C5	2.70	1.48	1.43
3	Q	1	NAG	O5-C5	2.69	1.48	1.43
3	R	1	NAG	O5-C5	2.69	1.48	1.43
3	Q	2	GAL	C1-C2	2.67	1.58	1.52
3	M	3	SIA	O6-C6	-2.61	1.39	1.44
3	Q	3	SIA	O6-C2	2.57	1.47	1.43
3	P	1	NAG	O5-C5	2.51	1.48	1.43
3	R	1	NAG	O5-C1	2.45	1.47	1.43
3	N	1	NAG	O5-C1	2.45	1.47	1.43
3	R	1	NAG	C3-C2	2.43	1.57	1.52
3	Q	1	NAG	O5-C1	2.41	1.47	1.43
3	P	1	NAG	C3-C2	2.39	1.57	1.52
3	P	2	GAL	C2-C3	2.36	1.56	1.52
3	O	1	NAG	C3-C2	2.34	1.57	1.52
3	P	1	NAG	O5-C1	2.33	1.47	1.43
3	Q	1	NAG	C3-C2	2.29	1.57	1.52
3	M	2	GAL	C1-C2	2.29	1.57	1.52
3	N	1	NAG	C3-C2	2.23	1.57	1.52
3	P	2	GAL	C1-C2	2.16	1.57	1.52
3	M	3	SIA	O1B-C1	-2.10	1.23	1.30
3	N	3	SIA	O6-C2	2.08	1.46	1.43
3	O	1	NAG	C1-C2	2.07	1.55	1.52
3	R	1	NAG	C1-C2	2.06	1.55	1.52
3	P	1	NAG	C4-C3	2.05	1.57	1.52
3	Q	3	SIA	O1B-C1	-2.05	1.23	1.30
3	N	3	SIA	O1B-C1	-2.04	1.23	1.30
3	P	1	NAG	C1-C2	2.03	1.55	1.52
3	N	2	GAL	C4-C5	2.02	1.57	1.53
3	R	2	GAL	C4-C5	2.01	1.57	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	3	SIA	C6-O6-C2	12.59	138.26	111.34
3	N	3	SIA	C6-O6-C2	12.47	138.00	111.34
3	P	3	SIA	C6-O6-C2	12.37	137.81	111.34
3	R	3	SIA	C6-O6-C2	12.37	137.81	111.34
3	O	3	SIA	C6-O6-C2	12.31	137.68	111.34
3	M	3	SIA	C6-O6-C2	12.13	137.28	111.34
3	M	3	SIA	O6-C2-C3	-4.45	104.33	110.46
3	N	3	SIA	O1B-C1-C2	4.33	125.39	113.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	3	SIA	O1B-C1-C2	4.27	125.21	113.03
3	P	3	SIA	O1B-C1-C2	4.21	125.06	113.03
3	O	3	SIA	O1B-C1-C2	4.20	125.03	113.03
3	R	3	SIA	O1B-C1-C2	4.20	125.01	113.03
3	M	3	SIA	O1B-C1-C2	4.06	124.61	113.03
3	P	3	SIA	O6-C2-C3	-3.89	105.11	110.46
3	Q	3	SIA	O6-C2-C3	-3.81	105.21	110.46
3	Q	3	SIA	O1A-C1-C2	-3.78	113.63	122.57
3	R	3	SIA	O1A-C1-C2	-3.73	113.77	122.57
3	N	3	SIA	O1A-C1-C2	-3.70	113.84	122.57
3	O	2	GAL	O5-C5-C6	3.64	112.91	107.20
3	R	3	SIA	O6-C2-C3	-3.62	105.48	110.46
3	N	3	SIA	O6-C2-C3	-3.60	105.51	110.46
3	O	3	SIA	O6-C2-C3	-3.59	105.52	110.46
3	P	2	GAL	O5-C5-C6	3.56	112.78	107.20
3	P	3	SIA	O1A-C1-C2	-3.53	114.22	122.57
3	O	3	SIA	O1A-C1-C2	-3.48	114.34	122.57
3	M	3	SIA	O1A-C1-C2	-3.37	114.62	122.57
3	M	3	SIA	C11-C10-N5	3.27	121.64	116.10
3	O	2	GAL	O5-C1-C2	-3.23	105.78	110.77
3	P	2	GAL	O5-C1-C2	-3.10	105.98	110.77
3	N	3	SIA	C11-C10-N5	3.05	121.27	116.10
3	P	1	NAG	O4-C4-C5	2.98	116.70	109.30
3	Q	3	SIA	C11-C10-N5	2.98	121.14	116.10
3	O	3	SIA	C11-C10-N5	2.98	121.14	116.10
3	R	3	SIA	C11-C10-N5	2.96	121.11	116.10
3	O	3	SIA	O4-C4-C3	-2.89	102.76	109.94
3	N	3	SIA	O4-C4-C3	-2.84	102.89	109.94
3	P	3	SIA	O4-C4-C3	-2.83	102.92	109.94
3	O	2	GAL	C6-C5-C4	-2.74	106.59	113.00
3	P	3	SIA	C11-C10-N5	2.73	120.72	116.10
3	R	3	SIA	O4-C4-C3	-2.70	103.24	109.94
3	Q	3	SIA	O4-C4-C3	-2.70	103.25	109.94
3	M	3	SIA	O4-C4-C3	-2.64	103.40	109.94
3	P	2	GAL	C6-C5-C4	-2.53	107.08	113.00
3	M	2	GAL	O5-C1-C2	-2.47	106.96	110.77
3	Q	3	SIA	C4-C5-N5	-2.46	105.50	110.38
3	N	2	GAL	O5-C5-C6	2.39	110.95	107.20
3	O	1	NAG	C4-C3-C2	-2.29	107.67	111.02
3	M	3	SIA	C5-N5-C10	2.23	128.60	123.18
3	Q	3	SIA	C5-N5-C10	2.19	128.51	123.18
3	R	2	GAL	O5-C5-C6	2.15	110.58	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	3	SIA	O10-C10-C11	-2.14	118.09	122.06
3	M	3	SIA	C4-C5-N5	-2.04	106.34	110.38

There are no chirality outliers.

All (20) torsion outliers are listed below:

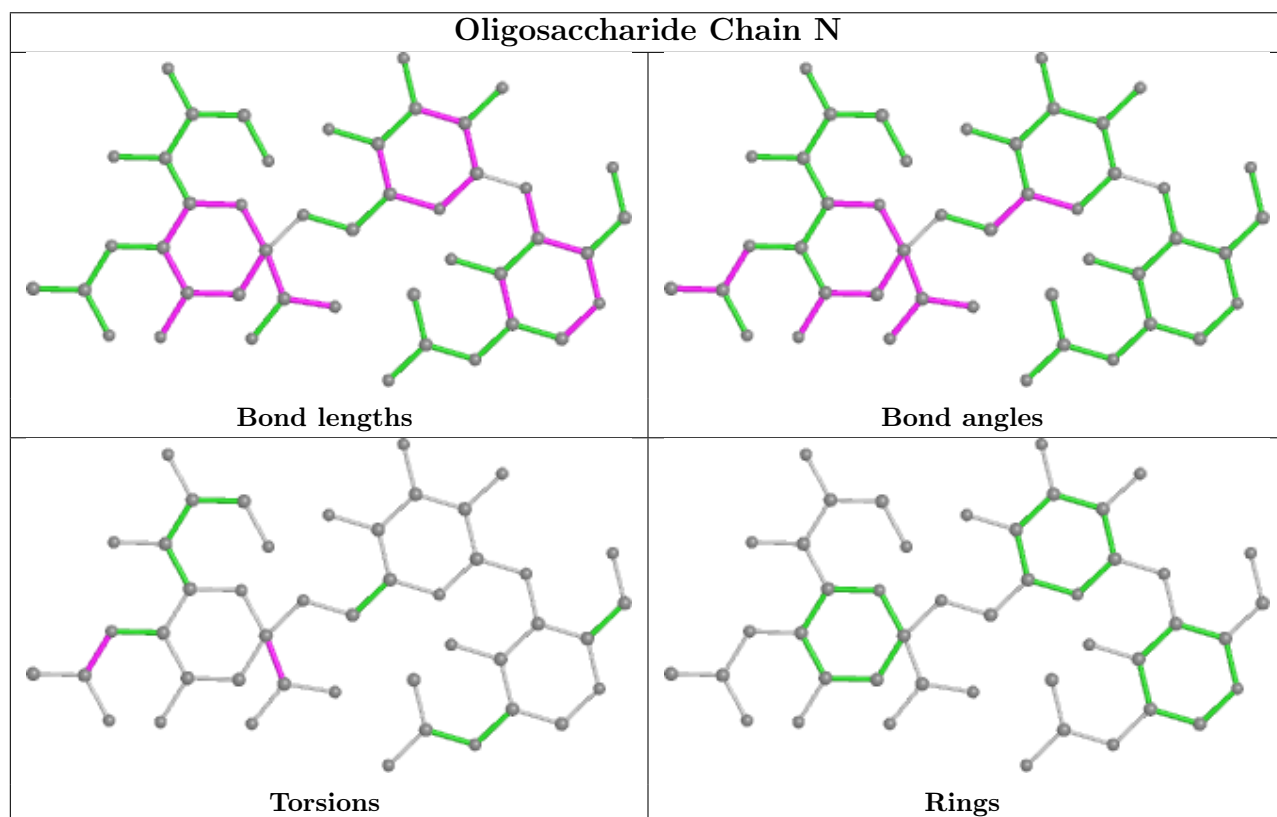
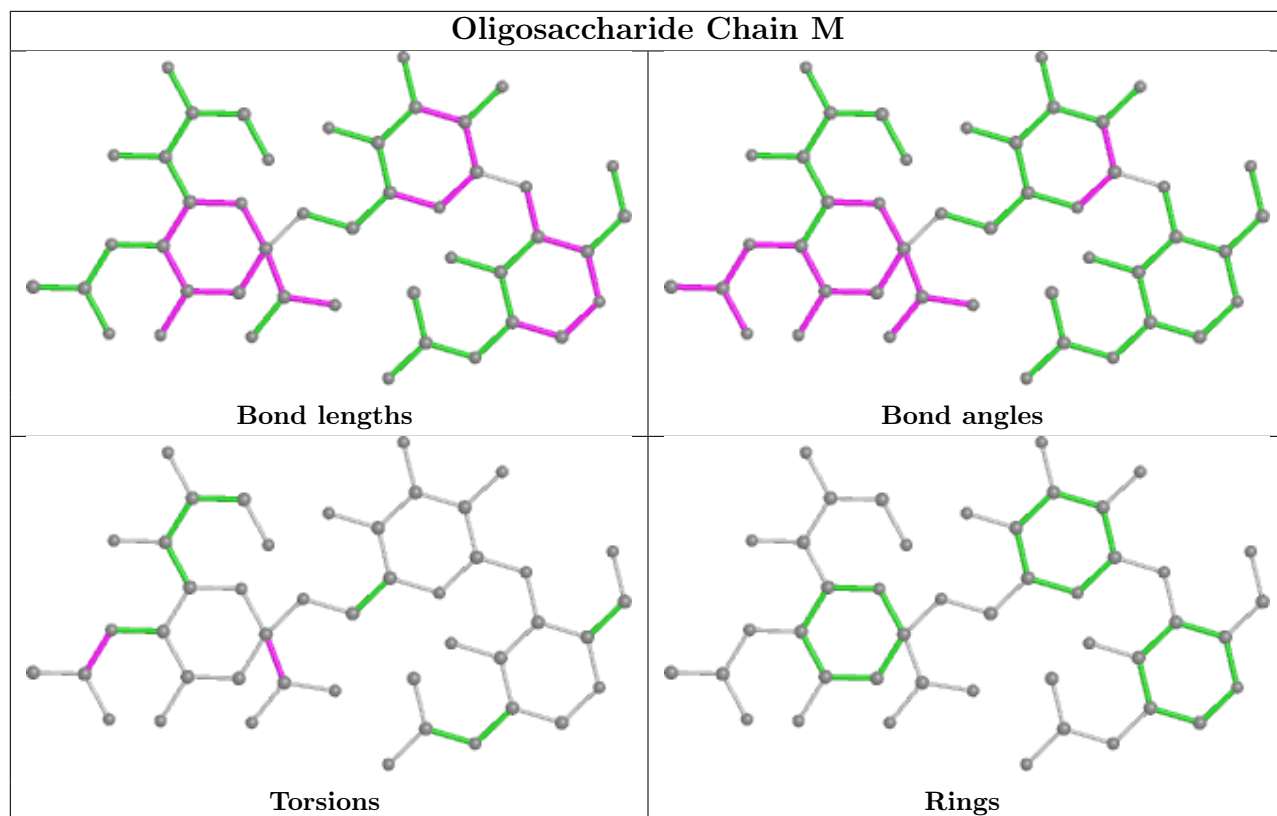
Mol	Chain	Res	Type	Atoms
3	M	3	SIA	C11-C10-N5-C5
3	O	3	SIA	C11-C10-N5-C5
3	M	3	SIA	O10-C10-N5-C5
3	O	3	SIA	O10-C10-N5-C5
3	Q	3	SIA	C11-C10-N5-C5
3	Q	3	SIA	O10-C10-N5-C5
3	R	3	SIA	C11-C10-N5-C5
3	R	3	SIA	O10-C10-N5-C5
3	N	3	SIA	C11-C10-N5-C5
3	N	3	SIA	O10-C10-N5-C5
3	P	3	SIA	C11-C10-N5-C5
3	P	3	SIA	O10-C10-N5-C5
3	M	3	SIA	O1A-C1-C2-C3
3	N	3	SIA	O1A-C1-C2-C3
3	O	3	SIA	O1A-C1-C2-C3
3	O	3	SIA	O1B-C1-C2-C3
3	P	3	SIA	O1A-C1-C2-C3
3	P	3	SIA	O1B-C1-C2-C3
3	Q	3	SIA	O1A-C1-C2-C3
3	R	3	SIA	O1A-C1-C2-C3

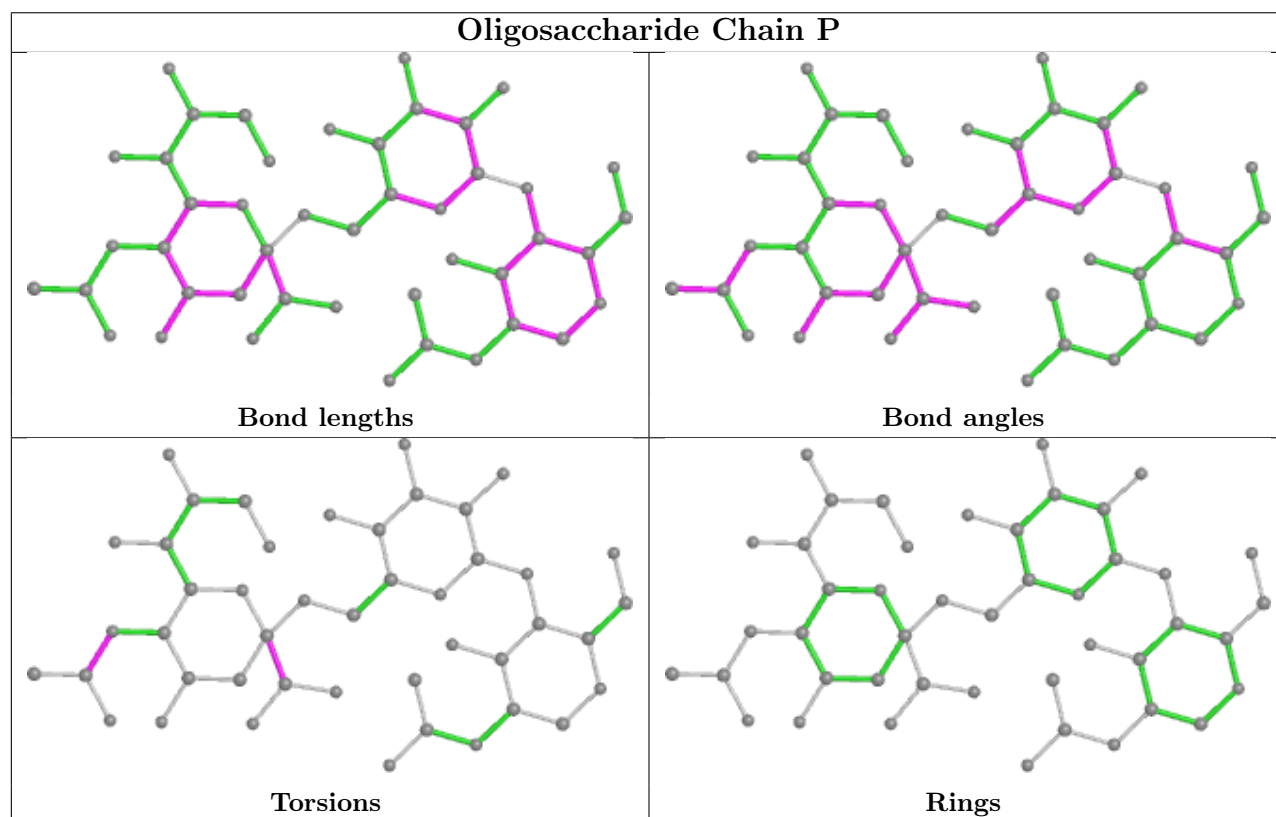
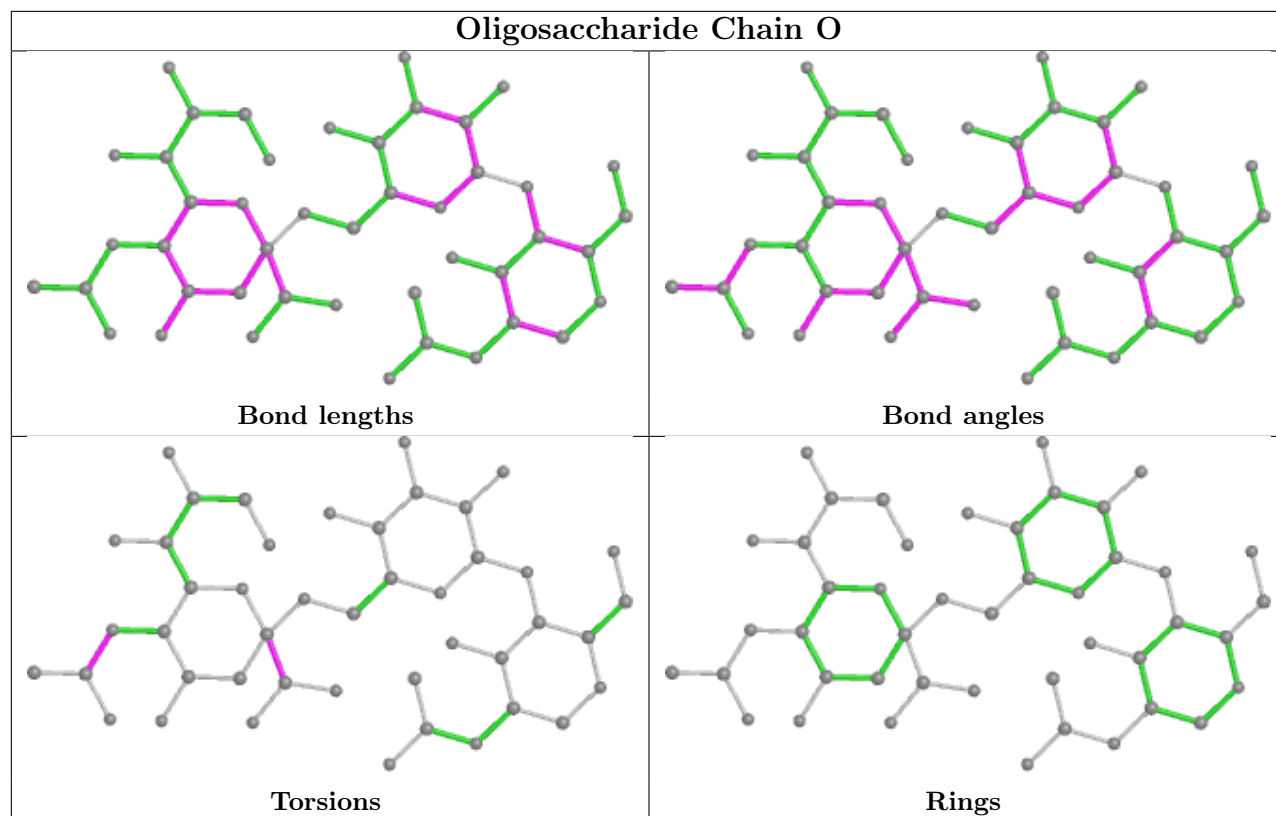
There are no ring outliers.

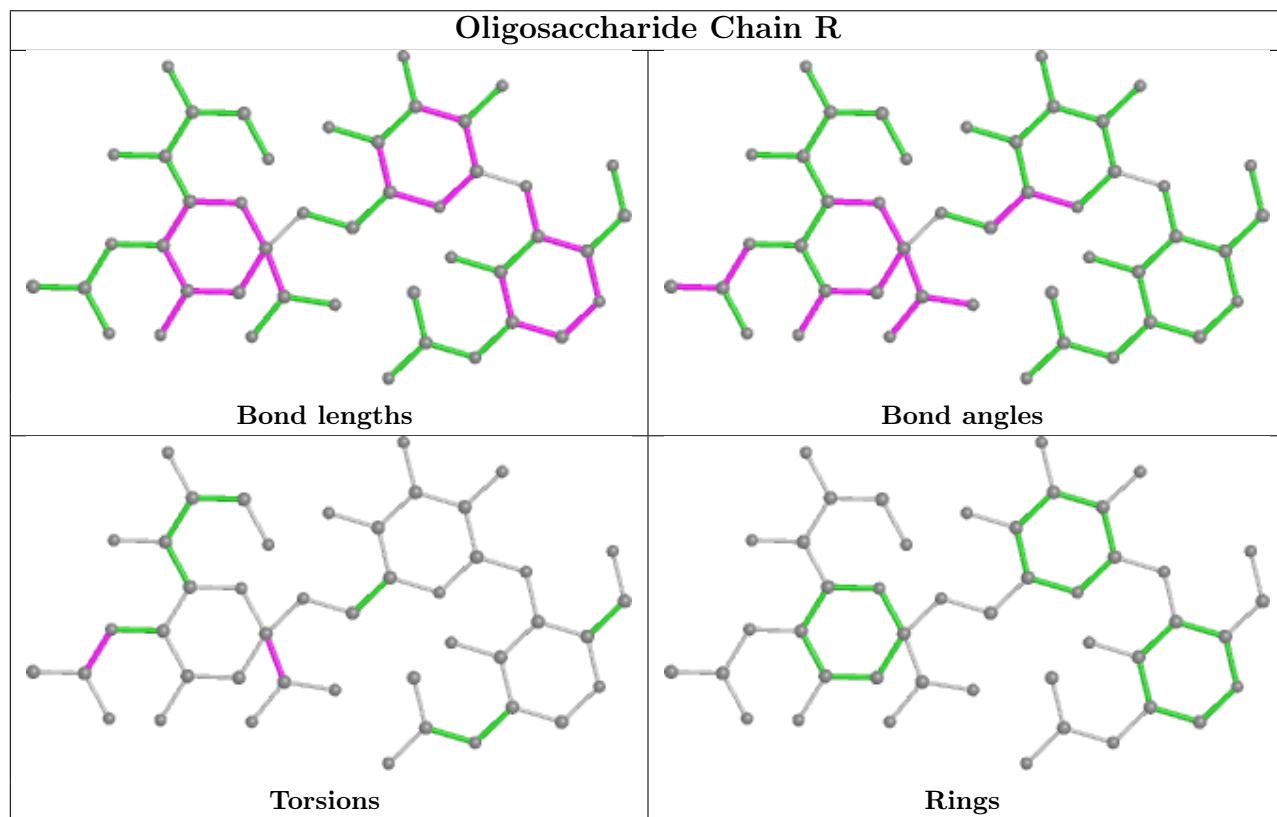
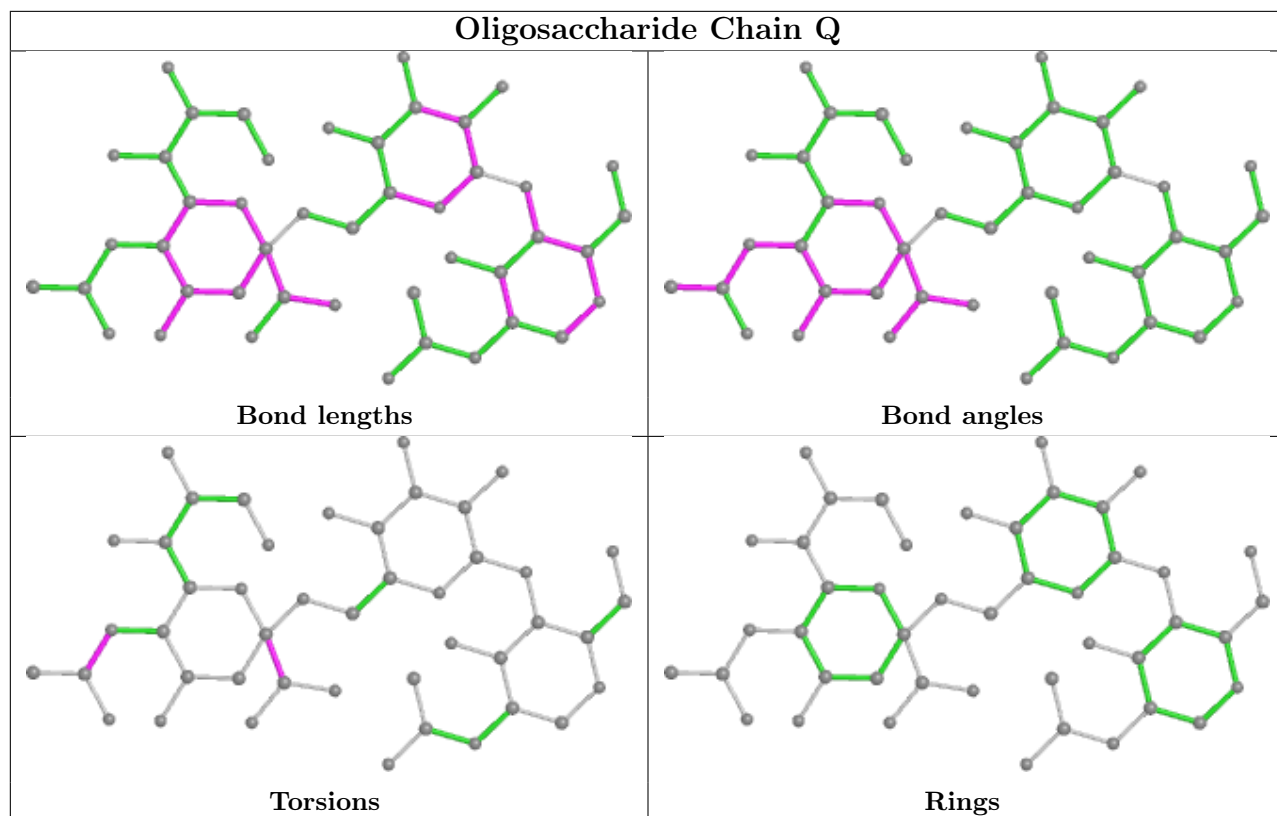
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	2	GAL	1	0
3	N	3	SIA	1	0
3	P	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	3331	-	15,15,15	0.48	0	21,21,21	0.60	0
4	NAG	E	3311	-	15,15,15	0.50	0	21,21,21	0.56	0
4	NAG	A	3321	-	15,15,15	0.47	0	21,21,21	0.68	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	3331	-	-	4/6/26/26	0/1/1/1
4	NAG	E	3311	-	-	4/6/26/26	0/1/1/1
4	NAG	A	3321	-	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3321	NAG	C8-C7-N2-C2
4	A	3321	NAG	O7-C7-N2-C2
4	E	3311	NAG	C8-C7-N2-C2
4	E	3311	NAG	O7-C7-N2-C2
4	F	3331	NAG	C8-C7-N2-C2
4	F	3331	NAG	O7-C7-N2-C2
4	F	3331	NAG	C3-C2-N2-C7
4	E	3311	NAG	C3-C2-N2-C7
4	F	3331	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	E	3311	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	3331	NAG	4	0
4	E	3311	NAG	4	0
4	A	3321	NAG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	42:ASN	C	44:GLY	N	2.61

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.