Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:03 PM GMT

PDB ID	:	1RVT
Title	:	1930 H1 Hemagglutinin in complex with LSTC
Authors	:	Skehel, J.J.; Gamblin, S.J.; Haire, L.F.; Russell, R.J.; Stevens, D.J.; Xiao, B.; Ha, Y.; Vasisht, N.; Steinhauer, D.A.; Daniels, R.S.
Deposited on	:	2003-12-15
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

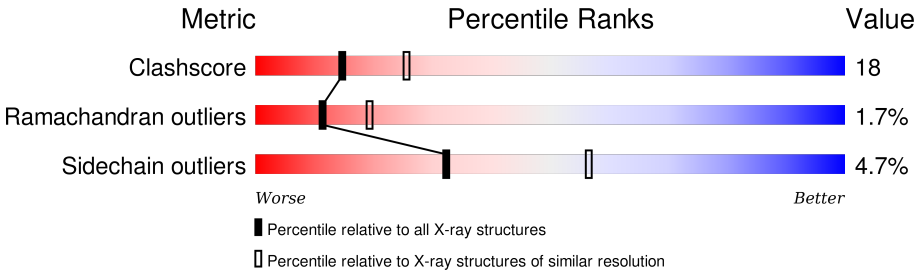
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	328	68% 28%
1	J	328	69% 27%
1	L	328	68% 28%
2	I	160	64% 31%
2	K	160	65% 29%
2	M	160	64% 31%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NDG	H	742	-	-	X	-
6	NDG	J	740	-	-	X	-
6	NDG	L	744	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12143 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.

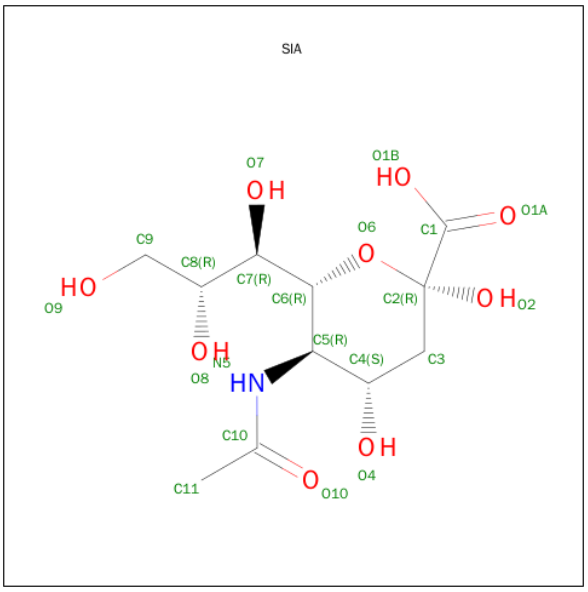
- Molecule 1 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	324	Total	C	N	O	S	0	0	0
			2511	1580	436	484	11			
1	J	324	Total	C	N	O	S	0	0	0
			2511	1580	436	484	11			
1	L	324	Total	C	N	O	S	0	0	0
			2511	1580	436	484	11			

- Molecule 2 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	160	Total	C	N	O	S	0	0	0
			1281	801	223	252	5			
2	K	160	Total	C	N	O	S	0	0	0
			1281	801	223	252	5			
2	M	160	Total	C	N	O	S	0	0	0
			1281	801	223	252	5			

- Molecule 3 is SUGAR (5-MER) (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).

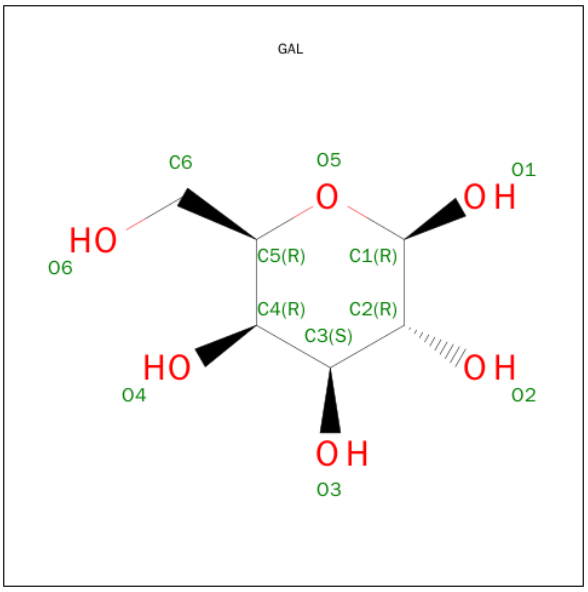


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total	C	N	O	0	0
			20	11	1	8		
3	H	1	Total	C	N	O	0	0
			20	11	1	8		
3	L	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

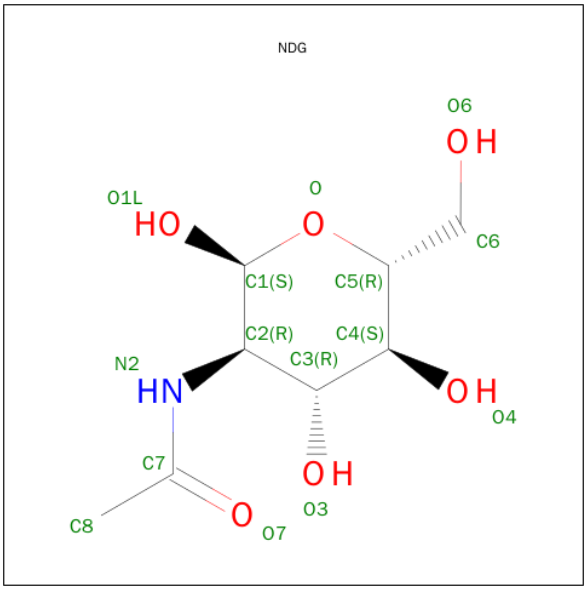
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	J	4	Total	C	N	O	0	0
			48	26	1	21		

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



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

- Molecule 6 is water (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total C N O 15 8 1 6	0	0
6	H	1	Total C N O 15 8 1 6	0	0

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	128	Total	O	0	0
			128	128		
7	I	36	Total	O	0	0
			36	36		
7	J	151	Total	O	0	0
			151	151		
7	K	44	Total	O	0	0
			44	44		
7	L	191	Total	O	0	0
			191	191		
7	M	42	Total	O	0	0
			42	42		

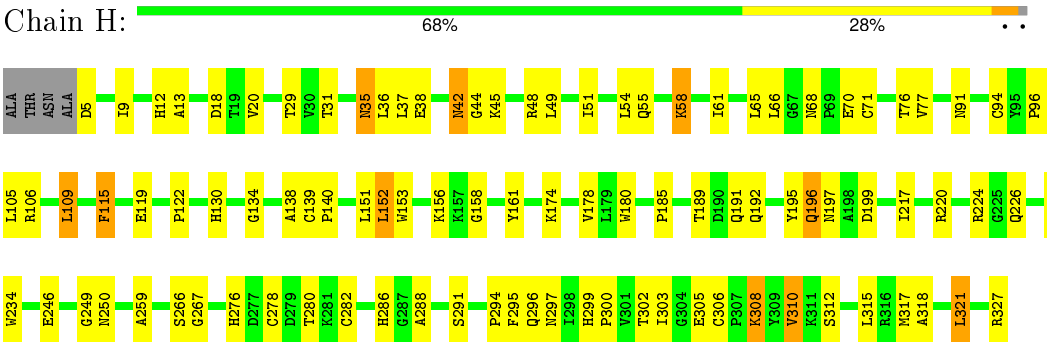
3 Residue-property plots (i)

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

Note EDS was not executed.

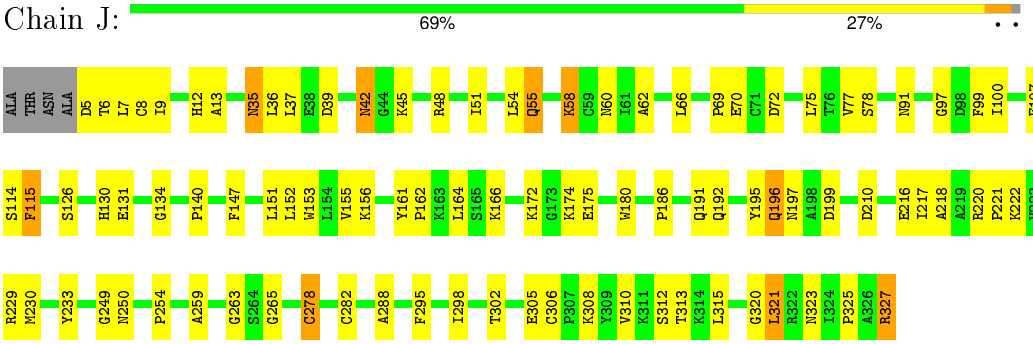
- Molecule 1: hemagglutinin

Chain H:



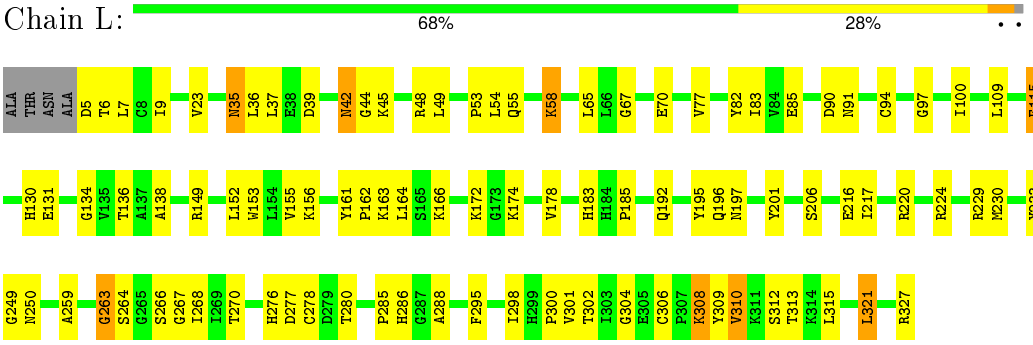
- Molecule 1: hemagglutinin

Chain J:



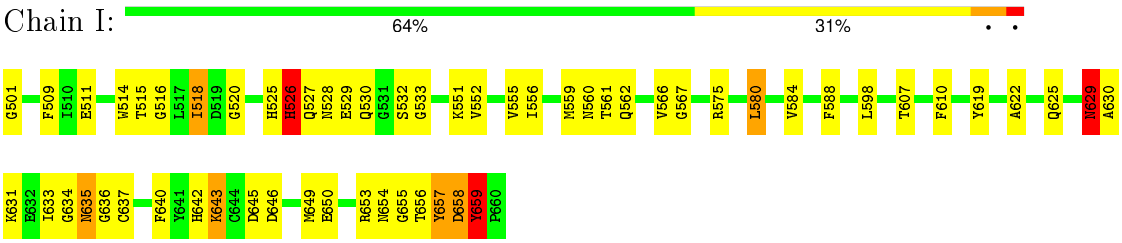
- Molecule 1: hemagglutinin

Chain L:



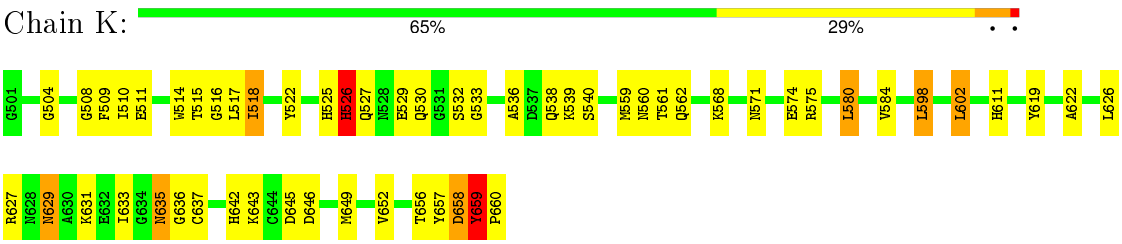
• Molecule 2: hemagglutinin

Chain I:



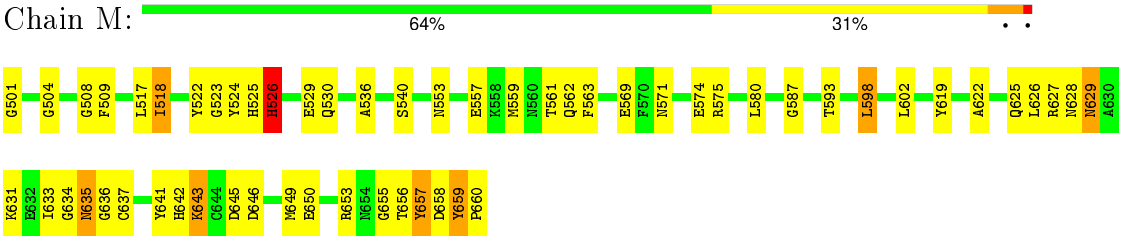
• Molecule 2: hemagglutinin

Chain K:



• Molecule 2: hemagglutinin

Chain M:



4 Data and refinement statistics (i)

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	204.30Å 83.30Å 177.38Å 90.00° 106.15° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12143	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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: GAL, SIA, BGC, NAG, NDG

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	H	0.39	0/2574	0.67	0/3507
1	J	0.36	0/2574	0.65	0/3507
1	L	0.39	0/2574	0.69	0/3507
2	I	0.35	0/1307	0.56	0/1761
2	K	0.34	0/1307	0.56	0/1761
2	M	0.36	0/1307	0.57	0/1761
All	All	0.37	0/11643	0.64	0/15804

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2511	0	2437	92	0
1	J	2511	0	2437	94	0
1	L	2511	0	2437	87	0
2	I	1281	0	1201	56	0
2	K	1281	0	1201	54	0
2	M	1281	0	1201	52	0
3	H	20	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	20	0	16	0	0
3	L	20	0	16	0	0
4	J	48	0	41	0	0
5	H	11	0	9	0	0
5	L	11	0	9	0	0
6	H	15	0	15	12	0
6	J	15	0	15	9	0
6	L	15	0	15	11	0
7	H	128	0	0	8	0
7	I	36	0	0	7	0
7	J	151	0	0	6	0
7	K	44	0	0	3	0
7	L	191	0	0	8	0
7	M	42	0	0	4	0
All	All	12143	0	11066	403	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (403) 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:L:91:ASN:HD21	6:L:744:NDG:C1	1.55	1.19
1:J:58:LYS:H	1:J:58:LYS:HD3	1.06	1.11
1:L:58:LYS:H	1:L:58:LYS:HD3	1.16	1.09
1:H:58:LYS:H	1:H:58:LYS:HD3	1.17	1.04
1:L:91:ASN:ND2	6:L:744:NDG:H1	1.73	1.04
1:J:224:ARG:NH2	6:J:740:NDG:H2	1.77	0.98
1:H:224:ARG:HH22	6:H:742:NDG:H2	1.26	0.96
1:L:224:ARG:NH2	6:L:744:NDG:H2	1.81	0.95
1:H:224:ARG:NH2	6:H:742:NDG:H2	1.82	0.93
1:L:91:ASN:ND2	6:L:744:NDG:C1	2.31	0.93
1:L:91:ASN:HD21	6:L:744:NDG:H1	1.27	0.91
2:M:530:GLN:NE2	2:M:645:ASP:HB2	1.87	0.88
2:I:530:GLN:NE2	2:I:645:ASP:HB2	1.87	0.88
1:L:224:ARG:HH22	6:L:744:NDG:H2	1.36	0.87
1:H:139:CYS:HA	6:H:742:NDG:H8C2	1.57	0.86
1:J:224:ARG:HH22	6:J:740:NDG:H2	1.38	0.86
1:J:58:LYS:CD	1:J:58:LYS:H	1.86	0.85
1:H:65:LEU:HD11	1:H:109:LEU:HD21	1.61	0.83
2:K:530:GLN:NE2	2:K:645:ASP:HB2	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:58:LYS:N	1:J:58:LYS:HD3	1.92	0.80
1:L:65:LEU:HD11	1:L:109:LEU:HD21	1.62	0.80
1:J:55:GLN:HG3	7:J:811:HOH:O	1.82	0.80
2:I:530:GLN:HE21	2:I:645:ASP:HB2	1.47	0.79
1:H:220:ARG:HD2	1:H:229:ARG:HG2	1.65	0.79
1:L:192:GLN:HG2	7:L:854:HOH:O	1.82	0.78
1:J:310:VAL:HG12	1:J:312:SER:H	1.50	0.77
1:J:156:LYS:HD2	1:J:196:GLN:HG2	1.67	0.76
1:H:100:ILE:HG13	1:H:233:TYR:CE2	2.21	0.76
2:M:501:GLY:HA3	7:M:661:HOH:O	1.86	0.76
2:M:629:ASN:N	2:M:629:ASN:HD22	1.83	0.75
1:L:100:ILE:HG13	1:L:233:TYR:CE2	2.22	0.74
1:H:192:GLN:HG2	7:H:813:HOH:O	1.88	0.74
1:H:156:LYS:HD2	1:H:196:GLN:HG2	1.69	0.74
1:L:58:LYS:N	1:L:58:LYS:HD3	1.99	0.74
1:H:158:GLY:HA3	7:H:830:HOH:O	1.88	0.73
1:J:199:ASP:HB2	7:J:856:HOH:O	1.89	0.72
1:L:58:LYS:HG3	7:L:887:HOH:O	1.89	0.71
2:I:561:THR:HG22	2:I:562:GLN:H	1.54	0.71
1:H:224:ARG:HH22	6:H:742:NDG:C2	2.00	0.70
2:K:518:ILE:HD13	2:K:518:ILE:H	1.57	0.69
1:J:35:ASN:ND2	1:J:37:LEU:H	1.89	0.69
2:K:571:ASN:OD1	2:K:574:GLU:HG3	1.93	0.69
2:I:629:ASN:N	2:I:629:ASN:HD22	1.88	0.69
1:J:5:ASP:OD2	2:K:529:GLU:HG3	1.93	0.69
1:J:113:SER:HB3	1:J:263:GLY:HA3	1.76	0.68
1:J:221:PRO:HG2	1:L:206:SER:HA	1.73	0.68
1:H:295:PHE:CZ	2:I:559:MET:HG3	2.29	0.68
1:L:224:ARG:HH22	6:L:744:NDG:C2	2.05	0.68
2:K:629:ASN:N	2:K:629:ASN:HD22	1.90	0.68
1:H:9:ILE:HD11	2:I:622:ALA:CB	2.25	0.67
1:H:5:ASP:OD2	2:I:529:GLU:HG3	1.93	0.67
1:J:42:ASN:ND2	1:J:45:LYS:H	1.93	0.66
1:J:100:ILE:HG13	1:J:233:TYR:CE2	2.30	0.66
2:M:530:GLN:NE2	2:M:646:ASP:H	1.94	0.66
2:M:530:GLN:HE21	2:M:645:ASP:HB2	1.59	0.66
1:H:42:ASN:C	1:H:42:ASN:HD22	1.99	0.66
1:H:61:ILE:HD13	1:H:106:ARG:NH1	2.10	0.66
2:I:516:GLY:O	2:I:518:ILE:HG23	1.95	0.65
1:H:139:CYS:HA	6:H:742:NDG:C8	2.27	0.65
2:I:561:THR:HG22	2:I:562:GLN:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:560:ASN:HA	7:I:687:HOH:O	1.96	0.64
1:L:35:ASN:ND2	1:L:37:LEU:H	1.94	0.64
2:K:561:THR:HG22	2:K:562:GLN:N	2.12	0.64
1:J:310:VAL:CG1	1:J:312:SER:H	2.11	0.64
2:M:569:GLU:HG3	7:M:675:HOH:O	1.97	0.64
1:J:9:ILE:HD11	2:K:622:ALA:CB	2.28	0.64
2:K:575:ARG:HD2	7:K:690:HOH:O	1.97	0.64
1:J:224:ARG:HH22	6:J:740:NDG:C2	2.11	0.63
1:H:35:ASN:HD22	1:H:36:LEU:N	1.96	0.63
1:L:5:ASP:OD2	2:M:529:GLU:HG3	1.99	0.63
2:K:518:ILE:N	2:K:518:ILE:HD13	2.14	0.63
1:J:156:LYS:NZ	1:J:196:GLN:HE21	1.97	0.63
1:J:42:ASN:C	1:J:42:ASN:HD22	2.02	0.63
1:L:220:ARG:HD2	1:L:229:ARG:CG	2.28	0.63
2:K:530:GLN:NE2	2:K:646:ASP:H	1.97	0.62
1:H:156:LYS:NZ	1:H:196:GLN:HE21	1.98	0.62
2:K:530:GLN:HE21	2:K:645:ASP:HB2	1.62	0.62
2:K:517:LEU:HD11	2:K:536:ALA:HB2	1.81	0.61
1:L:220:ARG:HD2	1:L:229:ARG:HG2	1.82	0.61
1:H:35:ASN:ND2	1:H:37:LEU:H	1.99	0.61
2:I:515:THR:HG23	7:I:669:HOH:O	2.00	0.61
1:H:140:PRO:HD2	6:H:742:NDG:H8C1	1.83	0.61
2:I:526:HIS:HD2	2:I:649:MET:HG3	1.66	0.61
2:K:509:PHE:O	2:K:635:ASN:HA	2.01	0.60
2:M:619:TYR:CE1	2:M:636:GLY:HA2	2.36	0.60
2:M:625:GLN:HE22	2:M:655:GLY:HA2	1.66	0.60
1:J:97:GLY:HA3	1:J:230:MET:O	2.02	0.60
1:H:308:LYS:HD2	7:I:689:HOH:O	2.02	0.60
1:L:302:THR:HB	1:L:306:CYS:SG	2.42	0.60
1:H:134:GLY:HA3	1:H:153:TRP:HB3	1.83	0.60
2:I:530:GLN:NE2	2:I:646:ASP:H	2.00	0.60
2:I:518:ILE:H	2:I:518:ILE:HD13	1.67	0.60
1:L:49:LEU:HD23	1:L:280:THR:O	2.02	0.59
2:I:631:LYS:HE3	2:I:633:ILE:CD1	2.31	0.59
1:H:220:ARG:HD2	1:H:229:ARG:CG	2.31	0.59
1:H:42:ASN:ND2	1:H:45:LYS:H	2.01	0.59
1:J:220:ARG:HD2	1:J:229:ARG:CG	2.32	0.59
2:M:629:ASN:N	2:M:629:ASN:ND2	2.49	0.59
6:H:742:NDG:H1	6:H:742:NDG:O7	2.01	0.59
1:H:94:CYS:HB2	1:H:138:ALA:O	2.02	0.59
2:K:619:TYR:CE1	2:K:636:GLY:HA2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:42:ASN:ND2	1:L:288:ALA:H	2.01	0.59
1:J:54:LEU:HD13	1:J:77:VAL:HG11	1.85	0.59
1:L:310:VAL:HG13	1:L:312:SER:H	1.67	0.58
1:H:13:ALA:O	2:I:515:THR:HA	2.04	0.58
2:K:658:ASP:O	2:K:659:TYR:HB2	2.04	0.58
1:J:9:ILE:HD12	2:K:619:TYR:HA	1.86	0.57
2:I:635:ASN:OD1	2:I:637:CYS:SG	2.62	0.57
1:L:7:LEU:HD11	2:M:524:TYR:HB3	1.86	0.57
2:K:635:ASN:HB2	7:K:698:HOH:O	2.03	0.57
1:J:321:LEU:N	1:J:321:LEU:HD23	2.20	0.57
1:J:48:ARG:HB2	1:J:51:ILE:O	2.03	0.57
2:K:627:ARG:NH1	2:K:660:PRO:HB3	2.18	0.57
1:H:189:THR:HG23	7:H:901:HOH:O	2.04	0.57
2:K:526:HIS:HB2	2:K:649:MET:HE3	1.86	0.57
2:M:517:LEU:HD11	2:M:536:ALA:HB2	1.87	0.57
1:H:66:LEU:HD22	1:H:151:LEU:HD11	1.87	0.57
1:J:174:LYS:HD2	1:J:259:ALA:HB1	1.86	0.56
1:H:174:LYS:HD2	1:H:259:ALA:HB1	1.86	0.56
1:J:91:ASN:ND2	6:J:740:NDG:O1L	2.38	0.56
2:K:631:LYS:HE3	2:K:633:ILE:HD13	1.88	0.56
2:M:525:HIS:O	2:M:526:HIS:ND1	2.36	0.56
1:L:172:LYS:HE2	7:L:825:HOH:O	2.05	0.56
1:J:156:LYS:NZ	1:J:196:GLN:NE2	2.55	0.55
1:J:42:ASN:HD21	1:J:288:ALA:H	1.54	0.55
2:K:526:HIS:HD2	2:K:649:MET:HG3	1.71	0.55
2:M:518:ILE:H	2:M:518:ILE:HD13	1.72	0.55
1:L:48:ARG:NH2	1:L:277:ASP:HA	2.22	0.55
1:H:70:GLU:HG3	6:H:742:NDG:O1L	2.07	0.55
1:H:302:THR:HB	1:H:306:CYS:SG	2.47	0.54
1:H:138:ALA:O	1:H:224:ARG:NH1	2.40	0.54
2:K:516:GLY:O	2:K:518:ILE:HG23	2.07	0.54
1:J:35:ASN:HD22	1:J:36:LEU:N	2.04	0.54
2:I:631:LYS:HE3	2:I:633:ILE:HD13	1.90	0.54
1:J:220:ARG:HD2	1:J:229:ARG:HG3	1.90	0.54
1:H:321:LEU:N	1:H:321:LEU:HD23	2.23	0.54
1:L:70:GLU:HG3	6:L:744:NDG:O1L	2.08	0.53
1:L:35:ASN:HD22	1:L:36:LEU:N	2.05	0.53
2:I:629:ASN:ND2	2:I:629:ASN:N	2.56	0.53
1:H:58:LYS:N	1:H:58:LYS:HD3	2.02	0.53
1:J:42:ASN:ND2	1:J:288:ALA:H	2.05	0.53
1:H:68:ASN:HB3	1:H:71:CYS:SG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:42:ASN:HD21	1:L:288:ALA:H	1.56	0.53
1:H:96:PRO:HG3	1:H:226:GLN:HB2	1.89	0.53
2:I:518:ILE:N	2:I:518:ILE:HD13	2.24	0.53
1:L:39:ASP:C	1:L:298:ILE:HD11	2.29	0.53
1:J:192:GLN:HG2	7:J:838:HOH:O	2.08	0.53
1:L:224:ARG:HH22	6:L:744:NDG:C3	2.22	0.53
1:J:42:ASN:HD22	1:J:45:LYS:H	1.56	0.53
1:J:70:GLU:HB2	1:J:91:ASN:ND2	2.24	0.52
1:H:310:VAL:HG13	1:H:312:SER:H	1.74	0.52
2:K:627:ARG:HH11	2:K:660:PRO:HB3	1.75	0.52
2:M:627:ARG:NH1	2:M:660:PRO:HB3	2.25	0.52
2:K:629:ASN:N	2:K:629:ASN:ND2	2.57	0.52
2:K:525:HIS:O	2:K:533:GLY:O	2.27	0.52
1:J:156:LYS:HZ1	1:J:196:GLN:NE2	2.07	0.52
2:M:634:GLY:O	2:M:636:GLY:N	2.42	0.52
2:M:631:LYS:HE3	2:M:633:ILE:CD1	2.40	0.52
1:J:156:LYS:CD	1:J:196:GLN:HG2	2.39	0.52
1:H:9:ILE:HD11	2:I:622:ALA:HB3	1.90	0.52
1:J:302:THR:HB	1:J:306:CYS:SG	2.50	0.52
1:L:91:ASN:ND2	6:L:744:NDG:O1L	2.28	0.52
2:M:530:GLN:HE22	2:M:645:ASP:HB2	1.71	0.52
2:K:561:THR:CG2	2:K:562:GLN:N	2.73	0.52
2:K:525:HIS:O	2:K:526:HIS:ND1	2.40	0.52
2:M:575:ARG:NE	7:M:673:HOH:O	2.43	0.52
1:L:197:ASN:ND2	7:L:920:HOH:O	2.42	0.52
1:H:220:ARG:HE	1:J:210:ASP:CG	2.12	0.52
1:J:156:LYS:HZ1	1:J:196:GLN:HE21	1.58	0.52
1:H:217:ILE:N	1:H:217:ILE:HD12	2.25	0.52
2:K:509:PHE:CD1	2:K:510:ILE:HG13	2.45	0.51
1:J:140:PRO:HD2	6:J:740:NDG:H8C1	1.92	0.51
2:M:625:GLN:NE2	2:M:655:GLY:HA2	2.25	0.51
1:H:36:LEU:HD11	1:H:317:MET:HG3	1.93	0.51
1:H:185:PRO:HG2	1:H:191:GLN:HE21	1.75	0.51
1:H:97:GLY:HA3	1:H:230:MET:O	2.10	0.51
2:I:634:GLY:O	2:I:636:GLY:N	2.44	0.51
2:M:642:HIS:O	2:M:643:LYS:O	2.29	0.51
2:I:566:VAL:HG22	7:I:675:HOH:O	2.11	0.51
2:K:504:GLY:O	2:K:508:GLY:HA3	2.11	0.51
1:H:295:PHE:HZ	2:I:559:MET:HG3	1.75	0.51
1:J:66:LEU:HD22	1:J:151:LEU:HD11	1.93	0.51
2:I:514:TRP:C	2:I:516:GLY:N	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:ASN:HD22	1:H:36:LEU:H	1.58	0.50
2:I:650:GLU:HA	2:I:653:ARG:HD2	1.93	0.50
2:M:561:THR:HG22	2:M:562:GLN:N	2.26	0.50
1:J:220:ARG:HD2	1:J:229:ARG:HG2	1.94	0.50
1:J:265:GLY:HA2	7:J:850:HOH:O	2.09	0.50
1:H:119:GLU:CD	1:H:122:PRO:HA	2.32	0.50
1:L:216:GLU:O	1:L:220:ARG:NH2	2.43	0.50
2:I:630:ALA:HB2	2:I:640:PHE:HA	1.92	0.50
2:K:530:GLN:HE22	2:K:645:ASP:HB2	1.76	0.50
1:J:172:LYS:HD2	7:J:896:HOH:O	2.11	0.50
1:J:327:ARG:C	1:J:327:ARG:NE	2.65	0.50
1:L:246:GLU:HG3	7:L:952:HOH:O	2.10	0.50
1:H:44:GLY:HA2	1:H:286:HIS:O	2.12	0.50
1:L:217:ILE:N	1:L:217:ILE:HD12	2.27	0.50
1:H:58:LYS:H	1:H:58:LYS:CD	2.00	0.49
2:M:622:ALA:O	2:M:626:LEU:HG	2.12	0.49
1:J:164:LEU:C	1:J:164:LEU:HD12	2.32	0.49
2:I:501:GLY:HA3	7:I:663:HOH:O	2.11	0.49
1:L:58:LYS:H	1:L:58:LYS:CD	1.96	0.49
1:L:220:ARG:HG3	1:L:220:ARG:HH11	1.76	0.49
2:M:627:ARG:HH11	2:M:660:PRO:HB3	1.77	0.49
1:H:246:GLU:HG3	7:H:894:HOH:O	2.12	0.49
1:H:18:ASP:O	1:H:29:THR:HA	2.13	0.49
1:L:9:ILE:HD11	2:M:622:ALA:CB	2.43	0.49
1:H:310:VAL:CG1	1:H:312:SER:H	2.26	0.49
1:J:107:GLU:OE2	2:K:568:LYS:NZ	2.42	0.49
1:H:266:SER:OG	1:H:267:GLY:N	2.46	0.48
1:H:49:LEU:CD1	1:H:303:ILE:HG22	2.42	0.48
1:H:42:ASN:C	1:H:42:ASN:ND2	2.66	0.48
1:L:131:GLU:HB3	1:L:155:VAL:HG23	1.94	0.48
1:J:175:GLU:HG2	7:J:879:HOH:O	2.14	0.48
1:L:134:GLY:HA3	1:L:153:TRP:HB3	1.94	0.48
1:H:42:ASN:HD21	1:H:288:ALA:H	1.61	0.48
1:H:199:ASP:HB2	7:H:888:HOH:O	2.13	0.48
1:L:83:ILE:O	1:L:268:ILE:HA	2.13	0.48
2:K:560:ASN:N	7:K:664:HOH:O	2.46	0.48
2:M:628:ASN:O	2:M:641:TYR:CD1	2.67	0.48
1:L:54:LEU:HD13	1:L:77:VAL:HG11	1.95	0.48
1:L:97:GLY:HA3	1:L:230:MET:O	2.14	0.48
1:L:164:LEU:HD12	1:L:164:LEU:C	2.33	0.48
1:H:38:GLU:OE1	1:H:291:SER:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:518:ILE:N	2:K:518:ILE:CD1	2.77	0.48
1:J:9:ILE:HD11	2:K:622:ALA:HB3	1.96	0.48
1:L:183:HIS:CE1	1:L:185:PRO:HG3	2.48	0.48
1:L:115:PHE:C	1:L:115:PHE:CD1	2.87	0.48
1:J:78:SER:O	1:J:114:SER:HB2	2.14	0.48
1:L:295:PHE:CZ	2:M:559:MET:HG3	2.49	0.47
1:L:321:LEU:HD23	1:L:321:LEU:N	2.29	0.47
1:J:282:CYS:HB2	1:J:305:GLU:O	2.12	0.47
2:M:518:ILE:HD13	2:M:518:ILE:N	2.30	0.47
2:M:635:ASN:OD1	2:M:637:CYS:SG	2.72	0.47
1:L:90:ASP:HB2	7:L:921:HOH:O	2.15	0.47
1:H:42:ASN:ND2	1:H:288:ALA:H	2.12	0.47
1:H:161:TYR:CZ	1:H:249:GLY:HA2	2.50	0.47
6:H:742:NDG:C1	6:H:742:NDG:O7	2.63	0.47
1:L:156:LYS:NZ	1:L:196:GLN:HE21	2.12	0.47
1:J:9:ILE:HD11	2:K:622:ALA:HB2	1.96	0.47
2:I:580:LEU:O	2:I:584:VAL:HG23	2.15	0.47
1:L:220:ARG:HD2	1:L:229:ARG:HG3	1.96	0.47
1:J:8:CYS:HA	2:K:637:CYS:HA	1.97	0.47
1:H:9:ILE:HD11	2:I:622:ALA:HB2	1.96	0.47
2:M:522:TYR:HD1	2:M:540:SER:HB3	1.79	0.47
1:L:53:PRO:HB3	1:L:82:TYR:CZ	2.50	0.47
1:H:48:ARG:HB2	1:H:51:ILE:O	2.15	0.47
2:I:656:THR:O	2:I:657:TYR:C	2.53	0.47
1:H:224:ARG:HH22	6:H:742:NDG:C3	2.28	0.46
1:L:115:PHE:C	1:L:115:PHE:HD1	2.18	0.46
1:H:294:PRO:HG2	1:H:295:PHE:CD1	2.50	0.46
1:J:134:GLY:HA3	1:J:153:TRP:HB3	1.96	0.46
1:H:105:LEU:HD12	1:H:105:LEU:O	2.15	0.46
6:L:744:NDG:O7	6:L:744:NDG:H1	2.14	0.46
1:L:266:SER:OG	1:L:267:GLY:N	2.48	0.46
1:L:310:VAL:HG22	2:M:593:THR:HA	1.96	0.46
1:J:91:ASN:ND2	6:J:740:NDG:C1	2.79	0.46
6:J:740:NDG:H1	6:J:740:NDG:O7	2.15	0.46
1:J:216:GLU:O	1:J:220:ARG:NH2	2.49	0.46
2:I:658:ASP:O	2:I:659:TYR:HB2	2.15	0.46
2:M:523:GLY:HA3	2:M:536:ALA:HA	1.98	0.46
1:J:131:GLU:HB3	1:J:155:VAL:HG23	1.98	0.46
2:M:571:ASN:OD1	2:M:574:GLU:HG3	2.15	0.46
1:L:161:TYR:CZ	1:L:249:GLY:HA2	2.50	0.46
2:I:526:HIS:O	2:I:526:HIS:ND1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:553:ASN:O	2:M:557:GLU:HG3	2.16	0.46
1:L:174:LYS:HD2	1:L:259:ALA:HB1	1.97	0.46
1:J:295:PHE:CZ	2:K:559:MET:HG3	2.51	0.46
1:H:115:PHE:C	1:H:115:PHE:CD1	2.90	0.46
1:J:91:ASN:HD21	6:J:740:NDG:C1	2.28	0.46
1:H:31:THR:HG23	1:H:321:LEU:O	2.15	0.46
1:J:217:ILE:HD12	1:J:217:ILE:N	2.31	0.46
2:M:598:LEU:HD13	2:M:602:LEU:HD22	1.98	0.46
1:L:42:ASN:ND2	1:L:45:LYS:H	2.14	0.45
1:L:45:LYS:HD2	1:L:276:HIS:CG	2.51	0.45
1:L:310:VAL:CG1	1:L:312:SER:H	2.28	0.45
2:K:598:LEU:HD13	2:K:602:LEU:HD22	1.99	0.45
1:J:130:HIS:CE1	1:J:162:PRO:HD2	2.51	0.45
1:H:276:HIS:HB3	7:H:846:HOH:O	2.15	0.45
1:H:54:LEU:HD13	1:H:77:VAL:HG11	1.99	0.45
1:J:58:LYS:O	1:J:91:ASN:HB2	2.16	0.45
1:H:37:LEU:HB2	1:H:315:LEU:HB2	1.97	0.45
1:H:115:PHE:C	1:H:115:PHE:HD1	2.20	0.45
1:J:13:ALA:O	2:K:515:THR:HA	2.16	0.45
1:H:130:HIS:HD2	7:H:852:HOH:O	1.99	0.45
1:J:222:LYS:HA	1:J:226:GLN:O	2.17	0.45
2:I:525:HIS:O	2:I:533:GLY:O	2.35	0.45
1:J:323:ASN:O	1:J:325:PRO:HD3	2.17	0.45
1:J:195:TYR:O	1:J:196:GLN:HB2	2.17	0.45
2:K:509:PHE:CE1	2:K:510:ILE:HG13	2.51	0.45
2:M:522:TYR:CD1	2:M:540:SER:HB3	2.52	0.45
1:J:249:GLY:C	1:J:250:ASN:HD22	2.20	0.45
1:J:191:GLN:HA	1:J:191:GLN:HE21	1.82	0.45
2:I:588:PHE:CZ	2:M:587:GLY:HA3	2.52	0.45
2:I:575:ARG:HD2	7:I:661:HOH:O	2.16	0.45
2:I:619:TYR:CE1	2:I:636:GLY:HA2	2.52	0.45
1:H:9:ILE:HD12	2:I:619:TYR:HA	1.98	0.44
2:I:635:ASN:OD1	2:I:635:ASN:C	2.56	0.44
2:M:625:GLN:HE22	2:M:655:GLY:CA	2.31	0.44
1:J:60:ASN:OD1	1:J:62:ALA:HB3	2.18	0.44
2:K:580:LEU:O	2:K:584:VAL:HG23	2.17	0.44
1:L:308:LYS:HD2	7:M:677:HOH:O	2.17	0.44
1:J:69:PRO:HG3	1:J:147:PHE:O	2.17	0.44
1:J:35:ASN:HD22	1:J:36:LEU:H	1.65	0.44
1:H:49:LEU:HD23	1:H:280:THR:O	2.17	0.44
1:L:249:GLY:C	1:L:250:ASN:HD22	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:91:ASN:ND2	6:J:740:NDG:H1	2.33	0.44
1:H:224:ARG:CZ	6:H:742:NDG:H2	2.44	0.44
1:J:39:ASP:C	1:J:298:ILE:HD11	2.38	0.44
1:J:320:GLY:O	2:K:611:HIS:CD2	2.70	0.44
2:I:561:THR:CG2	2:I:562:GLN:H	2.27	0.44
1:L:156:LYS:HD2	1:L:196:GLN:HG2	1.99	0.44
2:K:527:GLN:HG3	2:K:532:SER:OG	2.18	0.44
1:J:42:ASN:ND2	1:J:42:ASN:C	2.70	0.44
1:J:131:GLU:HB3	1:J:155:VAL:CG2	2.47	0.44
1:H:91:ASN:ND2	6:H:742:NDG:C1	2.81	0.43
1:H:37:LEU:HD21	1:H:297:ASN:ND2	2.33	0.43
2:I:509:PHE:O	2:I:635:ASN:HA	2.19	0.43
1:L:263:GLY:O	1:L:264:SER:HB3	2.18	0.43
2:K:522:TYR:HD1	2:K:540:SER:HB3	1.84	0.43
2:K:656:THR:O	2:K:658:ASP:N	2.51	0.43
1:L:285:PRO:HD3	1:L:301:VAL:O	2.18	0.43
1:L:94:CYS:HB2	1:L:138:ALA:O	2.19	0.43
1:L:48:ARG:HH22	1:L:277:ASP:CG	2.22	0.43
1:L:315:LEU:HA	1:L:315:LEU:HD23	1.88	0.43
2:K:538:GLN:O	2:K:539:LYS:C	2.56	0.43
2:M:526:HIS:CG	2:M:526:HIS:O	2.72	0.43
1:H:20:VAL:HG21	1:H:318:ALA:HB2	2.01	0.43
2:M:656:THR:O	2:M:657:TYR:C	2.57	0.43
2:I:561:THR:CG2	2:I:562:GLN:N	2.80	0.43
1:J:12:HIS:CG	1:J:13:ALA:N	2.87	0.43
1:L:300:PRO:HB3	1:L:309:TYR:CD2	2.54	0.43
1:J:126:SER:HB3	1:J:166:LYS:HE2	2.00	0.43
2:K:622:ALA:O	2:K:626:LEU:HG	2.18	0.42
1:L:6:THR:O	2:M:649:MET:HE1	2.19	0.42
1:L:117:LYS:CE	7:L:843:HOH:O	2.66	0.42
1:L:130:HIS:HD2	7:L:852:HOH:O	2.02	0.42
1:H:299:HIS:ND1	1:H:300:PRO:HD2	2.34	0.42
1:J:37:LEU:HB2	1:J:315:LEU:HB2	2.00	0.42
1:J:48:ARG:HG2	1:J:278:CYS:O	2.20	0.42
1:J:6:THR:O	2:K:526:HIS:HA	2.19	0.42
2:M:627:ARG:HD2	2:M:660:PRO:HA	2.01	0.42
1:J:180:TRP:HB3	1:J:254:PRO:HG3	2.01	0.42
2:I:634:GLY:C	2:I:636:GLY:N	2.72	0.42
1:H:38:GLU:O	1:H:296:GLN:HA	2.20	0.42
2:I:659:TYR:HD2	2:I:659:TYR:HA	1.75	0.42
1:J:161:TYR:CZ	1:J:249:GLY:HA2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:300:PRO:HD3	1:L:309:TYR:CZ	2.54	0.42
2:I:567:GLY:HA2	7:I:688:HOH:O	2.19	0.42
2:K:526:HIS:HB2	2:K:649:MET:CE	2.49	0.42
1:L:195:TYR:O	1:L:196:GLN:HB2	2.18	0.42
1:H:195:TYR:O	1:H:197:ASN:N	2.50	0.42
1:J:186:PRO:HA	1:J:218:ALA:O	2.20	0.42
2:I:607:THR:O	2:I:610:PHE:HB3	2.19	0.42
1:L:85:GLU:O	1:L:270:THR:HA	2.19	0.42
1:H:156:LYS:HZ2	1:H:196:GLN:HE21	1.68	0.42
2:I:634:GLY:C	2:I:636:GLY:H	2.22	0.42
1:L:67:GLY:O	1:L:149:ARG:HG2	2.20	0.42
2:M:650:GLU:OE2	2:M:653:ARG:HD2	2.20	0.42
2:M:504:GLY:O	2:M:508:GLY:HA3	2.19	0.42
1:J:195:TYR:O	1:J:197:ASN:N	2.53	0.42
1:H:42:ASN:HD22	1:H:45:LYS:H	1.65	0.42
1:L:44:GLY:HA2	1:L:286:HIS:O	2.19	0.42
1:J:115:PHE:C	1:J:115:PHE:HD1	2.23	0.42
1:H:180:TRP:CE2	1:H:233:TYR:HB2	2.55	0.41
2:M:509:PHE:O	2:M:635:ASN:HA	2.20	0.41
1:J:115:PHE:C	1:J:115:PHE:CD1	2.92	0.41
2:K:514:TRP:C	2:K:516:GLY:N	2.72	0.41
1:L:9:ILE:HD12	2:M:619:TYR:HA	2.01	0.41
1:L:130:HIS:CE1	1:L:162:PRO:HD2	2.55	0.41
2:M:559:MET:HA	2:M:559:MET:HE3	2.01	0.41
2:I:552:VAL:O	2:I:556:ILE:HG13	2.21	0.41
2:I:551:LYS:HG3	1:L:23:VAL:CG1	2.49	0.41
2:I:625:GLN:HE22	2:I:655:GLY:HA2	1.85	0.41
1:H:152:LEU:HD23	1:H:152:LEU:HA	1.91	0.41
2:K:561:THR:CG2	2:K:562:GLN:H	2.34	0.41
1:H:48:ARG:HG2	1:H:278:CYS:O	2.19	0.41
1:H:12:HIS:HB2	2:I:520:GLY:O	2.20	0.41
1:L:7:LEU:HA	2:M:526:HIS:HA	2.03	0.41
1:J:323:ASN:C	1:J:325:PRO:HD3	2.41	0.41
1:L:163:LYS:HE2	1:L:201:TYR:OH	2.20	0.41
1:L:178:VAL:O	1:L:234:TRP:HA	2.21	0.41
2:M:526:HIS:HD2	2:M:649:MET:HG3	1.85	0.41
1:L:304:GLY:O	2:M:563:PHE:HA	2.20	0.41
1:L:126:SER:HB3	1:L:166:LYS:HE2	2.02	0.41
1:L:42:ASN:C	1:L:42:ASN:HD22	2.24	0.41
2:K:633:ILE:HG22	2:K:633:ILE:O	2.20	0.41
1:H:249:GLY:C	1:H:250:ASN:HD22	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:642:HIS:O	2:I:643:LYS:O	2.38	0.41
2:I:528:ASN:ND2	2:I:645:ASP:HA	2.36	0.41
1:J:7:LEU:CD2	2:K:652:VAL:HG11	2.51	0.41
2:I:650:GLU:O	2:I:654:ASN:ND2	2.54	0.41
1:H:185:PRO:HG2	1:H:191:GLN:NE2	2.34	0.40
2:I:527:GLN:HG3	2:I:532:SER:OG	2.21	0.40
2:M:628:ASN:O	2:M:641:TYR:CE1	2.74	0.40
1:J:191:GLN:NE2	1:J:191:GLN:HA	2.36	0.40
1:H:178:VAL:O	1:H:234:TRP:HA	2.21	0.40
2:I:555:VAL:O	2:I:559:MET:HG2	2.21	0.40
1:H:282:CYS:HB2	1:H:305:GLU:O	2.22	0.40
1:L:9:ILE:HD11	2:M:622:ALA:HB3	2.03	0.40
1:J:7:LEU:HA	2:K:526:HIS:HA	2.04	0.40
1:H:76:THR:HG23	7:H:916:HOH:O	2.21	0.40
1:J:72:ASP:HA	1:J:75:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	322/328 (98%)	299 (93%)	22 (7%)	1 (0%)	46 68
1	J	322/328 (98%)	304 (94%)	17 (5%)	1 (0%)	46 68
1	L	322/328 (98%)	301 (94%)	20 (6%)	1 (0%)	46 68
2	I	158/160 (99%)	134 (85%)	16 (10%)	8 (5%)	2 2
2	K	158/160 (99%)	139 (88%)	12 (8%)	7 (4%)	3 3
2	M	158/160 (99%)	139 (88%)	13 (8%)	6 (4%)	4 5
All	All	1440/1464 (98%)	1316 (91%)	100 (7%)	24 (2%)	11 19

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	635	ASN
2	K	657	TYR
2	K	658	ASP
2	K	659	TYR
2	M	635	ASN
2	M	657	TYR
2	I	511	GLU
2	I	643	LYS
2	I	657	TYR
2	K	526	HIS
2	M	643	LYS
2	I	526	HIS
2	I	658	ASP
2	I	659	TYR
2	K	511	GLU
2	K	643	LYS
2	M	658	ASP
2	M	659	TYR
2	I	629	ASN
1	J	196	GLN
1	L	263	GLY
2	M	526	HIS
1	H	196	GLN
2	K	635	ASN

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	H	279/281 (99%)	268 (96%)	11 (4%)	39	66
1	J	279/281 (99%)	266 (95%)	13 (5%)	32	56
1	L	279/281 (99%)	265 (95%)	14 (5%)	30	53
2	I	134/134 (100%)	128 (96%)	6 (4%)	34	59
2	K	134/134 (100%)	126 (94%)	8 (6%)	24	43
2	M	134/134 (100%)	128 (96%)	6 (4%)	34	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1239/1245 (100%)	1181 (95%)	58 (5%)	32 56

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	35	ASN
1	H	42	ASN
1	H	55	GLN
1	H	58	LYS
1	H	109	LEU
1	H	115	PHE
1	H	152	LEU
1	H	308	LYS
1	H	310	VAL
1	H	321	LEU
1	H	327	ARG
2	I	518	ILE
2	I	526	HIS
2	I	580	LEU
2	I	598	LEU
2	I	629	ASN
2	I	659	TYR
1	J	35	ASN
1	J	42	ASN
1	J	55	GLN
1	J	58	LYS
1	J	99	PHE
1	J	109	LEU
1	J	115	PHE
1	J	152	LEU
1	J	278	CYS
1	J	308	LYS
1	J	313	THR
1	J	321	LEU
1	J	327	ARG
2	K	518	ILE
2	K	526	HIS
2	K	580	LEU
2	K	598	LEU
2	K	602	LEU
2	K	629	ASN
2	K	642	HIS

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Mol	Chain	Res	Type
2	K	659	TYR
1	L	35	ASN
1	L	42	ASN
1	L	55	GLN
1	L	58	LYS
1	L	115	PHE
1	L	136	THR
1	L	152	LEU
1	L	246	GLU
1	L	278	CYS
1	L	308	LYS
1	L	310	VAL
1	L	313	THR
1	L	321	LEU
1	L	327	ARG
2	M	518	ILE
2	M	526	HIS
2	M	580	LEU
2	M	598	LEU
2	M	629	ASN
2	M	659	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	35	ASN
1	H	42	ASN
1	H	91	ASN
1	H	159	ASN
1	H	191	GLN
1	H	196	GLN
1	H	250	ASN
1	H	276	HIS
2	I	530	GLN
2	I	625	GLN
2	I	629	ASN
1	J	35	ASN
1	J	42	ASN
1	J	91	ASN
1	J	130	HIS
1	J	159	ASN
1	J	171	ASN

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Mol	Chain	Res	Type
1	J	191	GLN
1	J	196	GLN
1	J	250	ASN
1	J	276	HIS
2	K	530	GLN
2	K	625	GLN
2	K	629	ASN
1	L	35	ASN
1	L	42	ASN
1	L	91	ASN
1	L	130	HIS
1	L	191	GLN
1	L	196	GLN
1	L	250	ASN
2	M	530	GLN
2	M	625	GLN
2	M	629	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

4 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	$\#\|Z\| > 2$
4	GAL	J	802	3,4	11,11,12	2.66	6 (54%)	14,15,17	1.51	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	J	803	4	14,14,15	1.86	6 (42%)	15,19,21	0.91	0
4	GAL	J	804	4	11,11,12	2.18	2 (18%)	14,15,17	0.96	1 (7%)
4	BGC	J	805	4	12,12,12	2.68	6 (50%)	17,17,17	0.62	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	GAL	J	802	3,4	-	0/2/19/22	0/1/1/1
4	NAG	J	803	4	-	0/6/23/26	0/1/1/1
4	GAL	J	804	4	-	0/2/19/22	0/1/1/1
4	BGC	J	805	4	-	0/2/22/22	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	803	NAG	C4-C3	2.01	1.57	1.52
4	J	805	BGC	O5-C5	2.07	1.49	1.44
4	J	803	NAG	O5-C5	2.13	1.48	1.43
4	J	803	NAG	C4-C5	2.18	1.57	1.53
4	J	803	NAG	O4-C4	2.56	1.49	1.43
4	J	803	NAG	C2-N2	2.61	1.50	1.46
4	J	804	GAL	O5-C1	2.77	1.48	1.43
4	J	805	BGC	C1-C2	2.80	1.58	1.52
4	J	802	GAL	C4-C3	2.81	1.59	1.52
4	J	802	GAL	O5-C1	2.96	1.48	1.43
4	J	805	BGC	C3-C2	3.14	1.60	1.52
4	J	803	NAG	O5-C1	3.17	1.49	1.43
4	J	802	GAL	C4-C5	3.46	1.60	1.53
4	J	802	GAL	C2-C3	3.58	1.57	1.52
4	J	802	GAL	C1-C2	3.58	1.60	1.52
4	J	802	GAL	O5-C5	3.99	1.52	1.43
4	J	805	BGC	C4-C5	4.06	1.61	1.53
4	J	805	BGC	O5-C1	4.11	1.50	1.43
4	J	805	BGC	O4-C4	4.75	1.54	1.43
4	J	804	GAL	O5-C5	5.37	1.55	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	802	GAL	C2-C3-C4	-2.13	107.42	111.04
4	J	804	GAL	O5-C5-C6	2.10	111.89	107.35
4	J	802	GAL	C1-O5-C5	3.80	117.07	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
6	NDG	H	742	-	15,15,15	0.43	0	17,21,21	0.74	0
3	SIA	H	806	5	16,20,21	2.92	5 (31%)	18,28,31	2.54	7 (38%)
5	GAL	H	807	3	11,11,12	2.95	6 (54%)	14,15,17	1.61	4 (28%)
6	NDG	J	740	-	15,15,15	0.44	0	17,21,21	0.67	0
3	SIA	J	801	4	16,20,21	3.01	4 (25%)	18,28,31	2.61	7 (38%)
6	NDG	L	744	-	15,15,15	0.50	0	17,21,21	0.64	0
3	SIA	L	808	5	16,20,21	3.01	5 (31%)	18,28,31	2.45	7 (38%)
5	GAL	L	809	3	11,11,12	2.73	6 (54%)	14,15,17	1.13	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NDG	H	742	-	-	0/6/26/26	0/1/1/1
3	SIA	H	806	5	-	0/14/34/38	0/1/1/1
5	GAL	H	807	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NDG	J	740	-	-	0/6/26/26	0/1/1/1
3	SIA	J	801	4	-	0/14/34/38	0/1/1/1
6	NDG	L	744	-	-	0/6/26/26	0/1/1/1
3	SIA	L	808	5	-	0/14/34/38	0/1/1/1
5	GAL	L	809	3	-	0/2/19/22	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	808	SIA	O4-C4	-7.39	1.26	1.43
3	J	801	SIA	O4-C4	-7.02	1.27	1.43
3	H	806	SIA	O4-C4	-6.76	1.28	1.43
3	J	801	SIA	O6-C6	-2.91	1.39	1.43
3	H	806	SIA	O6-C6	-2.82	1.39	1.43
3	L	808	SIA	O6-C6	-2.51	1.39	1.43
3	L	808	SIA	C7-C6	-2.05	1.50	1.52
3	H	806	SIA	C3-C2	-2.04	1.49	1.52
5	L	809	GAL	C4-C3	2.60	1.59	1.52
5	L	809	GAL	C2-C3	2.68	1.56	1.52
5	H	807	GAL	C4-C3	2.94	1.60	1.52
5	L	809	GAL	C4-C5	3.13	1.59	1.53
5	L	809	GAL	C1-C2	3.31	1.60	1.52
5	H	807	GAL	C2-C3	3.37	1.57	1.52
5	H	807	GAL	O5-C1	3.59	1.49	1.43
5	H	807	GAL	C4-C5	3.59	1.60	1.53
5	L	809	GAL	O5-C1	4.09	1.50	1.43
5	H	807	GAL	C1-C2	4.61	1.63	1.52
5	H	807	GAL	O5-C5	4.74	1.53	1.43
5	L	809	GAL	O5-C5	5.07	1.54	1.43
3	L	808	SIA	C6-C5	5.78	1.62	1.53
3	H	806	SIA	C3-C4	5.83	1.62	1.52
3	J	801	SIA	C3-C4	6.00	1.62	1.52
3	H	806	SIA	C6-C5	6.34	1.63	1.53
3	L	808	SIA	C3-C4	6.37	1.63	1.52
3	J	801	SIA	C6-C5	6.49	1.63	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	806	SIA	O6-C6-C5	-7.46	96.28	108.48
3	J	801	SIA	O6-C6-C5	-7.35	96.46	108.48
3	L	808	SIA	O6-C6-C5	-6.80	97.34	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	801	SIA	O6-C2-C3	-3.05	103.99	109.86
3	L	808	SIA	O6-C2-C3	-3.00	104.09	109.86
3	H	806	SIA	O6-C2-C3	-2.67	104.73	109.86
3	L	808	SIA	C6-C5-N5	-2.66	106.43	111.07
3	J	801	SIA	C3-C4-C5	-2.55	108.64	111.47
3	H	806	SIA	C6-C5-N5	-2.53	106.66	111.07
5	H	807	GAL	O5-C1-C2	-2.37	107.01	110.86
3	H	806	SIA	O4-C4-C3	-2.34	104.32	110.06
3	L	808	SIA	C3-C4-C5	-2.33	108.87	111.47
3	J	801	SIA	C6-C5-N5	-2.31	107.04	111.07
5	H	807	GAL	C2-C3-C4	-2.19	107.33	111.04
3	H	806	SIA	O10-C10-C11	-2.13	118.15	122.06
3	J	801	SIA	O10-C10-C11	-2.03	118.34	122.06
3	L	808	SIA	O10-C10-C11	-2.02	118.35	122.06
5	L	809	GAL	C2-C3-C4	-2.01	107.62	111.04
5	H	807	GAL	C1-C2-C3	2.11	112.03	109.54
5	L	809	GAL	C1-O5-C5	2.14	114.96	112.25
3	L	808	SIA	C5-N5-C10	3.23	131.39	123.10
3	H	806	SIA	C5-N5-C10	3.35	131.71	123.10
3	J	801	SIA	C5-N5-C10	3.61	132.36	123.10
5	H	807	GAL	C1-O5-C5	3.78	117.05	112.25
3	L	808	SIA	C11-C10-N5	3.79	123.37	116.11
3	H	806	SIA	C11-C10-N5	3.89	123.55	116.11
3	J	801	SIA	C11-C10-N5	4.05	123.85	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	742	NDG	12	0
6	J	740	NDG	9	0
6	L	744	NDG	11	0

5.7 Other polymers (i)

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.