



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:25 AM GMT

PDB ID : 1RVX
Title : 1934 H1 Hemagglutinin in complex with LSTA
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 : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

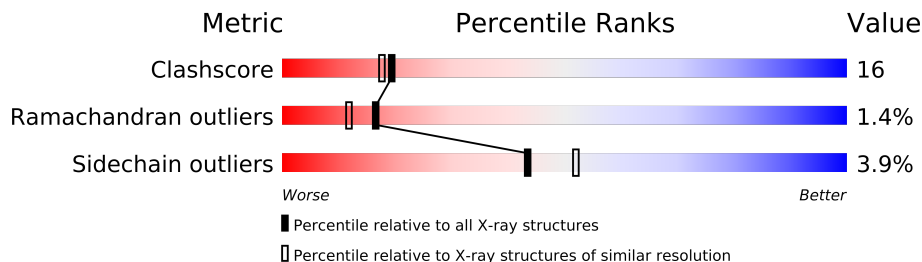
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	327	
1	C	327	
1	E	327	
1	G	327	
1	I	327	
1	K	327	
2	B	160	
2	D	160	
2	F	160	
2	H	160	
2	J	160	
2	L	160	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25966 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	323	Total	C	N	O	S	0	0	0
			2557	1612	450	482	13			
1	C	323	Total	C	N	O	S	0	0	0
			2557	1612	450	482	13			
1	E	323	Total	C	N	O	S	0	0	0
			2557	1612	450	482	13			
1	G	323	Total	C	N	O	S	0	0	0
			2557	1612	450	482	13			
1	I	323	Total	C	N	O	S	0	0	0
			2557	1612	450	482	13			
1	K	323	Total	C	N	O	S	0	0	0
			2557	1612	450	482	13			

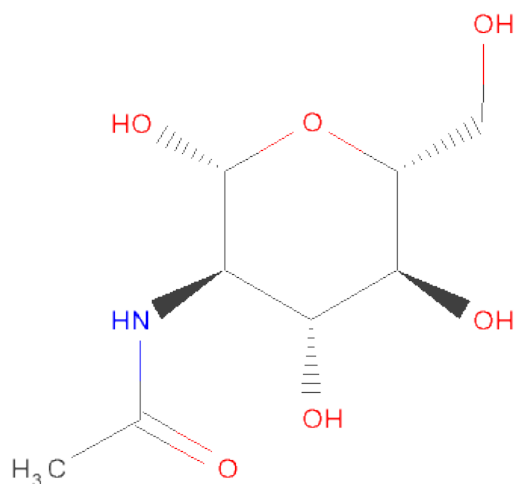
- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1283	805	218	253	7			
2	D	160	Total	C	N	O	S	0	0	0
			1283	805	218	253	7			
2	F	159	Total	C	N	O	S	0	0	0
			1275	800	217	251	7			
2	H	160	Total	C	N	O	S	0	0	0
			1283	805	218	253	7			
2	J	160	Total	C	N	O	S	0	0	0
			1283	805	218	253	7			
2	L	159	Total	C	N	O	S	0	0	0
			1275	800	217	251	7			

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			45	25	2	18		
3	C	3	Total	C	N	O	0	0
			45	25	2	18		
3	E	3	Total	C	N	O	0	0
			45	25	2	18		
3	G	3	Total	C	N	O	0	0
			45	25	2	18		
3	I	3	Total	C	N	O	0	0
			45	25	2	18		
3	K	3	Total	C	N	O	0	0
			45	25	2	18		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			15	8	1	6		
4	G	1	Total	C	N	O	0	0
			15	8	1	6		
4	I	1	Total	C	N	O	0	0
			15	8	1	6		
4	J	1	Total	C	N	O	0	0
			15	8	1	6		
4	K	1	Total	C	N	O	0	0
			15	8	1	6		

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	295	Total	O	0	0
			295	295		
5	B	107	Total	O	0	0
			107	107		
5	C	296	Total	O	0	0
			296	296		
5	D	122	Total	O	0	0
			122	122		
5	E	340	Total	O	0	0
			340	340		
5	F	122	Total	O	0	0
			122	122		
5	G	307	Total	O	0	0
			307	307		
5	H	101	Total	O	0	0
			101	101		
5	I	303	Total	O	0	0
			303	303		
5	J	105	Total	O	0	0
			105	105		
5	K	315	Total	O	0	0
			315	315		
5	L	109	Total	O	0	0
			109	109		

3 Residue-property plots

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

Note EDS was not executed.

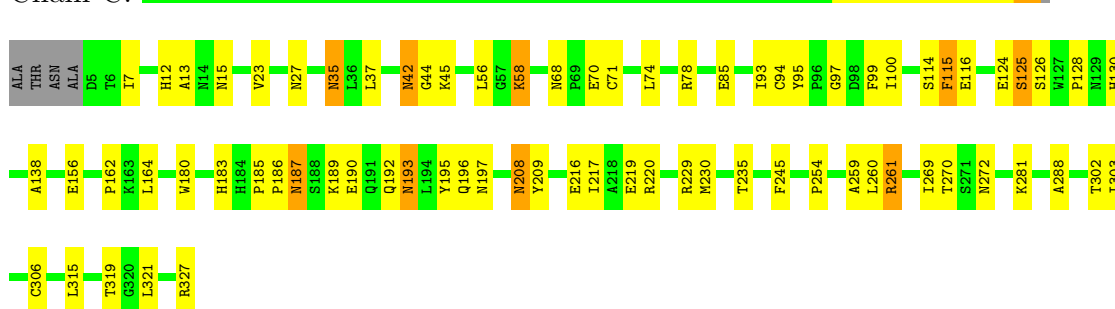
- Molecule 1: hemagglutinin

Chain A:



- Molecule 1: hemagglutinin

Chain C:



- Molecule 1: hemagglutinin

Chain E:



- Molecule 1: hemagglutinin

Chain G:



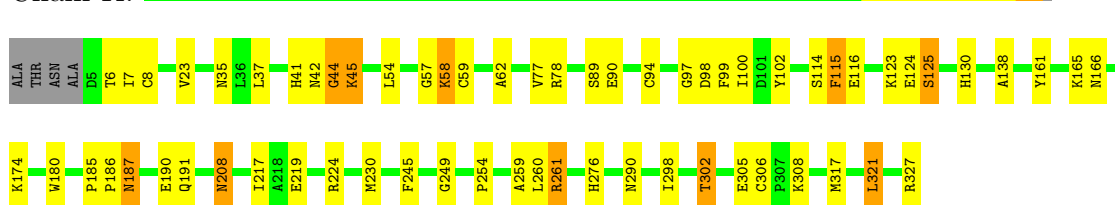
- Molecule 1: hemagglutinin

Chain I:



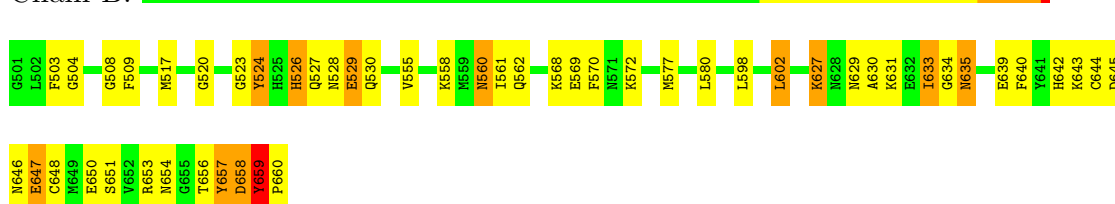
- Molecule 1: hemagglutinin

Chain K:



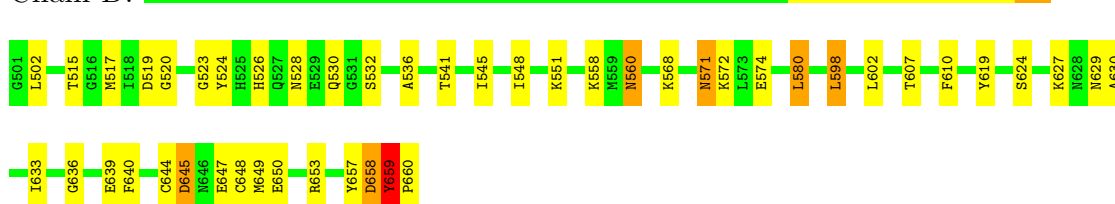
- Molecule 2: Hemagglutinin

Chain B:



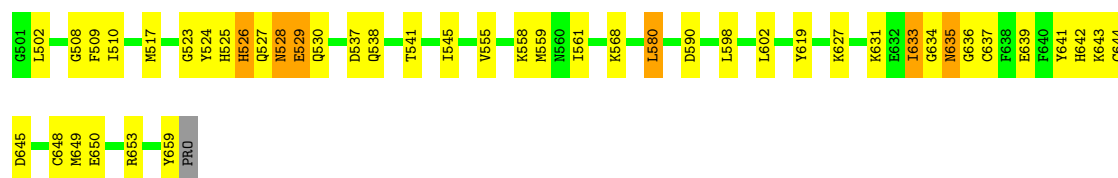
- Molecule 2: Hemagglutinin

Chain D:



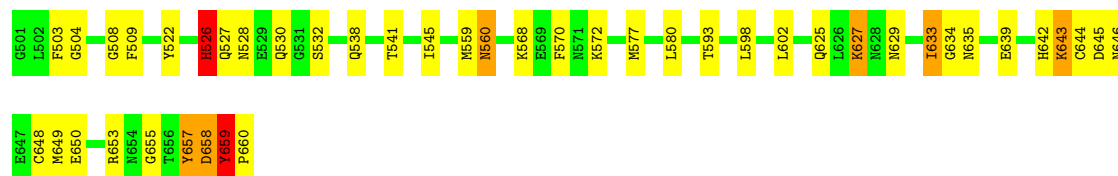
- Molecule 2: Hemagglutinin

Chain F: 



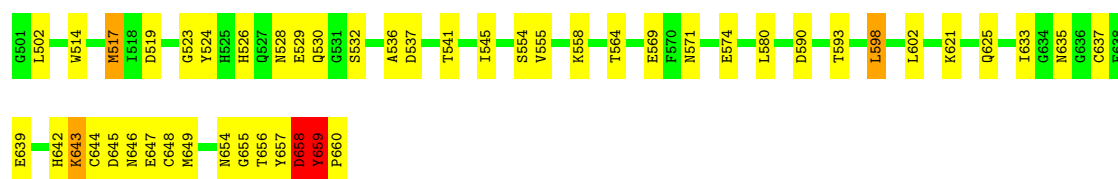
- Molecule 2: Hemagglutinin

Chain H: 



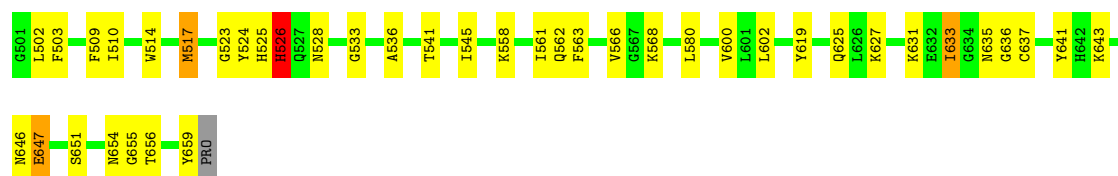
- Molecule 2: Hemagglutinin

Chain J: 



- Molecule 2: Hemagglutinin

Chain L: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	227.88Å 131.34Å 174.71Å 90.00° 110.09° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25966	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0/2621	0.61	0/3563
1	C	0.34	0/2621	0.62	0/3563
1	E	0.33	0/2620	0.62	0/3560
1	G	0.34	0/2621	0.63	0/3563
1	I	0.34	0/2620	0.62	0/3560
1	K	0.33	0/2621	0.64	1/3563 (0.0%)
2	B	0.32	0/1309	0.53	0/1761
2	D	0.33	0/1309	0.53	0/1761
2	F	0.33	0/1300	0.51	0/1749
2	H	0.32	0/1309	0.52	0/1761
2	J	0.32	0/1309	0.53	0/1761
2	L	0.32	0/1300	0.52	0/1749
All	All	0.33	0/23560	0.59	1/31914 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	44	GLY	N-CA-C	-8.24	92.50	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2557	0	2495	84	0
1	C	2557	0	2495	81	0
1	E	2557	0	2494	72	0
1	G	2557	0	2497	102	0
1	I	2557	0	2494	88	0
1	K	2557	0	2495	67	0
2	B	1283	0	1207	69	0
2	D	1283	0	1207	41	0
2	F	1275	0	1200	39	0
2	H	1283	0	1207	54	0
2	J	1283	0	1207	58	0
2	L	1275	0	1200	50	0
3	A	45	0	38	0	0
3	C	45	0	38	0	0
3	E	45	0	38	0	0
3	G	45	0	38	1	0
3	I	45	0	38	0	0
3	K	45	0	38	0	0
4	A	30	0	30	8	0
4	B	15	0	15	2	0
4	C	15	0	15	5	0
4	G	30	0	30	7	0
4	I	15	0	15	3	0
4	J	15	0	15	5	0
4	K	15	0	15	3	0
4	L	15	0	15	7	0
5	A	295	0	0	6	0
5	B	107	0	0	5	0
5	C	296	0	0	8	0
5	D	122	0	0	5	0
5	E	340	0	0	6	0
5	F	122	0	0	0	0
5	G	307	0	0	11	0
5	H	101	0	0	2	0
5	I	303	0	0	6	0
5	J	105	0	0	1	0
5	K	315	0	0	5	0
5	L	109	0	0	5	0
All	All	25966	0	22576	751	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 16.

All (751) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:15:ASN:HD21	4:C:3020:NAG:H61	1.08	1.19
1:A:27:ASN:HD21	4:A:3017:NAG:H4	1.04	1.14
1:A:238:LYS:H	1:A:238:LYS:CE	1.63	1.11
1:A:58:LYS:H	1:A:58:LYS:HD3	0.98	1.10
1:K:290:ASN:HD21	4:K:3015:NAG:H3	1.00	1.10
1:A:238:LYS:H	1:A:238:LYS:HE3	1.09	1.07
1:A:27:ASN:HD21	4:A:3017:NAG:C4	1.69	1.05
2:F:633:ILE:HD12	2:F:634:GLY:H	1.15	1.02
2:J:654:ASN:ND2	4:J:3014:NAG:H62	1.75	1.01
1:K:290:ASN:ND2	4:K:3015:NAG:H3	1.75	0.99
1:I:310:VAL:HG12	1:I:312:SER:H	1.27	0.99
2:B:659:TYR:H	2:B:660:PRO:HD3	1.32	0.94
1:A:27:ASN:ND2	4:A:3017:NAG:H4	1.84	0.91
1:A:58:LYS:N	1:A:58:LYS:HD3	1.83	0.91
2:D:659:TYR:H	2:D:660:PRO:HD3	1.35	0.91
2:D:571:ASN:OD1	2:D:574:GLU:HG3	1.70	0.90
2:H:530:GLN:NE2	2:H:645:ASP:HB2	1.88	0.89
1:C:190:GLU:HA	1:C:193:ASN:HD21	1.35	0.89
2:L:528:ASN:HD22	2:L:646:ASN:ND2	1.70	0.88
1:C:15:ASN:ND2	4:C:3020:NAG:H61	1.87	0.88
2:H:526:HIS:HB2	2:H:649:MET:HE3	1.52	0.88
2:H:659:TYR:H	2:H:660:PRO:HD3	1.37	0.87
1:G:27:ASN:ND2	4:G:3011:NAG:H61	1.90	0.87
1:G:280:THR:HG22	1:G:282:CYS:H	1.37	0.86
1:I:42:ASN:ND2	1:I:288:ALA:HB3	1.90	0.86
1:A:58:LYS:CD	1:A:58:LYS:H	1.83	0.86
1:C:42:ASN:O	1:C:45:LYS:N	2.07	0.86
2:F:633:ILE:CD1	2:F:634:GLY:H	1.87	0.86
1:A:238:LYS:N	1:A:238:LYS:HE3	1.90	0.85
2:B:642:HIS:HE1	2:B:644:CYS:HB3	1.41	0.85
2:J:528:ASN:HD22	2:J:646:ASN:ND2	1.73	0.85
2:B:644:CYS:HB2	2:B:648:CYS:HB3	1.59	0.85
1:E:317:MET:HE1	2:F:555:VAL:HG11	1.58	0.85
1:G:116:GLU:HG2	1:G:259:ALA:HB3	1.58	0.84
2:B:528:ASN:HD22	2:B:646:ASN:ND2	1.74	0.84
1:K:174:LYS:HE2	1:K:261:ARG:HG3	1.60	0.83
2:B:651:SER:HA	2:B:654:ASN:HD21	1.43	0.83
1:G:238:LYS:H	1:G:238:LYS:HZ2	1.25	0.83
1:C:42:ASN:O	1:C:42:ASN:ND2	2.13	0.82
2:J:654:ASN:HD21	4:J:3014:NAG:H62	1.40	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:528:ASN:HD21	2:J:645:ASP:HA	1.44	0.82
2:D:530:GLN:NE2	2:D:645:ASP:HB2	1.96	0.81
2:B:633:ILE:HD11	2:B:639:GLU:HB2	1.63	0.81
2:H:642:HIS:HE1	2:H:644:CYS:HB3	1.46	0.80
1:A:290:ASN:ND2	4:A:3018:NAG:H5	1.96	0.80
1:C:15:ASN:HD21	4:C:3020:NAG:C6	1.93	0.80
1:G:238:LYS:H	1:G:238:LYS:NZ	1.79	0.80
2:H:627:LYS:HD2	2:H:660:PRO:HB3	1.62	0.80
1:G:208:ASN:HD21	1:G:238:LYS:HE2	1.47	0.79
2:F:644:CYS:HB2	2:F:648:CYS:SG	2.22	0.79
1:G:208:ASN:ND2	1:G:238:LYS:HE2	1.96	0.79
2:J:659:TYR:N	2:J:660:PRO:HD3	1.98	0.78
1:I:78:ARG:HH21	1:I:261:ARG:HH22	1.31	0.78
2:J:642:HIS:HE1	2:J:644:CYS:HB3	1.50	0.77
1:G:310:VAL:HG23	2:H:593:THR:HA	1.66	0.77
2:B:530:GLN:NE2	2:B:645:ASP:HB2	2.00	0.76
1:A:290:ASN:HD21	4:A:3018:NAG:H1	1.50	0.76
2:H:530:GLN:HE22	2:H:645:ASP:HB2	1.52	0.75
1:C:58:LYS:HD3	1:C:58:LYS:H	1.52	0.74
2:B:529:GLU:OE1	2:B:530:GLN:HG3	1.88	0.74
2:F:633:ILE:HD12	2:F:634:GLY:N	1.98	0.73
2:B:528:ASN:HD21	2:B:645:ASP:HA	1.53	0.73
2:L:631:LYS:HE3	2:L:633:ILE:HG23	1.70	0.73
2:B:644:CYS:HB2	2:B:648:CYS:CB	2.17	0.73
2:H:528:ASN:HB3	2:H:646:ASN:HD21	1.53	0.73
2:H:644:CYS:HB2	2:H:648:CYS:HB3	1.70	0.72
2:J:526:HIS:CE1	2:J:649:MET:HG3	2.24	0.72
2:B:633:ILE:N	2:B:633:ILE:HD12	2.04	0.72
1:A:238:LYS:CE	1:A:238:LYS:N	2.48	0.72
2:B:530:GLN:HE21	2:B:645:ASP:HB2	1.54	0.72
2:D:659:TYR:N	2:D:660:PRO:HD3	2.04	0.71
1:I:187:ASN:ND2	1:I:190:GLU:H	1.88	0.71
1:I:116:GLU:HG2	1:I:259:ALA:HB3	1.72	0.71
2:B:659:TYR:H	2:B:660:PRO:CD	2.03	0.71
1:E:98:ASP:HB2	5:E:3304:HOH:O	1.89	0.71
2:D:560:ASN:HB3	5:D:758:HOH:O	1.91	0.71
1:C:116:GLU:HG2	1:C:259:ALA:HB3	1.73	0.70
2:H:528:ASN:HB3	2:H:646:ASN:ND2	2.06	0.70
2:J:528:ASN:HD22	2:J:646:ASN:HD22	1.35	0.70
5:G:3284:HOH:O	2:H:568:LYS:HG2	1.91	0.70
2:J:644:CYS:HB2	2:J:648:CYS:HB3	1.74	0.70
1:I:192:GLN:HE22	1:I:198:GLU:HB2	1.57	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:642:HIS:CE1	2:B:644:CYS:HB3	2.25	0.69
1:E:35:ASN:ND2	1:E:37:LEU:H	1.91	0.69
1:A:116:GLU:HG2	1:A:259:ALA:HB3	1.74	0.69
1:I:78:ARG:HH21	1:I:261:ARG:NH2	1.91	0.69
1:E:45:LYS:HG2	1:E:276:HIS:CD2	2.27	0.69
1:I:193:ASN:HD22	1:I:194:LEU:N	1.90	0.69
2:L:619:TYR:CE1	2:L:636:GLY:HA2	2.28	0.69
1:C:187:ASN:ND2	1:C:190:GLU:H	1.92	0.68
2:F:509:PHE:O	2:F:635:ASN:HB3	1.92	0.68
1:A:189:LYS:HE2	5:A:3276:HOH:O	1.93	0.68
1:G:58:LYS:CD	1:G:58:LYS:H	2.06	0.68
2:F:631:LYS:HE3	2:F:633:ILE:HG21	1.75	0.68
1:I:42:ASN:HD22	1:I:288:ALA:HB3	1.55	0.68
2:D:519:ASP:HB2	2:D:536:ALA:HB3	1.76	0.68
1:G:280:THR:HG21	1:G:288:ALA:HB1	1.76	0.67
1:C:189:LYS:HG3	5:C:3262:HOH:O	1.95	0.67
2:J:514:TRP:HE3	2:J:517:MET:HG3	1.59	0.67
2:B:528:ASN:HD22	2:B:646:ASN:HD22	1.42	0.66
1:G:135:VAL:HG12	1:G:145:SER:HB3	1.77	0.66
2:J:633:ILE:HD11	2:J:639:GLU:HG3	1.78	0.66
2:L:514:TRP:HE3	2:L:517:MET:HG3	1.61	0.66
1:I:317:MET:HE1	2:J:555:VAL:HG11	1.78	0.65
5:G:3271:HOH:O	1:K:98:ASP:HB2	1.95	0.65
2:B:644:CYS:HB2	2:B:648:CYS:SG	2.36	0.65
1:G:42:ASN:C	1:G:42:ASN:HD22	1.98	0.65
2:H:659:TYR:N	2:H:660:PRO:HD3	2.11	0.65
2:J:644:CYS:HB2	2:J:648:CYS:CB	2.27	0.65
1:E:187:ASN:ND2	1:E:190:GLU:H	1.94	0.65
1:G:222:LYS:HB3	1:G:225:ASP:HA	1.78	0.64
1:A:58:LYS:HG3	5:A:3268:HOH:O	1.98	0.64
2:L:528:ASN:HA	5:L:3095:HOH:O	1.98	0.64
2:H:659:TYR:H	2:H:660:PRO:CD	2.10	0.64
2:J:526:HIS:O	2:J:532:SER:HA	1.98	0.64
2:H:642:HIS:CE1	2:H:644:CYS:HB3	2.31	0.64
1:K:123:LYS:HE2	5:K:3204:HOH:O	1.98	0.64
1:K:58:LYS:HD3	1:K:58:LYS:H	1.63	0.64
1:K:302:THR:HG23	1:K:306:CYS:SG	2.38	0.63
1:C:71:CYS:HB3	1:C:74:LEU:HD12	1.80	0.63
1:E:208:ASN:HD22	1:E:208:ASN:H	1.45	0.63
2:L:656:THR:HG21	4:L:3016:NAG:H62	1.79	0.63
1:E:180:TRP:HB3	1:E:254:PRO:HG3	1.81	0.63
2:B:560:ASN:HD22	2:B:560:ASN:N	1.95	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:654:ASN:OD1	4:L:3016:NAG:H61	1.99	0.63
2:B:659:TYR:N	2:B:660:PRO:HD3	2.09	0.62
2:J:644:CYS:HB2	2:J:648:CYS:SG	2.39	0.62
1:A:238:LYS:H	1:A:238:LYS:HE2	1.59	0.62
1:C:124:GLU:O	1:C:125:SER:CB	2.47	0.62
2:B:629:ASN:HD22	2:B:657:TYR:HE2	1.47	0.62
2:B:651:SER:HA	2:B:654:ASN:ND2	2.12	0.62
2:D:633:ILE:HD11	2:D:639:GLU:HG3	1.82	0.62
2:H:560:ASN:N	2:H:560:ASN:HD22	1.98	0.61
2:H:644:CYS:HB2	2:H:648:CYS:CB	2.29	0.61
1:G:310:VAL:CG2	2:H:593:THR:HA	2.28	0.61
1:E:157:LYS:HG2	1:E:158:GLU:HG3	1.81	0.61
1:K:327:ARG:C	1:K:327:ARG:HD2	2.20	0.61
2:B:562:GLN:HG3	5:B:3026:HOH:O	1.99	0.61
1:K:208:ASN:H	1:K:208:ASN:HD22	1.48	0.61
2:L:525:HIS:O	2:L:526:HIS:ND1	2.32	0.61
1:I:45:LYS:HG2	1:I:276:HIS:CD2	2.36	0.61
2:L:633:ILE:CD1	2:L:637:CYS:HB2	2.30	0.61
1:E:41:HIS:HB3	1:E:298:ILE:HD13	1.82	0.61
1:C:23:VAL:HG22	2:D:602:LEU:HD12	1.83	0.61
2:L:517:MET:HE1	2:L:536:ALA:HB2	1.81	0.61
2:L:627:LYS:HB2	2:L:659:TYR:HE1	1.66	0.61
1:G:208:ASN:H	1:G:208:ASN:HD22	1.47	0.61
2:J:530:GLN:NE2	2:J:646:ASN:H	1.97	0.60
2:D:659:TYR:H	2:D:660:PRO:CD	2.12	0.60
1:C:58:LYS:H	1:C:58:LYS:CD	2.13	0.60
1:I:124:GLU:O	1:I:125:SER:CB	2.50	0.60
2:B:650:GLU:HA	2:B:653:ARG:HH11	1.67	0.60
1:I:124:GLU:O	1:I:125:SER:HB3	2.02	0.60
1:A:186:PRO:HD2	1:A:190:GLU:OE2	2.01	0.60
1:G:163:LYS:HE3	1:G:201:TYR:OH	2.01	0.60
1:I:290:ASN:ND2	4:I:3013:NAG:H61	2.17	0.60
2:J:659:TYR:H	2:J:660:PRO:HD3	1.64	0.60
1:I:35:ASN:ND2	1:I:37:LEU:H	1.99	0.60
1:G:42:ASN:ND2	1:G:45:LYS:H	2.00	0.60
2:B:627:LYS:HD2	2:B:660:PRO:HB3	1.83	0.59
1:G:280:THR:HG23	5:G:3063:HOH:O	2.03	0.59
1:A:97:GLY:HA3	1:A:230:MET:O	2.01	0.59
2:J:642:HIS:CE1	2:J:644:CYS:HB3	2.33	0.59
1:E:42:ASN:C	1:E:44:GLY:N	2.55	0.59
2:B:560:ASN:N	2:B:560:ASN:ND2	2.49	0.59
1:C:42:ASN:HD21	1:C:288:ALA:HB3	1.67	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:116:GLU:HG2	1:K:259:ALA:HB3	1.83	0.59
1:G:141:HIS:HD2	5:G:3203:HOH:O	1.86	0.59
2:H:526:HIS:HD2	2:H:649:MET:HG3	1.68	0.59
2:J:517:MET:HE1	2:J:536:ALA:HB2	1.84	0.59
1:K:321:LEU:HD23	1:K:321:LEU:N	2.17	0.59
2:H:509:PHE:O	2:H:635:ASN:HA	2.02	0.59
2:D:624:SER:O	2:D:627:LYS:HG3	2.03	0.59
1:A:23:VAL:HG21	2:B:602:LEU:HD12	1.85	0.58
1:I:42:ASN:HB3	1:I:45:LYS:HB2	1.84	0.58
1:C:78:ARG:NH2	1:C:261:ARG:HH22	2.01	0.58
1:I:188:SER:O	1:I:192:GLN:HG2	2.03	0.58
2:L:654:ASN:CG	4:L:3016:NAG:H61	2.22	0.58
1:C:190:GLU:HA	1:C:193:ASN:ND2	2.14	0.58
2:B:529:GLU:OE1	2:B:530:GLN:N	2.36	0.58
2:F:644:CYS:CB	2:F:648:CYS:SG	2.90	0.58
1:A:187:ASN:ND2	1:A:190:GLU:H	2.02	0.58
1:E:124:GLU:O	1:E:125:SER:CB	2.51	0.58
1:I:119:GLU:OE2	1:I:122:PRO:HA	2.03	0.58
1:A:290:ASN:CG	4:A:3018:NAG:H5	2.23	0.58
1:A:23:VAL:CG2	2:B:602:LEU:HD12	2.33	0.58
1:E:35:ASN:HD22	1:E:36:LEU:N	2.02	0.58
1:K:58:LYS:CD	1:K:58:LYS:H	2.17	0.58
2:D:560:ASN:ND2	5:D:675:HOH:O	2.36	0.58
2:D:519:ASP:HB2	2:D:536:ALA:CB	2.34	0.58
1:C:216:GLU:HB2	5:C:3198:HOH:O	2.03	0.58
1:G:47:CYS:SG	1:G:278:CYS:HB3	2.44	0.58
1:K:124:GLU:O	1:K:125:SER:CB	2.51	0.58
1:E:116:GLU:HG3	1:E:116:GLU:O	2.04	0.57
1:A:42:ASN:HD22	1:A:42:ASN:C	2.06	0.57
1:G:97:GLY:HA3	1:G:230:MET:O	2.04	0.57
1:K:260:LEU:C	1:K:261:ARG:HD2	2.25	0.57
1:C:124:GLU:O	1:C:125:SER:HB3	2.03	0.57
2:H:627:LYS:HD2	2:H:660:PRO:CB	2.33	0.57
1:G:27:ASN:CG	4:G:3011:NAG:H61	2.25	0.57
1:E:185:PRO:HG2	1:E:191:GLN:HE21	1.69	0.57
2:L:528:ASN:HD21	2:L:646:ASN:N	2.02	0.57
2:B:633:ILE:HG22	2:B:634:GLY:N	2.20	0.57
1:E:42:ASN:HB3	1:E:45:LYS:HB2	1.86	0.57
1:I:59:CYS:O	1:I:89:SER:HB2	2.04	0.57
4:A:3018:NAG:H62	5:A:3271:HOH:O	2.05	0.56
1:I:5:ASP:OD1	2:J:643:LYS:HB3	2.05	0.56
2:H:559:MET:HE3	5:H:745:HOH:O	2.04	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:124:GLU:O	1:A:125:SER:HB3	2.04	0.56
2:F:627:LYS:HB2	2:F:659:TYR:CE1	2.40	0.56
2:H:629:ASN:HD22	2:H:657:TYR:HE2	1.51	0.56
1:G:78:ARG:HH21	1:G:116:GLU:HB3	1.70	0.56
2:J:659:TYR:N	2:J:660:PRO:CD	2.66	0.56
2:F:631:LYS:HB3	2:F:641:TYR:OH	2.06	0.56
1:C:58:LYS:N	1:C:58:LYS:HD3	2.20	0.56
1:C:116:GLU:HG3	1:C:116:GLU:O	2.05	0.56
1:G:58:LYS:HD3	1:G:58:LYS:H	1.70	0.56
1:E:198:GLU:HG3	5:E:3329:HOH:O	2.06	0.56
1:C:208:ASN:HD22	1:C:208:ASN:H	1.53	0.56
2:H:650:GLU:OE2	2:H:653:ARG:HD2	2.05	0.56
1:E:54:LEU:HD13	1:E:77:VAL:HG11	1.88	0.56
1:I:78:ARG:NH2	1:I:261:ARG:HH22	2.01	0.56
1:I:290:ASN:ND2	4:I:3013:NAG:C6	2.68	0.56
1:G:186:PRO:HD2	1:G:190:GLU:OE2	2.05	0.56
1:E:6:THR:O	2:F:526:HIS:HA	2.06	0.56
2:D:659:TYR:N	2:D:660:PRO:CD	2.69	0.56
2:B:528:ASN:ND2	2:B:645:ASP:HA	2.21	0.56
1:C:23:VAL:CG2	2:D:602:LEU:HD12	2.35	0.56
1:E:188:SER:O	1:E:192:GLN:HG2	2.06	0.56
2:L:561:ILE:HD11	2:L:563:PHE:CZ	2.41	0.56
1:G:290:ASN:HD21	4:G:3012:NAG:C1	2.19	0.56
1:C:78:ARG:HH21	1:C:261:ARG:HH22	1.54	0.55
1:C:180:TRP:HB3	1:C:254:PRO:HG3	1.88	0.55
1:K:6:THR:HG22	1:K:7:ILE:N	2.21	0.55
1:A:208:ASN:HD22	1:A:208:ASN:H	1.53	0.55
2:D:629:ASN:HD21	2:D:660:PRO:HA	1.72	0.55
1:I:5:ASP:N	2:J:643:LYS:HD2	2.21	0.55
1:K:327:ARG:O	1:K:327:ARG:HD2	2.07	0.55
1:A:42:ASN:ND2	1:A:45:LYS:H	2.05	0.55
2:H:598:LEU:HD21	2:J:558:LYS:HG3	1.89	0.55
1:E:185:PRO:HG2	1:E:191:GLN:NE2	2.22	0.55
1:C:260:LEU:C	1:C:261:ARG:HD2	2.27	0.55
1:A:124:GLU:O	1:A:125:SER:CB	2.54	0.55
1:G:238:LYS:H	1:G:238:LYS:CE	2.19	0.55
2:L:633:ILE:H	2:L:633:ILE:HD12	1.72	0.55
1:I:95:TYR:CD2	1:I:230:MET:HB2	2.42	0.55
1:G:6:THR:HG22	2:H:639:GLU:HA	1.87	0.55
1:C:35:ASN:ND2	1:C:37:LEU:H	2.04	0.55
1:E:42:ASN:HB3	1:E:44:GLY:O	2.07	0.54
2:L:654:ASN:HD21	4:L:3016:NAG:H4	1.72	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:527:GLN:HG2	5:B:3089:HOH:O	2.07	0.54
2:H:644:CYS:HB2	2:H:648:CYS:SG	2.47	0.54
2:L:631:LYS:HB3	2:L:641:TYR:OH	2.06	0.54
2:H:650:GLU:HA	2:H:653:ARG:HH11	1.72	0.54
2:H:598:LEU:CD2	2:J:558:LYS:HG3	2.37	0.54
2:L:633:ILE:HD13	2:L:637:CYS:HB2	1.89	0.54
1:C:327:ARG:HD2	1:C:327:ARG:C	2.28	0.54
1:E:42:ASN:HB2	1:E:288:ALA:H	1.72	0.54
1:G:187:ASN:ND2	1:G:190:GLU:H	2.05	0.54
2:H:625:GLN:HE22	2:H:655:GLY:C	2.10	0.54
1:I:163:LYS:HE3	1:I:201:TYR:OH	2.07	0.54
2:F:644:CYS:HB2	2:F:648:CYS:CB	2.37	0.54
1:G:290:ASN:ND2	4:G:3012:NAG:O5	2.41	0.54
2:F:529:GLU:OE1	2:F:530:GLN:HG3	2.08	0.54
1:C:186:PRO:HD2	1:C:190:GLU:OE2	2.08	0.54
5:G:3162:HOH:O	1:K:219:GLU:HG3	2.08	0.54
2:J:647:GLU:CD	4:J:3014:NAG:H82	2.28	0.53
1:G:208:ASN:CG	1:G:238:LYS:HE2	2.29	0.53
1:E:116:GLU:HG2	1:E:259:ALA:HB3	1.89	0.53
1:A:302:THR:HB	1:A:306:CYS:SG	2.48	0.53
2:B:631:LYS:HG3	2:B:633:ILE:HD11	1.88	0.53
1:K:23:VAL:HG22	2:L:602:LEU:HD12	1.90	0.53
2:J:526:HIS:HE1	2:J:649:MET:HG3	1.70	0.53
2:J:654:ASN:CG	4:J:3014:NAG:H62	2.28	0.53
2:H:530:GLN:NE2	2:H:646:ASN:H	2.06	0.53
2:J:644:CYS:CB	2:J:648:CYS:SG	2.97	0.53
2:L:568:LYS:HE2	5:L:3099:HOH:O	2.07	0.53
2:B:528:ASN:HB3	2:B:646:ASN:ND2	2.24	0.53
1:I:116:GLU:HG3	1:I:116:GLU:O	2.08	0.53
2:F:525:HIS:O	2:F:526:HIS:ND1	2.38	0.53
2:H:633:ILE:HD11	2:H:639:GLU:HB2	1.89	0.53
1:E:208:ASN:HD22	1:E:208:ASN:N	2.05	0.53
2:H:560:ASN:N	2:H:560:ASN:ND2	2.55	0.53
1:K:41:HIS:HB3	1:K:298:ILE:HD13	1.90	0.53
1:A:35:ASN:ND2	1:A:37:LEU:H	2.07	0.53
2:B:630:ALA:HB2	2:B:640:PHE:HA	1.90	0.53
1:A:327:ARG:HD2	1:A:327:ARG:C	2.28	0.53
2:F:642:HIS:HE1	2:F:644:CYS:HB3	1.72	0.53
1:C:261:ARG:CD	1:C:261:ARG:N	2.72	0.53
1:E:302:THR:HB	1:E:306:CYS:SG	2.48	0.53
1:A:41:HIS:HB3	1:A:298:ILE:HD13	1.91	0.53
2:B:629:ASN:HD21	2:B:659:TYR:C	2.12	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:193:ASN:ND2	1:C:193:ASN:H	2.06	0.53
2:F:644:CYS:HB2	2:F:648:CYS:HB3	1.91	0.52
1:E:123:LYS:HG3	1:E:152:LEU:HD11	1.91	0.52
1:I:217:ILE:N	1:I:217:ILE:HD12	2.24	0.52
2:B:627:LYS:HD2	2:B:660:PRO:CB	2.39	0.52
1:C:281:LYS:HD2	5:C:3199:HOH:O	2.08	0.52
1:K:7:ILE:O	1:K:7:ILE:HG23	2.09	0.52
2:F:645:ASP:O	2:F:649:MET:HG2	2.09	0.52
5:A:3285:HOH:O	1:E:219:GLU:HG3	2.08	0.52
1:C:27:ASN:HB2	5:C:3252:HOH:O	2.10	0.52
1:A:27:ASN:ND2	4:A:3017:NAG:C4	2.53	0.52
1:C:272:ASN:HB2	5:C:3268:HOH:O	2.10	0.52
1:E:321:LEU:HD23	1:E:321:LEU:N	2.24	0.52
1:A:135:VAL:HG12	1:A:145:SER:HB3	1.92	0.52
1:K:78:ARG:NH2	1:K:261:ARG:HH22	2.08	0.52
1:E:132:THR:HB	1:E:152:LEU:HD13	1.92	0.52
1:I:302:THR:HB	1:I:306:CYS:SG	2.50	0.52
1:A:115:PHE:HD1	1:A:115:PHE:C	2.13	0.52
2:D:530:GLN:HE22	2:D:645:ASP:HB2	1.74	0.52
1:I:327:ARG:HD2	1:I:327:ARG:C	2.30	0.52
2:B:659:TYR:N	2:B:660:PRO:CD	2.67	0.51
1:C:302:THR:HB	1:C:306:CYS:SG	2.50	0.51
1:G:115:PHE:HD1	1:G:115:PHE:C	2.13	0.51
1:K:90:GLU:HG2	5:K:3315:HOH:O	2.10	0.51
1:K:116:GLU:O	1:K:116:GLU:HG3	2.09	0.51
1:A:7:ILE:HG23	1:A:7:ILE:O	2.09	0.51
1:C:219:GLU:HG3	5:E:3269:HOH:O	2.10	0.51
1:G:130:HIS:HD2	5:G:3093:HOH:O	1.92	0.51
1:K:45:LYS:HG2	1:K:276:HIS:CD2	2.45	0.51
1:A:115:PHE:CD1	1:A:115:PHE:C	2.84	0.51
1:G:180:TRP:CH2	1:G:235:THR:HG23	2.45	0.51
1:E:327:ARG:HD2	1:E:327:ARG:C	2.31	0.51
1:A:317:MET:HE3	2:B:555:VAL:HG11	1.91	0.51
1:I:42:ASN:O	1:I:44:GLY:N	2.44	0.51
2:L:654:ASN:HD21	4:L:3016:NAG:C4	2.24	0.51
1:E:23:VAL:HG22	2:F:602:LEU:HD12	1.93	0.51
1:K:124:GLU:O	1:K:125:SER:HB3	2.10	0.51
1:G:115:PHE:CD1	1:G:115:PHE:C	2.84	0.51
2:B:558:LYS:HG3	2:F:598:LEU:CD2	2.40	0.51
2:L:528:ASN:HD22	2:L:646:ASN:HD22	1.56	0.51
1:G:42:ASN:C	1:G:42:ASN:ND2	2.64	0.51
1:G:135:VAL:CG1	1:G:136:THR:N	2.74	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:115:PHE:CD1	1:K:115:PHE:C	2.85	0.51
1:K:35:ASN:ND2	1:K:37:LEU:H	2.09	0.51
1:K:78:ARG:HH21	1:K:261:ARG:HH22	1.58	0.51
2:D:530:GLN:HE21	2:D:645:ASP:HB2	1.73	0.51
2:J:598:LEU:CD2	2:L:558:LYS:HG3	2.41	0.51
1:A:54:LEU:HD13	1:A:77:VAL:HG11	1.94	0.50
1:C:95:TYR:HD2	1:C:230:MET:HB2	1.76	0.50
2:B:509:PHE:O	2:B:635:ASN:HB3	2.12	0.50
1:I:290:ASN:ND2	4:I:3013:NAG:O6	2.45	0.50
1:E:186:PRO:HD2	1:E:190:GLU:OE2	2.11	0.50
1:I:192:GLN:NE2	1:I:198:GLU:HB2	2.24	0.50
2:L:651:SER:HA	4:L:3016:NAG:O4	2.12	0.50
1:G:118:PHE:HB3	5:G:3097:HOH:O	2.12	0.50
2:D:598:LEU:CD2	2:F:558:LYS:HG3	2.41	0.50
1:I:95:TYR:HD2	1:I:230:MET:HB2	1.77	0.50
2:H:633:ILE:CD1	2:H:639:GLU:HB2	2.42	0.50
1:I:208:ASN:H	1:I:208:ASN:HD22	1.59	0.50
1:C:115:PHE:CD1	1:C:115:PHE:C	2.85	0.50
1:C:115:PHE:C	1:C:115:PHE:HD1	2.15	0.50
2:B:528:ASN:ND2	2:B:646:ASN:N	2.59	0.50
1:A:157:LYS:HG2	1:A:158:GLU:HG3	1.94	0.50
2:D:517:MET:SD	2:D:523:GLY:HA3	2.52	0.50
1:G:115:PHE:HD1	1:G:115:PHE:O	1.95	0.50
1:A:100:ILE:HD12	1:A:100:ILE:N	2.26	0.50
1:K:115:PHE:HD1	1:K:115:PHE:C	2.14	0.49
1:K:57:GLY:O	1:K:89:SER:HB3	2.11	0.49
1:K:97:GLY:HA3	1:K:230:MET:O	2.12	0.49
1:G:238:LYS:N	1:G:238:LYS:HZ2	2.02	0.49
1:G:180:TRP:HH2	1:G:235:THR:HG23	1.76	0.49
1:E:94:CYS:O	1:E:224:ARG:HD3	2.12	0.49
1:E:95:TYR:HD2	1:E:230:MET:HB2	1.76	0.49
1:C:100:ILE:HD12	1:C:100:ILE:N	2.27	0.49
1:I:115:PHE:HD1	1:I:115:PHE:C	2.15	0.49
2:H:503:PHE:CZ	2:L:502:LEU:HG	2.48	0.49
1:G:327:ARG:C	1:G:327:ARG:HD2	2.32	0.49
1:A:208:ASN:OD1	1:A:238:LYS:HD3	2.11	0.49
1:A:208:ASN:ND2	1:A:238:LYS:HZ2	2.10	0.49
2:D:528:ASN:HD22	2:D:645:ASP:HA	1.77	0.49
1:I:115:PHE:CD1	1:I:115:PHE:C	2.86	0.49
1:A:269:ILE:HG23	1:A:303:ILE:HD11	1.95	0.49
2:D:526:HIS:HB2	2:D:649:MET:CE	2.41	0.49
2:B:572:LYS:NZ	5:B:3038:HOH:O	2.38	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:647:GLU:OE2	4:B:3019:NAG:O7	2.30	0.49
1:G:208:ASN:HD22	1:G:208:ASN:N	2.07	0.49
1:I:261:ARG:N	1:I:261:ARG:CD	2.76	0.49
1:A:164:LEU:C	1:A:164:LEU:HD12	2.33	0.49
1:C:97:GLY:HA3	1:C:230:MET:O	2.13	0.49
1:G:41:HIS:HB3	1:G:298:ILE:HD13	1.95	0.49
1:K:317:MET:HE2	2:L:600:VAL:HG22	1.94	0.49
2:J:645:ASP:O	2:J:649:MET:HG2	2.12	0.49
1:K:42:ASN:HB3	1:K:44:GLY:O	2.12	0.49
1:E:61:ILE:HD11	1:E:268:ILE:HD13	1.93	0.49
1:K:180:TRP:HB3	1:K:254:PRO:HG3	1.94	0.49
1:I:51:ILE:HD12	1:I:51:ILE:N	2.28	0.49
2:J:646:ASN:HD22	2:J:646:ASN:N	2.11	0.49
1:K:261:ARG:CD	1:K:261:ARG:N	2.76	0.49
1:A:114:SER:O	1:A:261:ARG:HD3	2.13	0.49
1:I:193:ASN:HD22	1:I:193:ASN:C	2.16	0.49
1:K:42:ASN:C	1:K:44:GLY:O	2.41	0.49
2:D:644:CYS:O	2:D:648:CYS:HB3	2.12	0.48
1:I:57:GLY:O	1:I:89:SER:HB3	2.13	0.48
1:I:85:GLU:O	1:I:270:THR:HA	2.12	0.48
1:I:14:ASN:OD1	1:I:16:SER:HB3	2.13	0.48
1:E:7:ILE:HG23	1:E:7:ILE:O	2.12	0.48
1:E:35:ASN:HD22	1:E:36:LEU:H	1.60	0.48
1:A:135:VAL:CG1	1:A:136:THR:N	2.77	0.48
1:E:107:GLU:OE2	2:F:568:LYS:HE3	2.13	0.48
1:I:321:LEU:N	1:I:321:LEU:HD23	2.27	0.48
2:H:530:GLN:HE21	2:H:645:ASP:HB2	1.74	0.48
2:F:631:LYS:HE2	2:F:639:GLU:OE1	2.13	0.48
2:L:528:ASN:ND2	2:L:646:ASN:ND2	2.51	0.48
2:J:528:ASN:ND2	2:J:645:ASP:HA	2.21	0.48
1:A:42:ASN:ND2	1:A:288:ALA:H	2.11	0.48
1:A:42:ASN:O	1:A:45:LYS:HG3	2.13	0.48
1:G:164:LEU:HD12	1:G:164:LEU:C	2.33	0.48
1:I:93:ILE:O	1:I:93:ILE:HG13	2.13	0.48
1:I:164:LEU:C	1:I:164:LEU:HD12	2.33	0.48
1:K:185:PRO:HG2	1:K:191:GLN:HE21	1.78	0.48
1:C:269:ILE:HG23	1:C:303:ILE:HD11	1.96	0.48
1:A:51:ILE:N	1:A:51:ILE:HD12	2.28	0.48
1:E:119:GLU:HG3	1:E:256:TYR:CZ	2.49	0.48
2:B:633:ILE:CD1	2:B:639:GLU:HB2	2.39	0.48
1:K:58:LYS:N	1:K:58:LYS:HD3	2.28	0.48
1:C:56:LEU:HD12	1:C:85:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:208:ASN:N	1:K:208:ASN:HD22	2.08	0.48
2:H:570:PHE:CE1	2:H:577:MET:HG2	2.49	0.48
1:E:115:PHE:CD1	1:E:115:PHE:C	2.87	0.48
1:C:164:LEU:O	1:C:164:LEU:HD12	2.14	0.48
1:K:174:LYS:CE	1:K:261:ARG:HG3	2.39	0.48
2:B:558:LYS:HG3	2:F:598:LEU:HD21	1.95	0.48
2:J:571:ASN:OD1	2:J:574:GLU:HG3	2.14	0.48
1:C:58:LYS:HE2	1:C:70:GLU:O	2.14	0.48
2:J:502:LEU:HG	2:L:503:PHE:CZ	2.49	0.48
1:G:310:VAL:HG23	2:H:593:THR:CA	2.39	0.47
1:I:97:GLY:HA3	1:I:230:MET:O	2.14	0.47
2:H:527:GLN:HG3	2:H:527:GLN:O	2.13	0.47
1:E:53:PRO:HG3	1:E:82:TYR:CE2	2.49	0.47
1:G:135:VAL:HG12	1:G:136:THR:N	2.28	0.47
1:C:180:TRP:CH2	1:C:235:THR:HG23	2.48	0.47
1:K:54:LEU:HD13	1:K:77:VAL:HG11	1.95	0.47
1:G:100:ILE:N	1:G:100:ILE:HD12	2.29	0.47
2:B:598:LEU:HD21	2:D:558:LYS:HG3	1.95	0.47
1:A:208:ASN:HD21	1:A:238:LYS:NZ	2.12	0.47
1:C:187:ASN:HD22	1:C:190:GLU:H	1.61	0.47
1:A:7:ILE:CG2	2:B:640:PHE:HE1	2.27	0.47
1:K:8:CYS:O	2:L:524:TYR:HA	2.14	0.47
1:I:100:ILE:N	1:I:100:ILE:HD12	2.30	0.47
1:K:217:ILE:HD12	1:K:217:ILE:N	2.29	0.47
1:G:132:THR:HG22	1:G:154:LEU:CD2	2.44	0.47
1:E:53:PRO:HG3	1:E:82:TYR:CZ	2.49	0.47
1:G:27:ASN:ND2	4:G:3011:NAG:C6	2.72	0.47
1:G:42:ASN:HD22	1:G:44:GLY:N	2.12	0.47
2:D:560:ASN:HD22	2:D:560:ASN:C	2.17	0.47
1:A:185:PRO:HG2	1:A:191:GLN:NE2	2.30	0.47
1:E:164:LEU:C	1:E:164:LEU:HD12	2.35	0.47
1:E:85:GLU:O	1:E:270:THR:HA	2.15	0.47
1:C:192:GLN:O	1:C:196:GLN:HA	2.14	0.47
1:A:78:ARG:NH2	1:A:116:GLU:HB3	2.30	0.47
2:L:541:THR:O	2:L:545:ILE:HG13	2.15	0.47
2:B:650:GLU:HA	2:B:653:ARG:NH1	2.29	0.47
1:I:35:ASN:ND2	5:I:3157:HOH:O	2.48	0.47
1:G:37:LEU:HB2	1:G:315:LEU:HB2	1.97	0.47
1:C:130:HIS:HD2	5:C:3250:HOH:O	1.97	0.47
1:C:130:HIS:CE1	1:C:162:PRO:HD2	2.50	0.47
2:D:541:THR:O	2:D:545:ILE:HG13	2.15	0.47
1:G:310:VAL:HG22	1:G:312:SER:H	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:17:THR:HG22	5:I:3286:HOH:O	2.14	0.47
1:E:311:ARG:NH1	2:F:590:ASP:OD1	2.44	0.47
2:H:627:LYS:CD	2:H:660:PRO:HB3	2.40	0.46
1:I:42:ASN:C	1:I:44:GLY:N	2.69	0.46
1:I:44:GLY:O	1:I:45:LYS:HB2	2.16	0.46
1:G:294:PRO:HG2	1:G:295:TYR:CD1	2.50	0.46
1:C:37:LEU:HB2	1:C:315:LEU:HB2	1.98	0.46
1:C:13:ALA:O	2:D:515:THR:HA	2.14	0.46
1:G:8:CYS:C	1:G:9:ILE:HD12	2.36	0.46
1:K:187:ASN:ND2	1:K:190:GLU:H	2.13	0.46
4:K:3015:NAG:H82	4:K:3015:NAG:O1	2.16	0.46
2:B:656:THR:O	2:B:657:TYR:C	2.54	0.46
2:H:528:ASN:ND2	2:H:530:GLN:HG3	2.30	0.46
1:G:47:CYS:HG	1:G:278:CYS:HB3	1.79	0.46
2:L:517:MET:SD	2:L:523:GLY:HA3	2.55	0.46
2:B:517:MET:SD	2:B:523:GLY:HA3	2.55	0.46
1:I:48:ARG:CZ	5:I:3271:HOH:O	2.63	0.46
1:G:53:PRO:HD2	1:G:275:MET:CE	2.46	0.46
2:F:517:MET:SD	2:F:523:GLY:HA3	2.55	0.46
1:G:280:THR:HG22	1:G:281:LYS:N	2.30	0.46
1:E:115:PHE:HD1	1:E:115:PHE:C	2.17	0.46
1:E:8:CYS:O	2:F:524:TYR:HA	2.16	0.46
2:L:625:GLN:NE2	2:L:655:GLY:HA2	2.31	0.46
2:H:659:TYR:N	2:H:660:PRO:CD	2.73	0.46
1:K:94:CYS:O	1:K:224:ARG:HD3	2.16	0.46
1:I:9:ILE:N	1:I:9:ILE:HD12	2.30	0.46
1:C:193:ASN:HD22	1:C:193:ASN:N	2.14	0.46
1:A:115:PHE:HD1	1:A:115:PHE:O	1.99	0.46
1:C:193:ASN:ND2	1:C:193:ASN:N	2.62	0.46
2:J:519:ASP:HB2	2:J:536:ALA:CB	2.46	0.46
1:I:180:TRP:HB3	1:I:254:PRO:HG3	1.97	0.46
1:A:116:GLU:HG3	1:A:116:GLU:O	2.16	0.46
1:A:135:VAL:CG1	1:A:145:SER:HB3	2.45	0.46
1:C:164:LEU:HD12	1:C:164:LEU:C	2.35	0.46
1:G:9:ILE:N	1:G:9:ILE:HD12	2.31	0.46
1:I:78:ARG:NH2	1:I:261:ARG:NH2	2.60	0.46
2:L:568:LYS:CE	5:L:3099:HOH:O	2.64	0.46
2:F:619:TYR:CE1	2:F:636:GLY:HA2	2.51	0.46
2:D:630:ALA:HB2	2:D:640:PHE:HA	1.98	0.46
2:J:656:THR:O	2:J:658:ASP:N	2.48	0.46
2:B:644:CYS:CB	2:B:648:CYS:SG	3.02	0.45
1:G:171:LYS:HE3	5:G:3060:HOH:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:277:GLU:HB3	5:E:3341:HOH:O	2.16	0.45
2:B:633:ILE:CD1	2:B:633:ILE:N	2.75	0.45
1:G:163:LYS:CE	1:G:201:TYR:OH	2.64	0.45
1:I:58:LYS:C	1:I:89:SER:HA	2.36	0.45
1:K:305:GLU:HB3	2:L:561:ILE:HD12	1.98	0.45
1:G:75:LEU:N	1:G:76:PRO:HD2	2.31	0.45
1:E:217:ILE:N	1:E:217:ILE:HD12	2.30	0.45
2:L:509:PHE:O	2:L:635:ASN:HA	2.16	0.45
1:C:85:GLU:O	1:C:270:THR:HA	2.16	0.45
1:E:130:HIS:HD2	5:E:3071:HOH:O	2.00	0.45
1:G:6:THR:HG22	2:H:639:GLU:HG3	1.99	0.45
1:E:95:TYR:CD2	1:E:230:MET:HB2	2.50	0.45
1:A:208:ASN:ND2	1:A:238:LYS:NZ	2.64	0.45
1:G:208:ASN:OD1	1:G:238:LYS:HD3	2.17	0.45
2:L:566:VAL:HG23	5:L:3099:HOH:O	2.16	0.45
1:E:97:GLY:HA3	1:E:230:MET:O	2.17	0.45
1:A:78:ARG:NH2	1:A:261:ARG:HH22	2.15	0.45
1:C:180:TRP:HH2	1:C:235:THR:HG23	1.82	0.45
1:A:75:LEU:N	1:A:76:PRO:HD2	2.31	0.45
2:H:526:HIS:CD2	2:H:649:MET:HG3	2.51	0.45
1:I:276:HIS:ND1	5:I:3185:HOH:O	2.14	0.45
1:E:44:GLY:O	1:E:45:LYS:HB2	2.17	0.45
1:C:115:PHE:HD1	1:C:115:PHE:O	2.00	0.45
1:K:94:CYS:HB2	1:K:138:ALA:O	2.16	0.45
1:A:12:HIS:HB2	2:B:520:GLY:O	2.16	0.45
1:G:245:PHE:CZ	1:G:254:PRO:HG2	2.51	0.45
1:K:59:CYS:O	1:K:89:SER:HB2	2.17	0.45
5:I:3199:HOH:O	2:J:569:GLU:HG3	2.17	0.45
1:G:219:GLU:OE2	1:I:165:LYS:NZ	2.46	0.45
2:B:631:LYS:HE3	2:B:633:ILE:HG13	1.98	0.45
1:A:49(A):LYS:HE3	5:A:3254:HOH:O	2.16	0.45
1:C:183:HIS:CE1	1:C:185:PRO:HG3	2.52	0.45
2:D:571:ASN:CG	5:D:711:HOH:O	2.55	0.44
1:G:35:ASN:ND2	1:G:37:LEU:H	2.14	0.44
1:E:163:LYS:CE	1:E:201:TYR:OH	2.65	0.44
1:G:54:LEU:HD13	1:G:77:VAL:HG11	1.99	0.44
1:A:208:ASN:HD22	1:A:208:ASN:N	2.13	0.44
2:D:644:CYS:O	2:D:645:ASP:C	2.56	0.44
1:A:42:ASN:C	1:A:42:ASN:ND2	2.70	0.44
1:C:195:TYR:O	1:C:197:ASN:N	2.49	0.44
2:H:629:ASN:ND2	2:H:659:TYR:O	2.41	0.44
1:I:42:ASN:HB3	1:I:45:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:58:LYS:NZ	5:C:3159:HOH:O	2.49	0.44
1:E:42:ASN:ND2	1:E:288:ALA:HB3	2.33	0.44
1:G:135:VAL:HG13	1:G:146:SER:N	2.33	0.44
1:I:35:ASN:HD22	1:I:36:LEU:H	1.66	0.44
1:G:119:GLU:OE2	1:G:122:PRO:HA	2.17	0.44
1:I:310:VAL:HG13	2:J:593:THR:HG23	1.99	0.44
2:J:642:HIS:O	2:J:643:LYS:HB2	2.17	0.44
1:G:253:ALA:HA	1:G:254:PRO:HD3	1.84	0.44
1:K:161:TYR:CZ	1:K:249:GLY:HA2	2.52	0.44
2:B:568:LYS:HG2	5:B:3118:HOH:O	2.17	0.44
1:I:294:PRO:HG2	1:I:295:TYR:CD1	2.53	0.44
1:G:208:ASN:OD1	1:G:238:LYS:HE2	2.18	0.44
1:C:42:ASN:HB2	1:C:45:LYS:HE3	2.00	0.44
1:K:261:ARG:HD2	1:K:261:ARG:N	2.33	0.44
1:I:5:ASP:HB2	2:J:643:LYS:HD2	2.00	0.44
1:G:58:LYS:CE	1:G:58:LYS:H	2.30	0.44
1:K:6:THR:O	2:L:526:HIS:HA	2.18	0.44
1:G:302:THR:HG23	1:G:306:CYS:SG	2.57	0.44
1:I:54:LEU:HD13	1:I:77:VAL:HG11	1.99	0.44
1:G:281:LYS:HB2	1:G:281:LYS:NZ	2.32	0.44
1:C:126:SER:C	1:C:128:PRO:HD3	2.37	0.44
1:G:134:GLY:HA2	3:G:3030:SIA:H113	2.00	0.44
2:J:621:LYS:NZ	5:J:3041:HOH:O	2.51	0.44
1:E:100:ILE:HD12	1:E:100:ILE:N	2.32	0.44
1:A:94:CYS:O	1:A:224:ARG:HD3	2.17	0.44
2:D:528:ASN:HD21	2:D:530:GLN:HB2	1.83	0.44
1:A:116:GLU:CG	1:A:259:ALA:HB3	2.44	0.44
1:G:96:PRO:HB3	1:G:223:VAL:HB	2.00	0.44
1:K:7:ILE:HA	2:L:526:HIS:HA	2.00	0.43
1:C:245:PHE:CZ	1:C:254:PRO:HG2	2.53	0.43
2:D:607:THR:O	2:D:610:PHE:HB3	2.18	0.43
1:I:311:ARG:NH1	2:J:590:ASP:OD1	2.47	0.43
1:C:56:LEU:HD12	1:C:85:GLU:CG	2.48	0.43
1:A:165:LYS:HA	1:A:245:PHE:O	2.17	0.43
1:E:37:LEU:HB2	1:E:315:LEU:HB2	2.00	0.43
1:E:35:ASN:ND2	1:E:36:LEU:N	2.67	0.43
1:A:78:ARG:HH21	1:A:116:GLU:HB3	1.83	0.43
1:A:261:ARG:N	1:A:261:ARG:CD	2.82	0.43
2:L:525:HIS:O	2:L:533:GLY:O	2.36	0.43
1:G:180:TRP:HB3	1:G:254:PRO:HG3	2.01	0.43
2:L:643:LYS:HD3	2:L:643:LYS:HA	1.86	0.43
1:E:261:ARG:CD	1:E:261:ARG:N	2.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:650:GLU:OE2	2:B:653:ARG:HD2	2.19	0.43
1:A:269:ILE:CG2	1:A:303:ILE:HD11	2.48	0.43
1:A:238:LYS:NZ	1:A:241:ASP:OD1	2.51	0.43
2:H:642:HIS:O	2:H:643:LYS:O	2.37	0.43
1:G:135:VAL:CG1	1:G:145:SER:HB3	2.48	0.43
2:D:526:HIS:O	2:D:532:SER:HA	2.18	0.43
2:H:541:THR:O	2:H:545:ILE:HG13	2.19	0.43
1:G:261:ARG:N	1:G:261:ARG:CD	2.80	0.43
1:C:217:ILE:HD12	1:C:217:ILE:N	2.33	0.43
2:B:654:ASN:ND2	4:B:3019:NAG:H3	2.34	0.43
1:E:190:GLU:HA	1:E:193:ASN:OD1	2.19	0.43
1:E:327:ARG:HD2	1:E:327:ARG:O	2.18	0.43
1:A:102:TYR:CE2	1:A:106:ARG:HD2	2.53	0.43
2:D:568:LYS:HG2	5:D:765:HOH:O	2.17	0.43
2:J:647:GLU:CD	4:J:3014:NAG:HO1	2.22	0.43
2:B:503:PHE:CZ	2:F:502:LEU:HG	2.53	0.43
1:I:53:PRO:HG3	1:I:82:TYR:CE2	2.53	0.43
1:G:7:ILE:O	1:G:7:ILE:HG23	2.18	0.43
2:J:541:THR:O	2:J:545:ILE:HG13	2.18	0.43
1:G:98:ASP:HB2	5:I:3293:HOH:O	2.19	0.43
1:A:208:ASN:ND2	1:A:208:ASN:H	2.16	0.43
1:C:95:TYR:CD2	1:C:230:MET:HB2	2.54	0.43
1:G:30:VAL:HG21	1:G:318:VAL:HG23	2.00	0.43
1:C:7:ILE:O	1:C:7:ILE:HG23	2.19	0.43
2:J:554:SER:O	2:J:558:LYS:HG2	2.19	0.43
2:L:625:GLN:HE22	2:L:655:GLY:HA2	1.83	0.43
1:G:27:ASN:CG	4:G:3011:NAG:C6	2.87	0.42
1:I:186:PRO:HD2	1:I:190:GLU:OE2	2.18	0.42
1:A:23:VAL:CG1	2:D:551:LYS:HG3	2.49	0.42
1:C:209:TYR:CE1	1:C:235:THR:HG22	2.54	0.42
1:K:186:PRO:HD2	1:K:190:GLU:OE2	2.19	0.42
1:K:62:ALA:HB2	1:K:102:TYR:CE1	2.54	0.42
1:C:93:ILE:HG13	1:C:93:ILE:O	2.19	0.42
1:I:71:CYS:HB3	1:I:74:LEU:HD12	2.00	0.42
2:J:517:MET:HE3	2:J:536:ALA:N	2.35	0.42
1:I:37:LEU:HB2	1:I:315:LEU:HB2	2.01	0.42
2:B:504:GLY:O	2:B:508:GLY:HA3	2.20	0.42
2:F:541:THR:O	2:F:545:ILE:HG13	2.19	0.42
2:F:508:GLY:C	2:F:510:ILE:H	2.20	0.42
1:G:94:CYS:HB2	1:G:138:ALA:O	2.19	0.42
1:I:5:ASP:N	2:J:643:LYS:HZ2	2.17	0.42
2:B:560:ASN:ND2	2:B:560:ASN:H	2.17	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:281:LYS:HE3	5:C:3300:HOH:O	2.18	0.42
2:D:572:LYS:NZ	5:D:721:HOH:O	2.46	0.42
1:I:179:LEU:HD23	1:I:234:TRP:HB3	2.01	0.42
1:A:180:TRP:HB3	1:A:254:PRO:HG3	2.02	0.42
2:L:528:ASN:ND2	2:L:646:ASN:N	2.66	0.42
1:G:172:LYS:NZ	5:G:3097:HOH:O	2.48	0.42
1:A:8:CYS:O	2:B:524:TYR:HA	2.20	0.42
1:A:72:ASP:N	1:A:73:PRO:CD	2.83	0.42
1:C:208:ASN:H	1:C:208:ASN:ND2	2.17	0.42
2:H:633:ILE:HG22	2:H:634:GLY:N	2.35	0.42
1:K:130:HIS:HD2	5:K:3076:HOH:O	2.02	0.42
1:K:100:ILE:N	1:K:100:ILE:HD12	2.35	0.42
1:A:42:ASN:HD21	1:A:288:ALA:H	1.67	0.42
1:G:165:LYS:HA	1:G:245:PHE:O	2.20	0.42
1:I:30:VAL:HG11	1:I:318:VAL:HG21	2.01	0.42
2:J:625:GLN:HE22	2:J:655:GLY:C	2.23	0.42
1:G:135:VAL:HG13	1:G:146:SER:CA	2.50	0.42
1:K:185:PRO:HG2	1:K:191:GLN:NE2	2.35	0.42
1:E:52:ALA:HA	1:E:53:PRO:HD3	1.84	0.42
1:G:94:CYS:O	1:G:224:ARG:HD3	2.20	0.42
1:E:305:GLU:HB3	2:F:561:ILE:HG12	2.01	0.42
1:I:132:THR:HG22	1:I:154:LEU:CD2	2.50	0.42
1:C:12:HIS:HB2	2:D:520:GLY:O	2.19	0.42
2:D:619:TYR:CE1	2:D:636:GLY:HA2	2.54	0.42
2:L:528:ASN:HB3	5:L:3066:HOH:O	2.19	0.42
1:G:42:ASN:O	1:G:45:LYS:HE3	2.20	0.42
1:I:42:ASN:CB	1:I:44:GLY:O	2.68	0.42
2:J:633:ILE:HD12	2:J:637:CYS:HB2	2.01	0.42
1:K:58:LYS:HE3	5:K:3301:HOH:O	2.19	0.42
1:E:23:VAL:CG2	2:F:602:LEU:HD12	2.50	0.42
2:J:598:LEU:O	2:J:602:LEU:HD13	2.20	0.42
1:C:319:THR:O	2:D:548:ILE:HD13	2.20	0.42
2:L:627:LYS:HD2	2:L:659:TYR:CE1	2.55	0.41
1:I:119:GLU:HG3	1:I:256:TYR:CZ	2.55	0.41
2:H:527:GLN:HA	2:H:532:SER:HA	2.02	0.41
2:F:524:TYR:CE1	2:F:537:ASP:HB2	2.54	0.41
2:D:580:LEU:HD11	2:F:580:LEU:HD13	2.01	0.41
1:G:102:TYR:CE2	1:G:106:ARG:HD2	2.55	0.41
2:B:629:ASN:ND2	2:B:659:TYR:O	2.42	0.41
2:H:645:ASP:O	2:H:649:MET:HG2	2.20	0.41
1:K:208:ASN:H	1:K:208:ASN:ND2	2.16	0.41
1:K:23:VAL:CG2	2:L:602:LEU:HD12	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:327:ARG:HD2	1:I:327:ARG:O	2.20	0.41
2:H:504:GLY:O	2:H:508:GLY:HA3	2.20	0.41
2:H:633:ILE:HD11	2:H:639:GLU:CB	2.50	0.41
1:G:208:ASN:ND2	1:G:208:ASN:N	2.69	0.41
1:A:23:VAL:HG12	2:D:551:LYS:HG3	2.02	0.41
1:A:185:PRO:HG2	1:A:191:GLN:HE21	1.86	0.41
1:I:94:CYS:HB2	1:I:138:ALA:O	2.20	0.41
1:I:6:THR:HG22	1:I:7:ILE:N	2.35	0.41
1:I:7:ILE:HG23	1:I:7:ILE:O	2.19	0.41
5:A:3080:HOH:O	2:B:569:GLU:HG3	2.19	0.41
1:G:42:ASN:ND2	1:G:288:ALA:H	2.18	0.41
1:K:114:SER:O	1:K:261:ARG:HD3	2.20	0.41
1:I:217:ILE:CD1	1:I:217:ILE:N	2.83	0.41
1:G:219:GLU:HG2	5:G:3193:HOH:O	2.20	0.41
1:C:94:CYS:HB2	1:C:138:ALA:O	2.20	0.41
2:B:561:ILE:HA	5:B:3079:HOH:O	2.20	0.41
1:A:208:ASN:N	1:A:208:ASN:ND2	2.69	0.41
2:J:530:GLN:NE2	2:J:645:ASP:HB2	2.35	0.41
1:C:68:ASN:HB3	1:C:71:CYS:SG	2.60	0.41
2:L:647:GLU:OE2	4:L:3016:NAG:N2	2.54	0.41
1:G:295:TYR:CZ	2:H:559:MET:HG3	2.56	0.41
1:E:61:ILE:HD11	1:E:268:ILE:CD1	2.49	0.41
1:I:245:PHE:CZ	1:I:254:PRO:HG2	2.56	0.41
2:B:528:ASN:ND2	2:B:529:GLU:OE1	2.54	0.41
1:E:289:ILE:CD1	1:E:298:ILE:HD12	2.50	0.41
1:I:35:ASN:HD22	1:I:36:LEU:N	2.19	0.41
1:E:119:GLU:HG3	1:E:256:TYR:CE2	2.56	0.41
1:G:35:ASN:ND2	5:G:3077:HOH:O	2.54	0.41
1:G:114:SER:OG	1:G:261:ARG:NH1	2.54	0.41
1:I:303:ILE:HD13	2:J:564:THR:HG23	2.03	0.41
2:D:650:GLU:OE2	2:D:653:ARG:NH1	2.54	0.41
2:B:654:ASN:OD1	2:B:656:THR:HG23	2.20	0.41
1:C:187:ASN:HD22	1:C:187:ASN:C	2.24	0.41
2:J:528:ASN:HB2	2:J:649:MET:HE2	2.03	0.41
2:B:530:GLN:HB2	2:B:646:ASN:CG	2.40	0.41
1:I:187:ASN:ND2	1:I:189:LYS:HB3	2.35	0.41
2:J:633:ILE:HG22	2:J:635:ASN:ND2	2.36	0.41
1:I:53:PRO:HG3	1:I:82:TYR:CZ	2.56	0.41
2:F:650:GLU:OE2	2:F:653:ARG:NH1	2.50	0.41
2:H:572:LYS:HE3	5:H:702:HOH:O	2.21	0.41
1:K:308:LYS:HE3	2:L:562:GLN:OE1	2.21	0.41
1:E:71:CYS:HB3	1:E:74:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:15:ASN:ND2	4:C:3020:NAG:O4	2.54	0.41
1:K:6:THR:CG2	1:K:7:ILE:N	2.85	0.41
2:F:529:GLU:HG2	2:F:530:GLN:N	2.36	0.41
1:A:299:HIS:CG	1:A:300:PRO:HD2	2.56	0.41
2:B:570:PHE:CE1	2:B:577:MET:HG2	2.55	0.41
2:F:538:GLN:HA	2:F:538:GLN:OE1	2.20	0.41
1:A:9:ILE:N	1:A:9:ILE:HD12	2.36	0.41
4:C:3020:NAG:O1	4:C:3020:NAG:H82	2.21	0.40
2:B:528:ASN:HB3	2:B:646:ASN:HD21	1.86	0.40
1:K:35:ASN:ND2	5:K:3091:HOH:O	2.54	0.40
1:K:208:ASN:N	1:K:208:ASN:ND2	2.69	0.40
1:K:7:ILE:O	1:K:7:ILE:CG2	2.69	0.40
1:E:308:LYS:HD2	2:F:559:MET:HE1	2.02	0.40
1:I:310:VAL:HG13	2:J:593:THR:HA	2.03	0.40
2:L:633:ILE:N	2:L:633:ILE:HD12	2.36	0.40
1:C:269:ILE:CG2	1:C:303:ILE:HD11	2.51	0.40
1:G:46:LEU:HB2	1:G:275:MET:HA	2.02	0.40
1:G:20:VAL:HG21	1:G:318:VAL:HB	2.03	0.40
2:J:524:TYR:CE1	2:J:537:ASP:HB2	2.56	0.40
2:F:633:ILE:HD12	2:F:637:CYS:HB2	2.04	0.40
2:J:528:ASN:CG	2:J:529:GLU:H	2.24	0.40
2:L:619:TYR:HE1	2:L:636:GLY:HA2	1.81	0.40
2:J:517:MET:SD	2:J:523:GLY:HA3	2.62	0.40
1:I:115:PHE:O	1:I:115:PHE:HD1	2.05	0.40
1:G:53:PRO:HB3	1:G:82:TYR:CE2	2.56	0.40
2:L:509:PHE:CD1	2:L:510:ILE:HG13	2.57	0.40
1:E:260:LEU:C	1:E:261:ARG:HD2	2.41	0.40
1:K:165:LYS:HA	1:K:245:PHE:O	2.22	0.40
1:E:165:LYS:HA	1:E:245:PHE:O	2.22	0.40
1:E:272:ASN:ND2	5:E:3108:HOH:O	2.53	0.40
1:I:310:VAL:CG1	1:I:311:ARG:N	2.84	0.40
2:B:528:ASN:CG	2:B:529:GLU:N	2.74	0.40
1:C:114:SER:O	1:C:261:ARG:HD3	2.21	0.40
1:G:290:ASN:HD21	4:G:3012:NAG:H1	1.86	0.40
1:G:62:ALA:HB2	1:G:102:TYR:CE1	2.56	0.40
1:C:220:ARG:HD2	1:C:229:ARG:HG2	2.04	0.40
2:H:538:GLN:OE1	2:H:538:GLN:HA	2.21	0.40
1:A:126:SER:C	1:A:128:PRO:HD3	2.42	0.40
1:A:71:CYS:HB3	1:A:74:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/327 (98%)	309 (96%)	11 (3%)	1 (0%)	50	53
1	C	321/327 (98%)	311 (97%)	8 (2%)	2 (1%)	33	32
1	E	319/327 (98%)	309 (97%)	8 (2%)	2 (1%)	33	32
1	G	321/327 (98%)	308 (96%)	13 (4%)	0	100	100
1	I	319/327 (98%)	307 (96%)	10 (3%)	2 (1%)	33	32
1	K	321/327 (98%)	307 (96%)	12 (4%)	2 (1%)	33	32
2	B	158/160 (99%)	139 (88%)	11 (7%)	8 (5%)	3	1
2	D	158/160 (99%)	138 (87%)	16 (10%)	4 (2%)	9	4
2	F	157/160 (98%)	140 (89%)	11 (7%)	6 (4%)	5	2
2	H	158/160 (99%)	140 (89%)	11 (7%)	7 (4%)	4	1
2	J	158/160 (99%)	145 (92%)	9 (6%)	4 (2%)	9	4
2	L	157/160 (98%)	150 (96%)	6 (4%)	1 (1%)	33	32
All	All	2868/2922 (98%)	2703 (94%)	126 (4%)	39 (1%)	16	12

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	657	TYR
2	B	659	TYR
1	C	44	GLY
2	D	645	ASP
2	D	658	ASP
2	F	529	GLU
2	H	659	TYR
1	A	125	SER
2	B	627	LYS
2	B	635	ASN
1	C	125	SER
2	D	659	TYR
1	E	125	SER

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Mol	Chain	Res	Type
2	F	528	ASN
2	F	643	LYS
2	H	643	LYS
1	I	125	SER
2	J	657	TYR
1	K	45	LYS
1	K	125	SER
2	B	643	LYS
2	F	635	ASN
2	H	627	LYS
2	H	657	TYR
2	J	658	ASP
2	B	526	HIS
2	B	658	ASP
2	D	657	TYR
1	E	45	LYS
1	I	45	LYS
2	B	633	ILE
2	H	526	HIS
2	H	658	ASP
2	J	643	LYS
2	F	527	GLN
2	L	526	HIS
2	F	633	ILE
2	H	633	ILE
2	J	659	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/287 (99%)	274 (96%)	11 (4%)	43	52
1	C	285/287 (99%)	274 (96%)	11 (4%)	43	52
1	E	285/287 (99%)	277 (97%)	8 (3%)	56	67
1	G	285/287 (99%)	273 (96%)	12 (4%)	40	48
1	I	285/287 (99%)	275 (96%)	10 (4%)	48	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	285/287 (99%)	276 (97%)	9 (3%)	51	62
2	B	136/136 (100%)	127 (93%)	9 (7%)	24	25
2	D	136/136 (100%)	127 (93%)	9 (7%)	24	25
2	F	135/136 (99%)	132 (98%)	3 (2%)	64	76
2	H	136/136 (100%)	129 (95%)	7 (5%)	33	38
2	J	136/136 (100%)	131 (96%)	5 (4%)	45	54
2	L	135/136 (99%)	130 (96%)	5 (4%)	45	54
All	All	2524/2538 (99%)	2425 (96%)	99 (4%)	43	52

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	58	LYS
1	A	99	PHE
1	A	115	PHE
1	A	156	GLU
1	A	166	ASN
1	A	187	ASN
1	A	208	ASN
1	A	238	LYS
1	A	261	ARG
1	A	321	LEU
2	B	524	TYR
2	B	526	HIS
2	B	529	GLU
2	B	560	ASN
2	B	580	LEU
2	B	602	LEU
2	B	647	GLU
2	B	658	ASP
2	B	659	TYR
1	C	35	ASN
1	C	42	ASN
1	C	58	LYS
1	C	99	PHE
1	C	115	PHE
1	C	156	GLU
1	C	187	ASN
1	C	193	ASN

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Mol	Chain	Res	Type
1	C	208	ASN
1	C	261	ARG
1	C	321	LEU
2	D	502	LEU
2	D	524	TYR
2	D	560	ASN
2	D	571	ASN
2	D	580	LEU
2	D	598	LEU
2	D	647	GLU
2	D	658	ASP
2	D	659	TYR
1	E	35	ASN
1	E	115	PHE
1	E	156	GLU
1	E	166	ASN
1	E	187	ASN
1	E	208	ASN
1	E	261	ARG
1	E	321	LEU
2	F	526	HIS
2	F	528	ASN
2	F	580	LEU
1	G	42	ASN
1	G	58	LYS
1	G	99	PHE
1	G	115	PHE
1	G	156	GLU
1	G	166	ASN
1	G	187	ASN
1	G	208	ASN
1	G	238	LYS
1	G	261	ARG
1	G	302	THR
1	G	321	LEU
2	H	522	TYR
2	H	526	HIS
2	H	560	ASN
2	H	580	LEU
2	H	602	LEU
2	H	658	ASP
2	H	659	TYR

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Mol	Chain	Res	Type
1	I	99	PHE
1	I	115	PHE
1	I	156	GLU
1	I	166	ASN
1	I	187	ASN
1	I	193	ASN
1	I	208	ASN
1	I	225	ASP
1	I	261	ARG
1	I	321	LEU
2	J	517	MET
2	J	580	LEU
2	J	598	LEU
2	J	658	ASP
2	J	659	TYR
1	K	58	LYS
1	K	99	PHE
1	K	115	PHE
1	K	166	ASN
1	K	187	ASN
1	K	208	ASN
1	K	261	ARG
1	K	302	THR
1	K	321	LEU
2	L	517	MET
2	L	526	HIS
2	L	580	LEU
2	L	633	ILE
2	L	647	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	35	ASN
1	A	42	ASN
1	A	91	ASN
1	A	130	HIS
1	A	187	ASN
1	A	191	GLN
1	A	208	ASN
1	A	250	ASN

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Mol	Chain	Res	Type
1	A	290	ASN
2	B	530	GLN
2	B	560	ASN
2	B	625	GLN
2	B	629	ASN
2	B	635	ASN
2	B	646	ASN
2	B	654	ASN
1	C	15	ASN
1	C	27	ASN
1	C	35	ASN
1	C	91	ASN
1	C	130	HIS
1	C	187	ASN
1	C	191	GLN
1	C	193	ASN
1	C	197	ASN
1	C	208	ASN
1	C	250	ASN
2	D	528	ASN
2	D	530	GLN
2	D	543	ASN
2	D	560	ASN
2	D	625	GLN
2	D	629	ASN
2	D	635	ASN
2	D	646	ASN
1	E	35	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	276	HIS
2	F	528	ASN
2	F	560	ASN
2	F	625	GLN
2	F	635	ASN
2	F	646	ASN
1	G	27	ASN

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Mol	Chain	Res	Type
1	G	35	ASN
1	G	42	ASN
1	G	91	ASN
1	G	130	HIS
1	G	187	ASN
1	G	191	GLN
1	G	208	ASN
1	G	250	ASN
1	G	290	ASN
2	H	528	ASN
2	H	530	GLN
2	H	543	ASN
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	193	ASN
1	I	208	ASN
1	I	250	ASN
1	I	290	ASN
2	J	530	GLN
2	J	625	GLN
2	J	628	ASN
2	J	629	ASN
2	J	635	ASN
2	J	646	ASN
1	K	35	ASN
1	K	55	GLN
1	K	91	ASN
1	K	130	HIS
1	K	187	ASN
1	K	191	GLN
1	K	208	ASN
1	K	250	ASN
1	K	290	ASN

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Mol	Chain	Res	Type
2	L	530	GLN
2	L	625	GLN
2	L	629	ASN
2	L	642	HIS
2	L	646	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

18 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$
3	SIA	A	3021	3	20,20,21	5.16	5 (25%)	23,28,31	2.67	1 (4%)
3	GAL	A	3022	3	10,11,12	1.32	2 (20%)	11,15,17	1.04	1 (9%)
3	NAG	A	3023	3	12,14,15	0.88	0	15,19,21	0.54	0
3	SIA	C	3024	3	20,20,21	5.36	5 (25%)	23,28,31	2.67	1 (4%)
3	GAL	C	3025	3	10,11,12	1.34	2 (20%)	11,15,17	0.95	1 (9%)
3	NAG	C	3026	3	12,14,15	0.96	0	15,19,21	0.62	0
3	SIA	E	3027	3	20,20,21	5.28	5 (25%)	23,28,31	2.68	1 (4%)
3	GAL	E	3028	3	10,11,12	1.25	1 (10%)	11,15,17	1.01	1 (9%)
3	NAG	E	3029	3	12,14,15	0.93	0	15,19,21	0.61	0
3	SIA	G	3030	3	20,20,21	5.27	5 (25%)	23,28,31	2.67	1 (4%)
3	GAL	G	3031	3	10,11,12	1.32	2 (20%)	11,15,17	0.97	1 (9%)
3	NAG	G	3032	3	12,14,15	0.80	0	15,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SIA	I	3033	3	20,20,21	5.45	5 (25%)	23,28,31	2.69	1 (4%)
3	GAL	I	3034	3	10,11,12	1.41	1 (10%)	11,15,17	0.96	1 (9%)
3	NAG	I	3035	3	12,14,15	1.46	2 (16%)	15,19,21	0.81	0
3	SIA	K	3036	3	20,20,21	5.35	5 (25%)	23,28,31	2.75	1 (4%)
3	GAL	K	3037	3	10,11,12	1.34	1 (10%)	11,15,17	0.92	1 (9%)
3	NAG	K	3038	3	12,14,15	0.83	0	15,19,21	0.56	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
3	SIA	A	3021	3	-	0/15/34/38	0/1/1/1
3	GAL	A	3022	3	-	0/2/19/22	0/1/1/1
3	NAG	A	3023	3	-	0/6/23/26	0/1/1/1
3	SIA	C	3024	3	-	0/15/34/38	0/1/1/1
3	GAL	C	3025	3	-	0/2/19/22	0/1/1/1
3	NAG	C	3026	3	-	0/6/23/26	0/1/1/1
3	SIA	E	3027	3	-	0/15/34/38	0/1/1/1
3	GAL	E	3028	3	-	0/2/19/22	0/1/1/1
3	NAG	E	3029	3	-	0/6/23/26	0/1/1/1
3	SIA	G	3030	3	-	0/15/34/38	0/1/1/1
3	GAL	G	3031	3	-	0/2/19/22	0/1/1/1
3	NAG	G	3032	3	-	0/6/23/26	0/1/1/1
3	SIA	I	3033	3	-	0/15/34/38	0/1/1/1
3	GAL	I	3034	3	-	0/2/19/22	0/1/1/1
3	NAG	I	3035	3	-	0/6/23/26	0/1/1/1
3	SIA	K	3036	3	-	0/15/34/38	0/1/1/1
3	GAL	K	3037	3	-	0/2/19/22	0/1/1/1
3	NAG	K	3038	3	-	0/6/23/26	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3033	SIA	O6-C2	23.12	1.49	1.28
3	K	3036	SIA	O6-C2	22.74	1.48	1.28
3	C	3024	SIA	O6-C2	22.73	1.48	1.28
3	E	3027	SIA	O6-C2	22.28	1.48	1.28
3	G	3030	SIA	O6-C2	22.25	1.48	1.28
3	A	3021	SIA	O6-C2	21.79	1.48	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3033	SIA	C3-C4	4.36	1.57	1.52
3	K	3036	SIA	C3-C4	4.08	1.57	1.52
3	C	3024	SIA	C3-C4	4.05	1.57	1.52
3	A	3021	SIA	C3-C4	3.97	1.57	1.52
3	E	3027	SIA	C3-C4	3.89	1.56	1.52
3	G	3030	SIA	C3-C4	3.81	1.56	1.52
3	G	3030	SIA	C3-C2	3.73	1.59	1.46
3	K	3036	SIA	C3-C2	3.68	1.59	1.46
3	E	3027	SIA	C3-C2	3.55	1.59	1.46
3	A	3021	SIA	C3-C2	3.54	1.59	1.46
3	I	3033	SIA	C3-C2	3.54	1.59	1.46
3	G	3030	SIA	C6-C5	3.48	1.58	1.53
3	C	3024	SIA	C3-C2	3.47	1.59	1.46
3	E	3027	SIA	C4-C5	3.31	1.56	1.53
3	E	3027	SIA	C6-C5	3.29	1.58	1.53
3	C	3024	SIA	C4-C5	3.25	1.56	1.53
3	I	3033	SIA	C6-C5	3.15	1.58	1.53
3	A	3021	SIA	C6-C5	2.97	1.58	1.53
3	K	3036	SIA	C6-C5	2.89	1.57	1.53
3	C	3024	SIA	C6-C5	2.89	1.57	1.53
3	G	3030	SIA	C4-C5	2.76	1.55	1.53
3	I	3034	GAL	C4-C5	2.75	1.59	1.53
3	A	3021	SIA	C4-C5	2.70	1.55	1.53
3	I	3033	SIA	C4-C5	2.66	1.55	1.53
3	I	3035	NAG	C2-N2	2.56	1.49	1.46
3	K	3037	GAL	C4-C5	2.50	1.58	1.53
3	G	3031	GAL	C4-C5	2.50	1.58	1.53
3	A	3022	GAL	C4-C5	2.48	1.58	1.53
3	I	3035	NAG	O4-C4	2.34	1.48	1.43
3	C	3025	GAL	C4-C5	2.25	1.58	1.53
3	E	3028	GAL	C4-C5	2.25	1.58	1.53
3	C	3025	GAL	O5-C5	2.09	1.49	1.45
3	A	3022	GAL	O5-C5	2.09	1.49	1.45
3	G	3031	GAL	O5-C5	2.06	1.49	1.45
3	K	3036	SIA	C4-C5	2.04	1.54	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	3036	SIA	O6-C2-C3	-12.47	108.61	124.91
3	I	3033	SIA	O6-C2-C3	-12.27	108.88	124.91
3	E	3027	SIA	O6-C2-C3	-12.20	108.97	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3030	SIA	O6-C2-C3	-12.15	109.03	124.91
3	A	3021	SIA	O6-C2-C3	-12.14	109.05	124.91
3	C	3024	SIA	O6-C2-C3	-12.09	109.12	124.91
3	E	3028	GAL	O5-C5-C6	2.51	109.62	106.98
3	A	3022	GAL	O5-C5-C6	2.45	109.55	106.98
3	G	3031	GAL	O5-C5-C6	2.40	109.50	106.98
3	C	3025	GAL	O5-C5-C6	2.39	109.49	106.98
3	I	3034	GAL	O5-C5-C6	2.33	109.42	106.98
3	K	3037	GAL	O5-C5-C6	2.27	109.36	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

10 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	A	3017	-	15,15,15	0.50	0	21,21,21	0.79	0
4	NAG	A	3018	-	15,15,15	0.43	0	21,21,21	0.51	0
4	NAG	B	3019	-	15,15,15	0.47	0	21,21,21	0.58	0
4	NAG	C	3020	-	15,15,15	0.48	0	21,21,21	0.54	0
4	NAG	G	3011	-	15,15,15	0.53	0	21,21,21	0.62	0
4	NAG	G	3012	-	15,15,15	0.40	0	21,21,21	0.52	0
4	NAG	I	3013	-	15,15,15	0.62	0	21,21,21	0.64	0
4	NAG	J	3014	-	15,15,15	0.47	0	21,21,21	0.56	0
4	NAG	K	3015	-	15,15,15	0.48	0	21,21,21	0.64	0
4	NAG	L	3016	-	15,15,15	0.53	0	21,21,21	0.57	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
4	NAG	A	3017	-	-	0/6/26/26	0/1/1/1
4	NAG	A	3018	-	-	0/6/26/26	0/1/1/1
4	NAG	B	3019	-	-	0/6/26/26	0/1/1/1
4	NAG	C	3020	-	-	0/6/26/26	0/1/1/1
4	NAG	G	3011	-	-	0/6/26/26	0/1/1/1
4	NAG	G	3012	-	-	0/6/26/26	0/1/1/1
4	NAG	I	3013	-	-	0/6/26/26	0/1/1/1
4	NAG	J	3014	-	-	0/6/26/26	0/1/1/1
4	NAG	K	3015	-	-	0/6/26/26	0/1/1/1
4	NAG	L	3016	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.