Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:20 AM GMT

PDB ID	:	2GK1
Title	:	X-ray crystal structure of NGT-bound HexA
Authors	:	Lemieux, M.J.; Mark, B.L.; Cherney, M.M.; Withers, S.G.; Mahuran, D.J.; James, M.N.
Deposited on	:	2006-03-31
Resolution	:	3.25 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

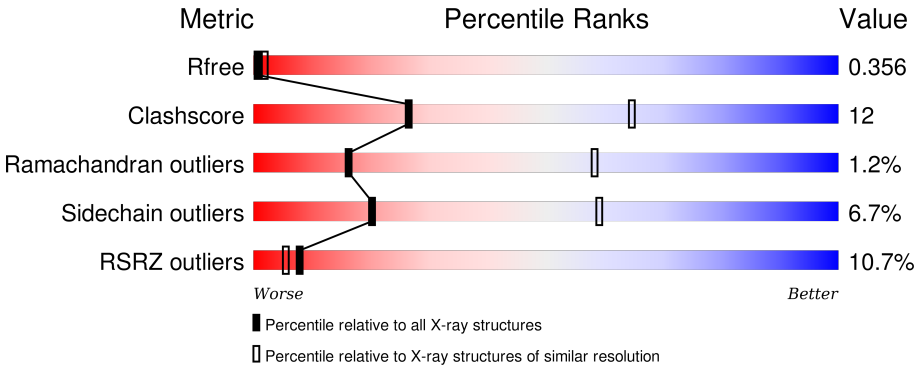
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	507	2% 63% 29% 5% •
1	C	507	4% 67% 26% • •
1	E	507	11% 67% 27% • •
1	G	507	15% 63% 31% • •
2	B	503	5% 72% 22% • 5%

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Mol	Chain	Length	Quality of chain
2	D	503	4% 71% 23% • 5%
2	F	503	14% 66% 28% • 5%
2	H	503	26% 72% 22% • 5%

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
3	NAG	C	12	-	-	X	-
3	NAG	C	13	X	-	-	-
3	NAG	G	531	X	-	-	-
4	NAG	D	15	X	-	-	-
4	NAG	D	16	X	-	-	-
4	NAG	E	17	X	-	X	-
4	NAG	E	18	X	-	-	-
4	NAG	F	19	X	-	-	-
4	NAG	F	20	X	-	-	-
4	NAG	G	21	-	-	X	-
4	NAG	G	22	X	-	-	-
4	NAG	H	27	X	-	-	-
5	NGT	A	21	-	-	X	-
5	NGT	C	530	-	-	X	-
5	NGT	E	530	-	-	X	-
5	NGT	G	533	-	-	X	-
5	NGT	H	28	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 32011 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 Beta-hexosaminidase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			4006	2598	650	744	14			
1	C	492	Total	C	N	O	S	0	0	0
			4006	2598	650	744	14			
1	E	492	Total	C	N	O	S	0	0	0
			4006	2598	650	744	14			
1	G	492	Total	C	N	O	S	0	0	0
			4006	2598	650	744	14			

- Molecule 2 is a protein called Beta-hexosaminidase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	480	Total	C	N	O	S	0	0	0
			3877	2505	643	716	13			
2	D	479	Total	C	N	O	S	0	0	0
			3871	2502	642	714	13			
2	F	480	Total	C	N	O	S	0	0	0
			3877	2505	643	716	13			
2	H	480	Total	C	N	O	S	0	0	0
			3877	2505	643	716	13			

- 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
			39	22	2	15		
3	A	3	Total	C	N	O	0	0
			39	22	2	15		
3	B	3	Total	C	N	O	0	0
			39	22	2	15		
3	C	3	Total	C	N	O	0	0
			39	22	2	15		

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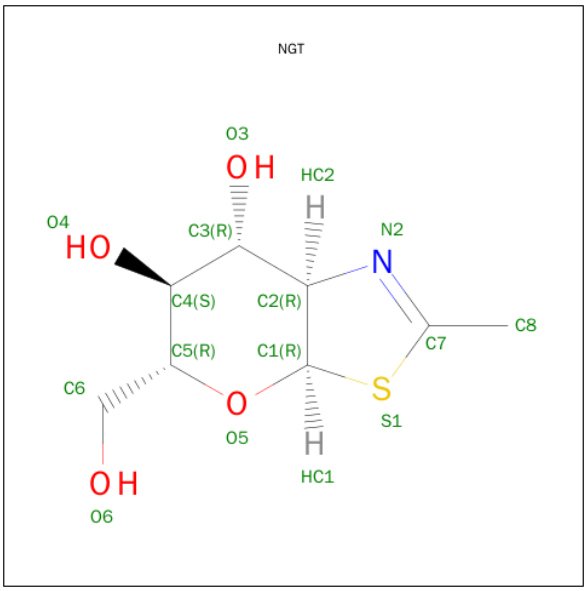
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TETRA HYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (three-letter code: NGT) (formula: $C_8H_{13}NO_4S$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
5	C	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
5	D	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
5	E	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
5	F	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
5	G	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
5	H	1	Total	C	N	O	S	0	0
			14	8	1	4	1		

- Molecule 6 is water.

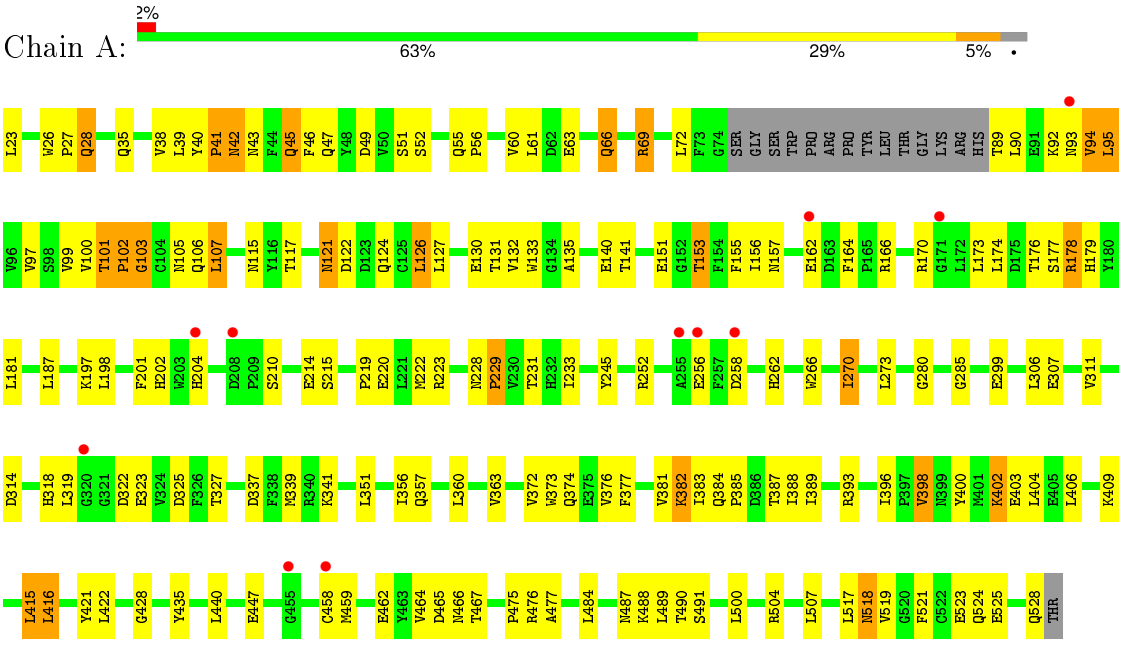
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		
6	B	1	Total	O	0	0
			1	1		
6	C	2	Total	O	0	0
			2	2		
6	D	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

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

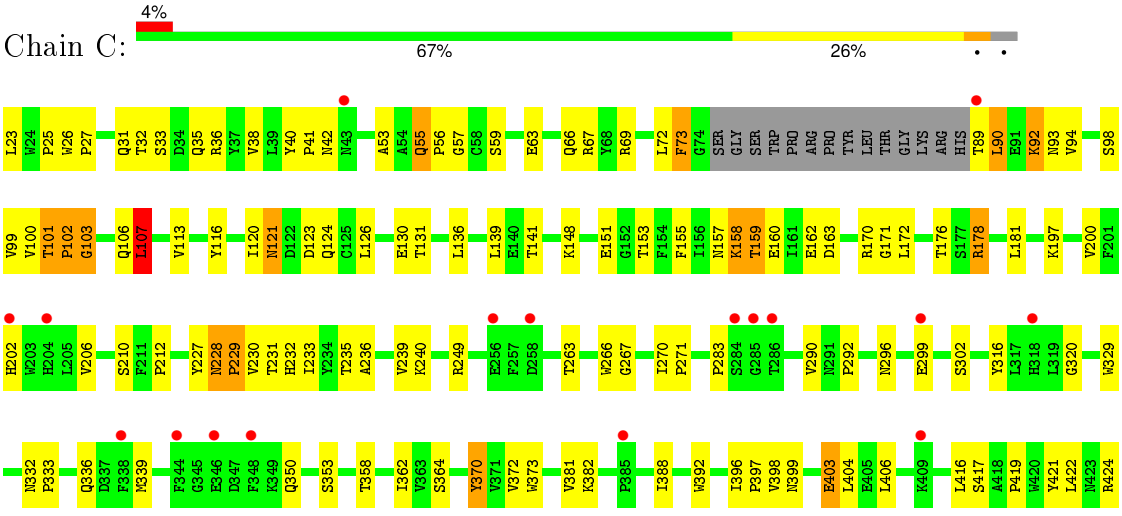
- Molecule 1: Beta-hexosaminidase alpha chain

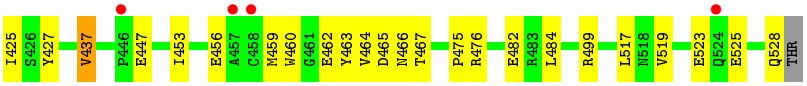
Chain A:



- Molecule 1: Beta-hexosaminidase alpha chain

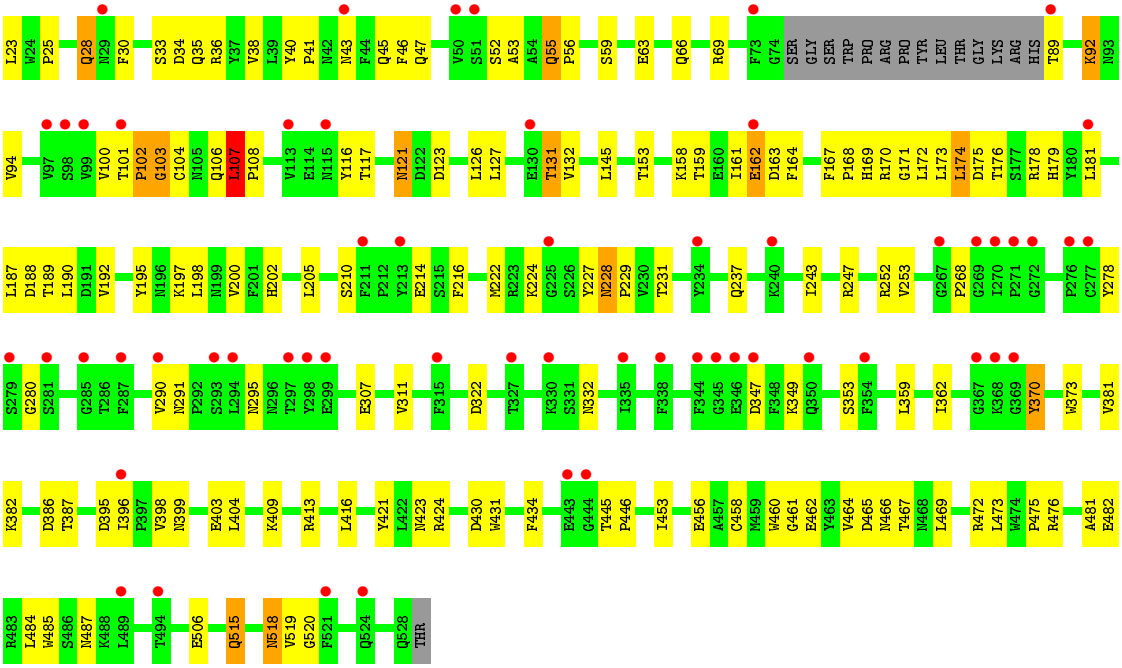
Chain C:





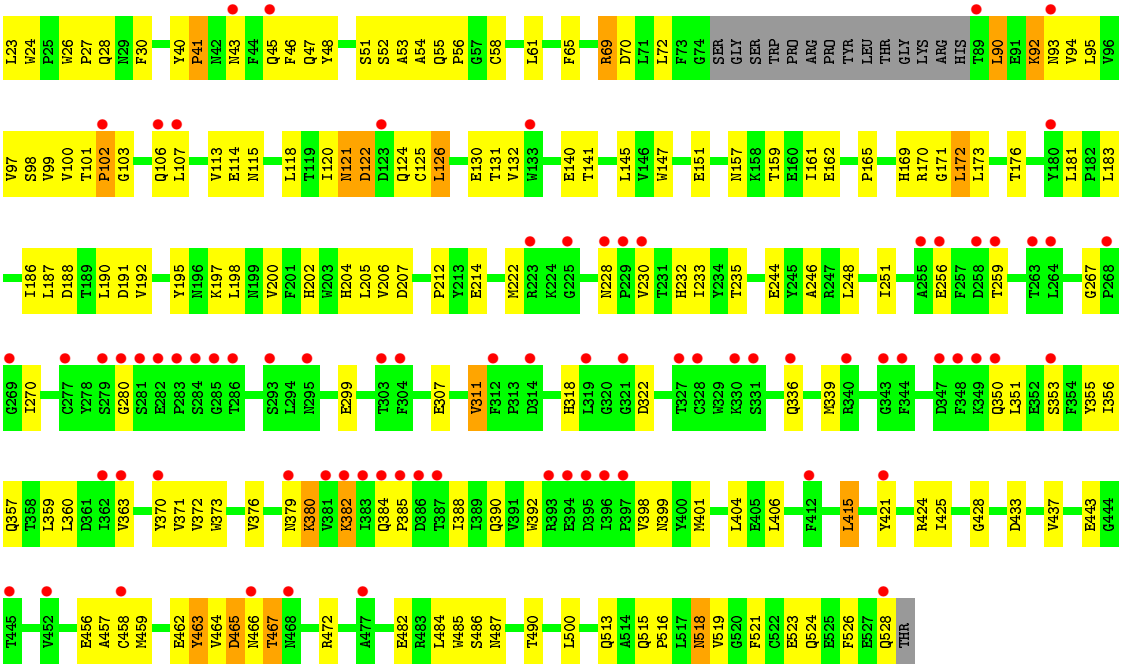
• Molecule 1: Beta-hexosaminidase alpha chain

Chain E:



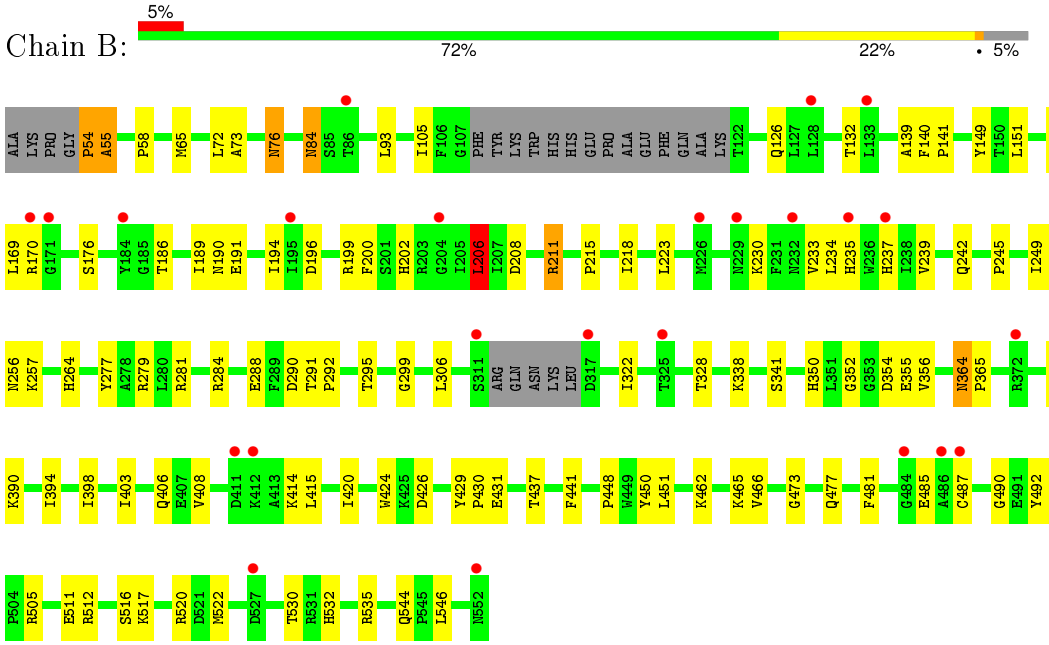
• Molecule 1: Beta-hexosaminidase alpha chain

Chain G:



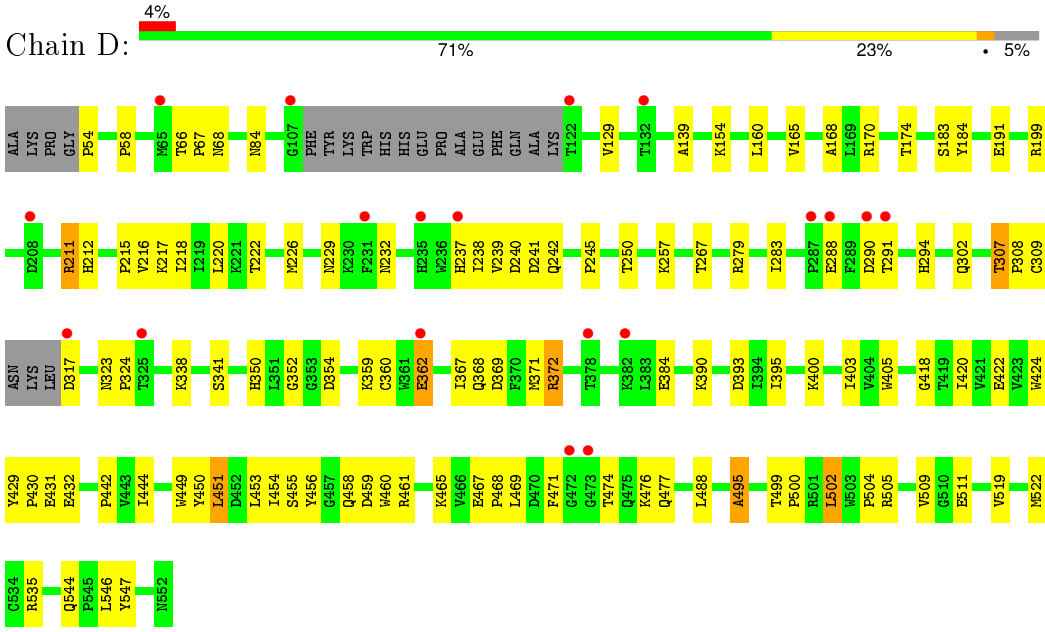
• Molecule 2: Beta-hexosaminidase beta chain

Chain B:



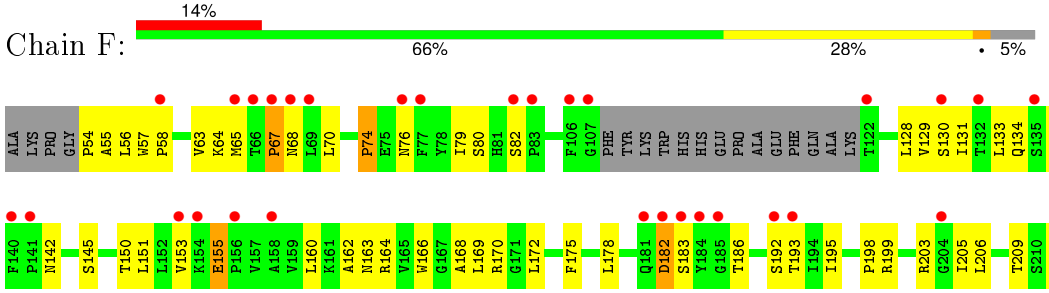
• Molecule 2: Beta-hexosaminidase beta chain

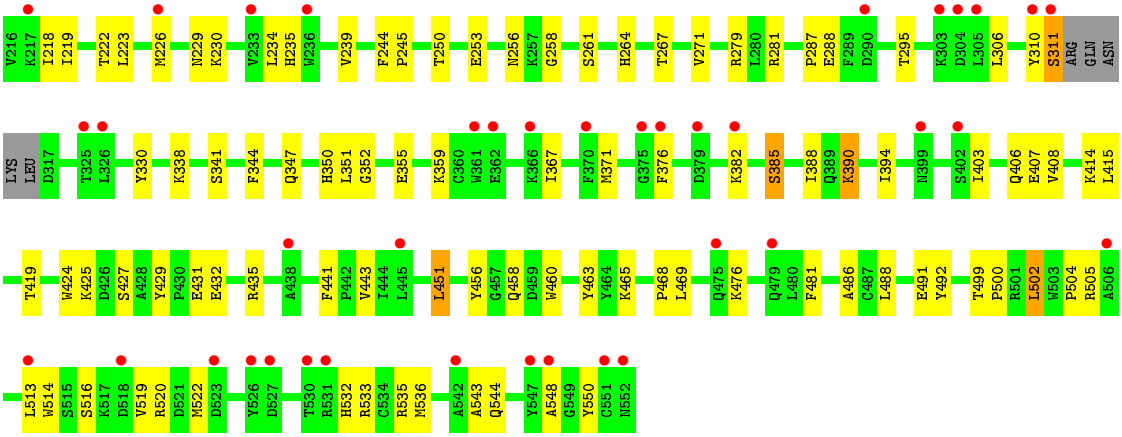
Chain D:



• Molecule 2: Beta-hexosaminidase beta chain

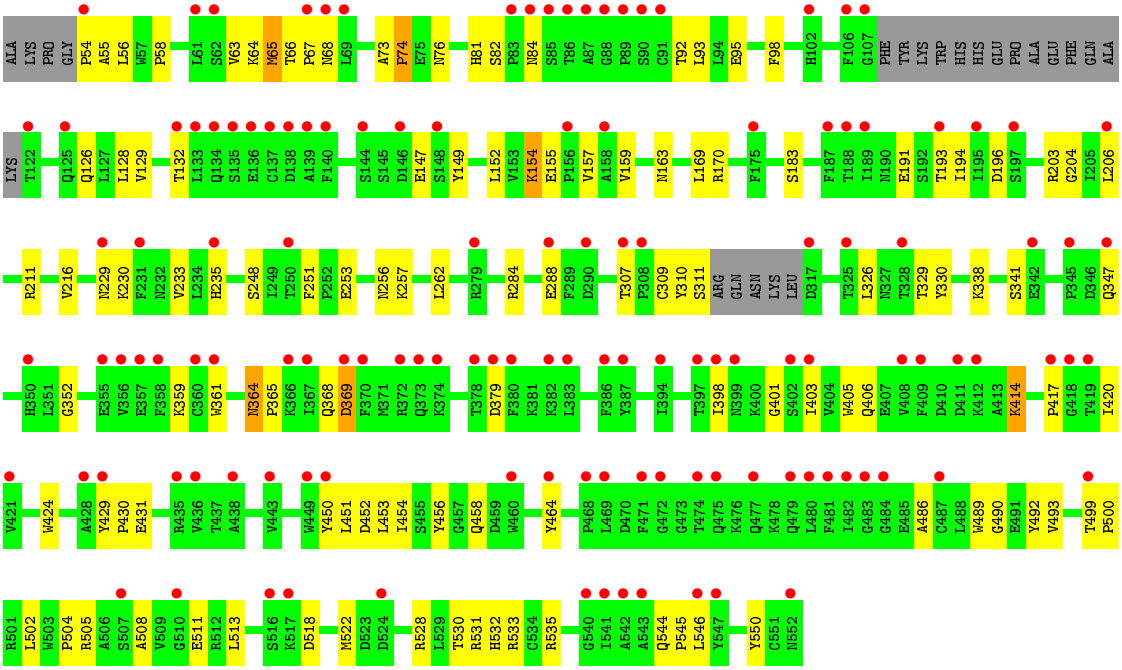
Chain F:





- Molecule 2: Beta-hexosaminidase beta chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	322.25Å 109.80Å 132.76Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	29.99 – 3.25 29.98 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.99-3.25) 97.8 (29.98-3.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.274 , 0.322 0.315 , 0.356	Depositor DCC
R_{free} test set	3599 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	89.4	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 15.6	EDS
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 71490 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	32011	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NGT, BMA, 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	0.40	0/4128	0.57	0/5628
1	C	0.40	0/4128	0.53	1/5628 (0.0%)
1	E	0.40	0/4128	0.53	1/5628 (0.0%)
1	G	0.40	0/4128	0.54	0/5628
2	B	0.94	4/3988 (0.1%)	0.57	2/5423 (0.0%)
2	D	0.39	0/3982	0.56	1/5415 (0.0%)
2	F	0.42	0/3988	0.54	0/5423
2	H	0.36	0/3988	0.48	0/5423
All	All	0.50	4/32458 (0.0%)	0.54	5/44196 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
3	C	1	0
3	G	1	0
4	D	2	0
4	E	2	0
4	F	2	0
4	G	1	0
4	H	1	0
All	All	10	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	PRO	N-CA	42.00	2.18	1.47
2	B	54	PRO	N-CD	32.56	1.93	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	55	ALA	CA-CB	7.07	1.67	1.52
2	B	54	PRO	CG-CD	5.16	1.67	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	54	PRO	CA-N-CD	-12.34	94.23	111.50
2	D	309	CYS	N-CA-C	8.31	133.45	111.00
1	E	107	LEU	CA-CB-CG	5.67	128.33	115.30
1	C	107	LEU	CA-CB-CG	5.21	127.28	115.30
2	B	206	LEU	CA-CB-CG	5.11	127.05	115.30

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	13	NAG	C5
4	D	15	NAG	C1
4	D	16	NAG	C1
4	E	17	NAG	C1
4	E	18	NAG	C1
4	F	19	NAG	C1
4	F	20	NAG	C1
4	G	22	NAG	C1
3	G	531	NAG	C1
4	H	27	NAG	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	308	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4006	0	3839	133	0
1	C	4006	0	3838	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4006	0	3838	111	0
1	G	4006	0	3835	123	1
2	B	3877	0	3784	72	0
2	D	3871	0	3777	85	0
2	F	3877	0	3782	92	0
2	H	3877	0	3782	73	1
3	A	78	0	68	6	0
3	B	39	0	34	1	0
3	C	39	0	33	7	0
3	G	39	0	34	1	0
4	C	28	0	25	1	0
4	D	28	0	25	2	0
4	E	28	0	25	9	0
4	F	28	0	25	2	0
4	G	28	0	25	7	0
4	H	28	0	25	3	0
5	A	14	0	13	6	0
5	B	14	0	13	3	0
5	C	14	0	13	12	0
5	D	14	0	13	4	0
5	E	14	0	13	6	0
5	F	14	0	13	2	0
5	G	14	0	13	8	0
5	H	14	0	13	6	0
6	A	5	0	0	1	0
6	B	1	0	0	0	0
6	C	2	0	0	1	0
6	D	2	0	0	0	0
All	All	32011	0	30898	765	1

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 12.

All (765) 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:C:157:ASN:HD21	3:C:12:NAG:C1	1.16	1.58
1:A:115:ASN:HD21	3:A:1:NAG:C1	1.18	1.53
1:A:157:ASN:HD21	3:A:4:NAG:C1	1.34	1.40
2:B:54:PRO:N	2:B:54:PRO:CD	1.93	1.30
1:E:462:GLU:OE1	5:E:530:NGT:HC62	1.19	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:450:TYR:HE2	5:H:28:NGT:S1	1.61	1.23
1:A:66:GLN:HA	1:A:66:GLN:HE21	0.98	1.13
1:C:421:TYR:OH	5:C:530:NGT:HC81	1.47	1.12
1:A:100:VAL:HG12	1:A:102:PRO:HD2	1.33	1.10
1:E:170:ARG:HG2	1:E:484:LEU:HB3	1.35	1.09
2:B:54:PRO:N	2:B:54:PRO:CA	2.18	1.06
1:G:55:GLN:HG3	1:G:56:PRO:HD2	1.36	1.04
2:H:450:TYR:CE2	5:H:28:NGT:S1	2.52	1.03
1:A:459:MET:HE1	1:A:464:VAL:HG11	1.45	0.98
1:E:462:GLU:OE1	5:E:530:NGT:C6	2.13	0.96
2:B:532:HIS:HD2	2:B:535:ARG:HH21	1.10	0.95
1:A:66:GLN:HA	1:A:66:GLN:NE2	1.82	0.94
2:H:452:ASP:OD2	5:H:28:NGT:HC62	1.68	0.92
1:G:130:GLU:HG2	4:G:21:NAG:H82	1.52	0.91
1:G:55:GLN:HG3	1:G:56:PRO:CD	1.99	0.91
2:B:532:HIS:CD2	2:B:535:ARG:HH21	1.88	0.90
1:E:178:ARG:HD2	1:E:462:GLU:OE2	1.71	0.90
1:A:66:GLN:HE21	1:A:66:GLN:CA	1.81	0.89
1:C:427:TYR:CD1	2:D:453:LEU:HA	2.08	0.89
1:E:36:ARG:HB3	4:E:17:NAG:H82	1.54	0.88
1:C:157:ASN:CG	3:C:12:NAG:C1	2.43	0.87
1:E:36:ARG:HB3	4:E:17:NAG:C8	2.06	0.86
1:G:130:GLU:HG2	4:G:21:NAG:C8	2.06	0.86
1:A:170:ARG:HG2	1:A:484:LEU:HB3	1.56	0.85
2:B:364:ASN:HD22	2:B:365:PRO:HD2	1.41	0.85
2:D:58:PRO:HB3	2:D:511:GLU:HA	1.58	0.85
1:A:100:VAL:CG1	1:A:102:PRO:HD2	2.07	0.85
1:G:30:PHE:HD2	1:G:161:ILE:HG12	1.42	0.84
2:F:355:GLU:OE1	5:F:26:NGT:HC2	1.78	0.84
2:F:67:PRO:O	4:F:19:NAG:H62	1.79	0.83
2:D:307:THR:HG21	2:D:367:ILE:HD11	1.60	0.83
1:G:373:TRP:CE2	5:G:533:NGT:C8	2.62	0.82
2:F:142:ASN:HB2	2:F:347:GLN:OE1	1.79	0.82
1:E:462:GLU:CD	5:E:530:NGT:HC62	2.00	0.81
1:E:465:ASP:OD2	1:E:467:THR:HG22	1.81	0.81
1:C:421:TYR:OH	5:C:530:NGT:C8	2.28	0.81
2:D:239:VAL:HG12	2:D:245:PRO:HD2	1.63	0.80
2:F:205:ILE:HD13	2:F:486:ALA:HB3	1.62	0.80
2:F:350:HIS:HD2	2:F:352:GLY:H	1.30	0.79
2:D:420:ILE:HD13	2:D:442:PRO:HB2	1.63	0.79
1:G:90:LEU:HD13	1:G:92:LYS:HE3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ALA:HB1	1:C:101:THR:HA	1.65	0.79
2:B:406:GLN:NE2	2:B:424:TRP:H	1.80	0.79
1:E:55:GLN:HG3	1:E:56:PRO:HD2	1.63	0.79
1:E:34:ASP:HA	4:E:17:NAG:HN2	1.51	0.76
1:A:467:THR:HG21	2:B:544:GLN:HA	1.67	0.76
2:D:450:TYR:OH	5:D:24:NGT:S1	2.43	0.75
2:D:532:HIS:HD2	2:D:535:ARG:HH21	1.32	0.75
1:G:100:VAL:HG12	1:G:102:PRO:HD2	1.67	0.75
1:A:322:ASP:OD2	5:A:21:NGT:N2	2.20	0.75
1:G:121:ASN:HD21	1:G:124:GLN:HG2	1.51	0.74
1:C:424:ARG:HA	2:D:456:TYR:CD1	2.22	0.74
1:E:467:THR:HG21	2:F:544:GLN:HA	1.69	0.74
2:F:432:GLU:HG2	2:F:435:ARG:HH21	1.51	0.74
1:A:131:THR:HG22	1:A:133:TRP:H	1.54	0.73
2:D:532:HIS:CD2	2:D:535:ARG:HH21	2.05	0.73
1:A:117:THR:HG22	1:A:162:GLU:HG3	1.69	0.73
2:F:504:PRO:HG3	2:F:533:ARG:HG3	1.70	0.73
1:C:100:VAL:HG12	1:C:102:PRO:HD2	1.68	0.73
1:A:170:ARG:NH2	1:A:197:LYS:O	2.22	0.73
2:B:211:ARG:NH2	5:B:22:NGT:O4	2.22	0.73
2:H:365:PRO:HA	2:H:368:GLN:HB2	1.71	0.72
2:B:451:LEU:O	2:B:505:ARG:NH2	2.22	0.72
1:A:229:PRO:HA	1:A:233:ILE:HD11	1.70	0.72
2:H:203:ARG:HG2	2:H:513:LEU:HB3	1.71	0.72
2:D:211:ARG:HD2	2:D:242:GLN:OE1	1.89	0.72
2:D:170:ARG:NH2	2:D:232:ASN:HB3	2.04	0.72
1:A:115:ASN:CG	3:A:1:NAG:C1	2.58	0.71
1:C:121:ASN:ND2	1:C:124:GLN:H	1.88	0.71
1:A:151:GLU:HG2	1:C:38:VAL:HG11	1.71	0.71
1:A:421:TYR:HB2	6:A:534:HOH:O	1.90	0.70
1:C:398:VAL:HG12	1:C:403:GLU:HG2	1.73	0.70
2:B:406:GLN:HE21	2:B:424:TRP:H	1.36	0.70
1:C:392:TRP:CD2	5:C:530:NGT:HC83	2.26	0.70
1:A:89:THR:HG22	1:A:90:LEU:H	1.56	0.70
1:E:214:GLU:HG3	1:E:222:MET:HE2	1.74	0.70
2:F:451:LEU:O	2:F:505:ARG:NH2	2.25	0.70
1:C:427:TYR:HD1	2:D:453:LEU:HA	1.57	0.69
1:E:107:LEU:HB2	1:E:108:PRO:HD2	1.74	0.69
2:B:295:THR:HG21	2:B:322:ILE:HD11	1.73	0.69
2:B:141:PRO:O	2:B:284:ARG:HG2	1.92	0.69
2:B:235:HIS:HB2	2:B:485:GLU:OE2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:ARG:CD	1:E:462:GLU:OE2	2.42	0.68
1:E:100:VAL:HG12	1:E:102:PRO:HD2	1.73	0.68
1:E:43:ASN:HD22	1:E:92:LYS:HG2	1.59	0.68
1:E:45:GLN:HB3	2:H:262:LEU:HD23	1.76	0.68
2:H:229:ASN:OD1	2:H:532:HIS:HE1	1.77	0.67
1:E:192:VAL:HA	1:E:195:TYR:CD2	2.28	0.67
2:F:229:ASN:OD1	2:F:532:HIS:HE1	1.78	0.67
1:C:178:ARG:NH1	5:C:530:NGT:O4	2.26	0.67
1:E:170:ARG:NH2	1:E:197:LYS:O	2.27	0.67
1:A:377:PHE:HB2	1:A:389:ILE:HD12	1.75	0.67
1:A:55:GLN:HG3	1:A:56:PRO:HD2	1.76	0.67
1:C:157:ASN:OD1	3:C:12:NAG:C1	2.43	0.67
1:G:99:VAL:HG22	1:G:130:GLU:HA	1.76	0.67
2:D:307:THR:CG2	2:D:367:ILE:HD11	2.25	0.67
2:F:183:SER:O	2:H:74:PRO:HD2	1.94	0.67
1:G:113:VAL:HG11	4:G:21:NAG:C8	2.25	0.66
1:G:228:ASN:HD22	1:G:230:VAL:H	1.42	0.66
1:E:101:THR:N	1:E:102:PRO:HD2	2.11	0.66
1:E:35:GLN:C	4:E:17:NAG:H83	2.15	0.66
1:E:45:GLN:HB3	2:H:262:LEU:CD2	2.26	0.66
2:B:215:PRO:O	2:B:218:ILE:HG22	1.96	0.66
1:G:459:MET:HE1	1:G:464:VAL:HG21	1.78	0.66
2:F:390:LYS:O	2:F:394:ILE:HD12	1.96	0.65
2:F:136:GLU:OE2	2:F:166:TRP:NE1	2.26	0.65
1:C:421:TYR:HE1	5:C:530:NGT:S1	2.20	0.65
2:D:307:THR:HG21	2:D:367:ILE:CD1	2.26	0.65
1:G:173:LEU:HA	1:G:202:HIS:HB3	1.78	0.65
1:G:94:VAL:HA	1:G:125:CYS:SG	2.37	0.65
1:A:447:GLU:CD	1:A:447:GLU:H	2.00	0.65
1:A:121:ASN:HD21	1:A:124:GLN:HG2	1.60	0.65
1:G:30:PHE:CD2	1:G:161:ILE:HG12	2.30	0.64
1:G:371:VAL:HG22	1:G:388:ILE:HD12	1.79	0.64
1:A:115:ASN:ND2	3:A:1:NAG:C2	2.59	0.64
1:E:36:ARG:CB	4:E:17:NAG:C8	2.76	0.64
1:G:373:TRP:CE2	5:G:533:NGT:HC82	2.33	0.64
1:A:465:ASP:OD2	1:A:467:THR:HG22	1.97	0.64
2:D:451:LEU:O	2:D:505:ARG:NH2	2.30	0.64
1:E:121:ASN:HD22	1:E:123:ASP:H	1.44	0.64
1:A:49:ASP:OD1	1:A:51:SER:N	2.24	0.64
1:G:58:CYS:SG	1:G:61:LEU:HG	2.37	0.64
2:F:166:TRP:HA	2:F:169:LEU:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:373:TRP:CD2	5:G:533:NGT:C8	2.82	0.63
1:C:170:ARG:HG2	1:C:484:LEU:HB3	1.80	0.63
1:C:89:THR:HG22	1:C:90:LEU:H	1.62	0.63
2:F:425:LYS:O	2:F:429:TYR:HB3	1.98	0.63
2:D:67:PRO:HA	4:D:15:NAG:O5	1.98	0.63
2:H:310:TYR:HE1	2:H:364:ASN:ND2	1.96	0.63
2:H:58:PRO:HB3	2:H:511:GLU:HA	1.79	0.63
1:G:173:LEU:HB3	1:G:458:CYS:HA	1.81	0.62
2:F:415:LEU:HB2	2:F:441:PHE:CZ	2.33	0.62
1:C:206:VAL:HG12	1:C:212:PRO:HD2	1.82	0.62
2:F:533:ARG:HA	2:F:536:MET:CE	2.29	0.62
2:F:499:THR:HB	2:F:500:PRO:HD3	1.81	0.61
1:C:102:PRO:O	1:C:103:GLY:O	2.18	0.61
1:E:53:ALA:HB1	1:E:101:THR:HA	1.83	0.61
2:B:132:THR:HB	2:B:163:ASN:HA	1.83	0.61
2:H:489:TRP:CD1	5:H:28:NGT:HC5	2.34	0.61
2:B:58:PRO:HB3	2:B:511:GLU:HA	1.81	0.61
2:D:372:ARG:CG	2:D:372:ARG:HH11	2.14	0.61
1:A:178:ARG:NH1	5:A:21:NGT:O4	2.34	0.61
1:G:46:PHE:CD2	1:G:94:VAL:HG11	2.36	0.61
1:G:48:TYR:CZ	1:G:65:PHE:HE2	2.19	0.61
1:G:463:TYR:O	2:H:545:PRO:HG2	2.01	0.61
1:A:153:THR:HG23	1:C:151:GLU:HB3	1.83	0.60
1:G:43:ASN:HD22	1:G:92:LYS:HG2	1.66	0.60
2:D:67:PRO:HB3	4:D:15:NAG:O6	2.01	0.60
1:A:101:THR:N	1:A:102:PRO:HD2	2.16	0.60
1:A:121:ASN:ND2	1:A:124:GLN:HG2	2.16	0.60
1:G:359:LEU:O	1:G:363:VAL:HG23	2.02	0.60
1:G:52:SER:HA	1:G:97:VAL:HG23	1.83	0.60
2:B:126:GLN:HB3	2:B:157:VAL:HG13	1.83	0.60
1:A:151:GLU:HB3	1:C:153:THR:HG23	1.82	0.60
1:G:339:MET:SD	1:G:351:LEU:HD22	2.41	0.60
1:G:131:THR:HG22	1:G:132:VAL:H	1.66	0.60
2:H:424:TRP:HB2	2:H:450:TYR:OH	2.02	0.60
2:B:239:VAL:HG12	2:B:245:PRO:HD2	1.84	0.60
1:E:55:GLN:HG3	1:E:56:PRO:CD	2.32	0.59
2:D:222:THR:O	2:D:226:MET:HG3	2.00	0.59
2:F:206:LEU:HA	2:F:235:HIS:HB3	1.82	0.59
1:C:157:ASN:ND2	3:C:12:NAG:C2	2.63	0.59
2:D:372:ARG:NH1	2:D:372:ARG:HG3	2.16	0.59
2:B:190:ASN:ND2	3:B:7:NAG:C1	2.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLN:HG3	1:A:93:ASN:ND2	2.17	0.59
1:C:467:THR:HG21	2:D:544:GLN:HA	1.84	0.59
1:A:459:MET:HE1	1:A:464:VAL:CG1	2.27	0.59
2:D:372:ARG:HH11	2:D:372:ARG:HG3	1.66	0.59
1:C:417:SER:O	1:C:421:TYR:CE2	2.56	0.59
1:G:515:GLN:HB2	1:G:516:PRO:HD2	1.84	0.59
2:B:465:LYS:O	2:B:520:ARG:NH2	2.36	0.59
2:D:403:ILE:HG12	2:D:420:ILE:HB	1.84	0.58
2:B:532:HIS:HD2	2:B:535:ARG:NH2	1.92	0.58
2:B:490:GLY:HA2	2:B:493:VAL:HB	1.86	0.58
2:H:67:PRO:HA	4:H:26:NAG:H2	1.85	0.58
2:B:473:GLY:HA2	2:B:477:GLN:NE2	2.19	0.58
1:E:170:ARG:HG2	1:E:484:LEU:CB	2.22	0.58
1:E:36:ARG:N	4:E:17:NAG:H83	2.19	0.58
1:C:121:ASN:HD21	1:C:124:GLN:H	1.50	0.58
1:E:169:HIS:NE2	1:E:200:VAL:HG11	2.19	0.58
2:F:310:TYR:O	2:F:311:SER:HB2	2.02	0.58
1:A:404:LEU:HD11	1:A:416:LEU:HG	1.84	0.57
2:B:403:ILE:HG23	2:B:420:ILE:HB	1.86	0.57
1:C:422:LEU:O	1:C:476:ARG:NH2	2.34	0.57
1:A:459:MET:CE	1:A:464:VAL:HG11	2.28	0.57
1:C:228:ASN:HD22	1:C:230:VAL:H	1.52	0.57
2:B:415:LEU:HB2	2:B:441:PHE:CE1	2.40	0.57
1:C:101:THR:O	1:C:102:PRO:C	2.42	0.57
1:E:108:PRO:HG2	1:E:252:ARG:HG2	1.86	0.57
2:F:229:ASN:OD1	2:F:532:HIS:CE1	2.56	0.57
1:C:171:GLY:HA3	1:C:456:GLU:HG2	1.86	0.57
1:E:25:PRO:HD2	1:E:197:LYS:HD2	1.86	0.56
2:H:149:TYR:CZ	2:H:196:ASP:HB3	2.40	0.56
1:A:262:HIS:CE1	5:A:21:NGT:O3	2.58	0.56
1:E:145:LEU:HD11	1:E:161:ILE:HD11	1.88	0.56
1:E:462:GLU:OE2	5:E:530:NGT:O4	2.21	0.56
1:G:113:VAL:HG11	4:G:21:NAG:H82	1.87	0.56
1:A:373:TRP:CE2	5:A:21:NGT:HC82	2.41	0.56
1:G:48:TYR:HH	1:G:65:PHE:HE2	1.51	0.56
2:D:488:LEU:HD22	2:D:502:LEU:HG	1.88	0.56
2:F:350:HIS:CD2	2:F:352:GLY:H	2.17	0.56
1:C:171:GLY:HA2	1:C:200:VAL:O	2.06	0.56
2:B:341:SER:OG	2:B:398:ILE:HD12	2.05	0.56
1:E:398:VAL:HG12	1:E:403:GLU:HG2	1.88	0.56
2:D:215:PRO:O	2:D:218:ILE:HG22	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:LEU:HA	1:G:186:ILE:HD12	1.87	0.55
2:H:132:THR:HB	2:H:163:ASN:HA	1.87	0.55
1:G:318:HIS:HE1	1:G:373:TRP:CD1	2.23	0.55
1:A:467:THR:CG2	2:B:544:GLN:HA	2.36	0.55
2:H:65:MET:HB2	4:H:26:NAG:H83	1.89	0.55
1:A:319:LEU:HD12	1:A:360:LEU:HD23	1.89	0.55
1:C:463:TYR:CE1	2:D:547:TYR:HD1	2.24	0.55
1:C:178:ARG:HH12	5:C:530:NGT:HO4	1.54	0.55
2:F:129:VAL:HG22	2:F:160:LEU:HD23	1.89	0.55
2:H:73:ALA:HB3	2:H:76:ASN:HB3	1.87	0.55
2:B:58:PRO:HD2	2:B:230:LYS:HD2	1.88	0.55
2:F:533:ARG:HA	2:F:536:MET:HE2	1.89	0.55
1:C:90:LEU:HD13	1:C:92:LYS:HE3	1.87	0.55
1:E:518:ASN:ND2	2:F:492:TYR:CE1	2.74	0.55
2:H:341:SER:OG	2:H:398:ILE:HD12	2.07	0.55
1:G:204:HIS:HE1	1:G:207:ASP:OD1	1.89	0.55
1:E:38:VAL:HG11	1:G:151:GLU:HG2	1.89	0.54
2:F:443:VAL:HG12	2:F:481:PHE:HA	1.88	0.54
1:G:52:SER:HB3	1:G:55:GLN:HE22	1.73	0.54
2:B:170:ARG:HB3	2:B:230:LYS:HE3	1.88	0.54
1:E:176:THR:OG1	1:E:205:LEU:HA	2.07	0.54
2:H:450:TYR:HD2	5:H:28:NGT:O6	1.90	0.54
1:C:392:TRP:CE3	5:C:530:NGT:HC83	2.42	0.54
1:E:100:VAL:HG12	1:E:102:PRO:CD	2.38	0.54
1:C:170:ARG:NH2	1:C:197:LYS:O	2.40	0.54
2:D:424:TRP:CZ2	2:D:425:LYS:HE2	2.43	0.54
1:G:101:THR:N	1:G:102:PRO:HD2	2.23	0.54
2:D:450:TYR:CZ	5:D:24:NGT:S1	3.00	0.54
1:A:170:ARG:HG2	1:A:484:LEU:CB	2.33	0.54
1:A:228:ASN:HD22	1:A:231:THR:H	1.56	0.54
1:C:136:LEU:HA	1:C:139:LEU:HD12	1.88	0.53
1:A:38:VAL:HG22	1:A:155:PHE:HE1	1.72	0.53
1:C:421:TYR:HH	5:C:530:NGT:HC81	1.67	0.53
1:E:519:VAL:HG12	2:F:491:GLU:HA	1.90	0.53
3:C:12:NAG:H61	3:C:13:NAG:N2	2.24	0.53
1:A:23:LEU:HD21	1:A:141:THR:HG23	1.89	0.53
1:G:372:VAL:HG21	1:G:376:VAL:HG21	1.90	0.53
2:B:211:ARG:HD2	2:B:242:GLN:OE1	2.09	0.53
2:H:352:GLY:HA2	2:H:405:TRP:CD1	2.44	0.53
2:D:424:TRP:HB2	2:D:450:TYR:OH	2.09	0.53
2:H:81:HIS:HE1	2:H:95:GLU:OE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:467:THR:HG21	2:H:544:GLN:HA	1.91	0.53
1:A:45:GLN:HG3	1:A:93:ASN:HD21	1.74	0.53
1:G:23:LEU:HD11	1:G:141:THR:HG23	1.91	0.53
1:G:28:GLN:NE2	1:G:487:ASN:HD22	2.07	0.53
1:E:423:ASN:HB3	1:E:460:TRP:H	1.74	0.53
1:A:102:PRO:O	1:A:103:GLY:O	2.27	0.53
2:D:450:TYR:CE2	5:D:24:NGT:S1	3.03	0.52
1:G:228:ASN:ND2	1:G:230:VAL:H	2.07	0.52
1:G:373:TRP:CD2	5:G:533:NGT:HC81	2.44	0.52
1:C:99:VAL:HG22	1:C:130:GLU:HA	1.90	0.52
2:H:58:PRO:HD2	2:H:230:LYS:HD2	1.91	0.52
1:G:170:ARG:HG2	1:G:484:LEU:HB3	1.91	0.52
1:E:173:LEU:HA	1:E:202:HIS:HB3	1.91	0.52
1:C:392:TRP:CG	5:C:530:NGT:HC83	2.45	0.52
2:B:390:LYS:O	2:B:394:ILE:HG13	2.09	0.52
1:G:147:TRP:NE1	1:G:157:ASN:OD1	2.39	0.52
1:A:525:GLU:OE1	2:B:264:HIS:HE1	1.93	0.52
1:A:61:LEU:HD11	1:A:135:ALA:CB	2.40	0.52
1:C:417:SER:O	1:C:421:TYR:HE2	1.93	0.52
1:G:459:MET:HE1	1:G:464:VAL:HG11	1.92	0.52
3:G:530:NAG:H61	3:G:531:NAG:O7	2.09	0.52
2:H:429:TYR:N	2:H:430:PRO:CD	2.72	0.52
2:F:406:GLN:HE21	2:F:424:TRP:H	1.57	0.52
2:F:415:LEU:HD22	2:F:419:THR:HG21	1.92	0.52
2:H:451:LEU:O	2:H:505:ARG:NH2	2.32	0.52
2:F:465:LYS:O	2:F:520:ARG:NH2	2.43	0.52
2:D:459:ASP:OD1	2:D:505:ARG:HD2	2.10	0.51
2:F:267:THR:O	2:F:271:VAL:HG23	2.09	0.51
2:D:504:PRO:HG3	2:D:533:ARG:HG3	1.92	0.51
1:A:402:LYS:HD2	1:A:406:LEU:HD13	1.92	0.51
1:E:467:THR:CG2	2:F:544:GLN:HA	2.39	0.51
2:H:310:TYR:CE1	2:H:364:ASN:ND2	2.77	0.51
2:F:407:GLU:OE2	2:F:424:TRP:HZ2	1.92	0.51
1:C:210:SER:HB2	1:C:227:TYR:CE2	2.45	0.51
1:A:101:THR:N	1:A:102:PRO:CD	2.73	0.51
1:G:518:ASN:ND2	1:G:519:VAL:H	2.09	0.51
2:F:170:ARG:HD2	2:F:230:LYS:HG2	1.92	0.51
1:C:392:TRP:HE3	1:C:421:TYR:HH	1.57	0.51
1:C:460:TRP:NE1	5:C:530:NGT:S1	2.83	0.51
2:D:395:ILE:HG22	2:D:400:LYS:O	2.09	0.51
1:C:320:GLY:HA2	1:C:373:TRP:CD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:ILE:HG13	1:C:397:PRO:HA	1.92	0.51
2:F:55:ALA:O	2:F:535:ARG:NH2	2.40	0.51
2:H:235:HIS:NE2	2:H:288:GLU:OE1	2.38	0.51
1:E:107:LEU:HB3	1:E:247:ARG:HG3	1.91	0.51
1:A:61:LEU:HD23	1:A:61:LEU:N	2.25	0.51
2:H:55:ALA:HB1	2:H:531:ARG:HG3	1.92	0.51
2:D:499:THR:HB	2:D:500:PRO:HD3	1.93	0.51
2:D:294:HIS:CE1	5:D:24:NGT:O3	2.64	0.51
2:F:235:HIS:NE2	2:F:288:GLU:OE1	2.37	0.51
2:H:64:LYS:HE3	2:H:193:THR:HB	1.93	0.51
2:F:199:ARG:HH21	2:F:469:LEU:HD12	1.76	0.51
2:F:203:ARG:HG2	2:F:513:LEU:HB3	1.92	0.51
1:G:46:PHE:CD2	1:G:94:VAL:CG1	2.93	0.51
1:G:172:LEU:HD23	1:G:457:ALA:HB3	1.93	0.51
1:C:113:VAL:HG21	4:C:10:NAG:H82	1.93	0.51
1:A:524:GLN:O	1:A:524:GLN:HG2	2.10	0.51
2:B:299:GLY:HA3	2:B:306:LEU:HD12	1.93	0.51
1:A:97:VAL:HG12	1:A:126:LEU:HD21	1.93	0.51
2:B:364:ASN:HD22	2:B:365:PRO:CD	2.19	0.51
4:H:26:NAG:H61	4:H:27:NAG:O7	2.11	0.51
1:A:252:ARG:HB3	1:A:314:ASP:OD1	2.10	0.51
2:B:151:LEU:HD23	2:B:194:ILE:HD13	1.94	0.50
2:D:362:GLU:O	2:D:368:GLN:NE2	2.44	0.50
2:B:202:HIS:CD2	2:B:233:VAL:HG21	2.46	0.50
2:H:504:PRO:HG3	2:H:533:ARG:HG3	1.92	0.50
2:H:530:THR:HG23	2:H:546:LEU:HD12	1.92	0.50
1:C:101:THR:N	1:C:102:PRO:HD2	2.26	0.50
1:C:202:HIS:ND1	1:C:456:GLU:OE1	2.44	0.50
1:E:424:ARG:HA	2:F:456:TYR:CD1	2.47	0.50
1:A:99:VAL:CG2	1:A:100:VAL:N	2.74	0.50
1:A:55:GLN:HG3	1:A:56:PRO:CD	2.42	0.50
2:D:474:THR:H	2:D:477:GLN:NE2	2.09	0.50
2:H:326:LEU:O	2:H:329:THR:HG22	2.11	0.50
2:H:126:GLN:HB3	2:H:157:VAL:HG13	1.94	0.50
2:D:302:GLN:HA	2:D:302:GLN:HE21	1.76	0.50
1:C:475:PRO:HG2	1:C:517:LEU:CD1	2.41	0.50
1:C:350:GLN:HA	1:C:353:SER:HB2	1.94	0.50
2:F:367:ILE:O	2:F:371:MET:HG2	2.12	0.50
1:C:23:LEU:HD11	1:C:141:THR:HG23	1.94	0.50
2:D:430:PRO:O	2:D:471:PHE:HB2	2.12	0.50
1:E:30:PHE:CD2	1:E:161:ILE:HG12	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:SER:HA	1:E:381:VAL:HG13	1.93	0.50
1:G:214:GLU:HA	1:G:222:MET:HB2	1.94	0.50
2:B:249:ILE:HG12	1:C:57:GLY:HA2	1.93	0.50
1:E:187:LEU:HA	1:E:190:LEU:HD12	1.93	0.50
2:B:223:LEU:HD21	2:B:234:LEU:HD22	1.94	0.50
1:E:228:ASN:HD22	1:E:231:THR:H	1.58	0.50
1:E:30:PHE:HD2	1:E:161:ILE:HG12	1.75	0.50
1:A:319:LEU:HD11	1:A:363:VAL:HG21	1.94	0.50
1:C:235:THR:O	1:C:239:VAL:HG23	2.12	0.50
1:C:55:GLN:HG3	1:C:56:PRO:HD2	1.93	0.50
1:A:39:LEU:HD11	1:A:156:ILE:HB	1.94	0.49
1:G:53:ALA:HB1	1:G:101:THR:HG23	1.94	0.49
1:E:46:PHE:CD2	1:E:94:VAL:CG1	2.94	0.49
2:H:248:SER:HB3	2:H:251:PHE:O	2.12	0.49
2:F:388:ILE:HG21	2:F:408:VAL:HG13	1.94	0.49
1:G:357:GLN:CD	1:G:382:LYS:HB3	2.32	0.49
1:E:198:LEU:HD11	1:E:481:ALA:HB2	1.94	0.49
1:G:307:GLU:O	1:G:311:VAL:HG23	2.11	0.49
1:A:428:GLY:HA2	2:B:492:TYR:CE2	2.47	0.49
2:D:461:ARG:O	2:D:465:LYS:HB2	2.13	0.49
1:G:113:VAL:HG11	4:G:21:NAG:H83	1.93	0.49
1:E:178:ARG:HD3	2:F:548:ALA:HB2	1.94	0.49
1:A:101:THR:O	1:A:103:GLY:N	2.46	0.49
1:G:55:GLN:CG	1:G:56:PRO:HD2	2.26	0.49
2:F:355:GLU:OE1	5:F:26:NGT:C2	2.56	0.49
1:E:409:LYS:HB2	1:E:409:LYS:HZ2	1.77	0.49
1:A:220:GLU:HA	1:A:223:ARG:HB2	1.95	0.49
1:A:325:ASP:OD2	1:A:327:THR:HB	2.13	0.49
1:C:25:PRO:HB3	1:C:482:GLU:HA	1.95	0.49
2:H:329:THR:HG23	2:H:330:TYR:CD2	2.48	0.49
2:F:253:GLU:HA	2:F:256:ASN:HB2	1.94	0.49
1:E:421:TYR:HA	1:E:458:CYS:HB2	1.94	0.49
1:A:101:THR:H	1:A:102:PRO:HD2	1.77	0.49
2:H:504:PRO:HD3	2:H:544:GLN:O	2.13	0.49
1:G:176:THR:HG22	1:G:181:LEU:HB2	1.94	0.49
1:A:100:VAL:HG23	1:A:130:GLU:HG3	1.95	0.49
2:F:460:TRP:HA	2:F:463:TYR:HD2	1.77	0.49
1:G:169:HIS:HE1	1:G:456:GLU:OE2	1.96	0.49
1:E:347:ASP:HB2	1:E:349:LYS:HE3	1.94	0.49
1:A:28:GLN:HE22	1:A:487:ASN:HD22	1.60	0.49
1:A:151:GLU:CG	1:C:38:VAL:HG11	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:451:LEU:HD11	2:H:486:ALA:HB1	1.94	0.48
2:B:350:HIS:HD2	2:B:352:GLY:H	1.61	0.48
1:A:101:THR:H	1:A:102:PRO:CD	2.26	0.48
1:G:48:TYR:HE2	1:G:61:LEU:HD12	1.79	0.48
1:G:24:TRP:CZ3	1:G:500:LEU:HB2	2.48	0.48
1:A:131:THR:HG21	1:A:133:TRP:CD1	2.48	0.48
2:F:175:PHE:O	2:F:178:LEU:HB2	2.14	0.48
1:G:318:HIS:CE1	1:G:373:TRP:CD1	3.01	0.48
2:F:142:ASN:CB	2:F:347:GLN:OE1	2.56	0.48
2:B:277:TYR:O	2:B:281:ARG:NH1	2.45	0.48
2:F:533:ARG:HG2	2:F:543:ALA:HB3	1.96	0.48
2:D:459:ASP:OD2	2:D:505:ARG:NH1	2.45	0.48
1:G:425:ILE:HB	2:H:454:ILE:HD12	1.96	0.48
1:C:421:TYR:HB2	6:C:7:HOH:O	2.13	0.48
1:A:422:LEU:O	1:A:476:ARG:NH2	2.46	0.48
1:A:43:ASN:O	1:A:43:ASN:CG	2.52	0.48
2:D:170:ARG:HH21	2:D:232:ASN:HB3	1.77	0.48
1:E:43:ASN:ND2	1:E:92:LYS:HG2	2.28	0.48
1:C:107:LEU:HD22	1:C:107:LEU:H	1.78	0.48
1:C:419:PRO:HB2	1:C:437:VAL:HG21	1.95	0.48
1:E:117:THR:HG22	1:E:162:GLU:HG2	1.94	0.48
1:A:204:HIS:CD2	1:A:256:GLU:OE1	2.66	0.48
1:C:421:TYR:HH	5:C:530:NGT:C8	2.24	0.48
1:G:114:GLU:CD	1:G:170:ARG:HH12	2.17	0.48
1:A:307:GLU:O	1:A:311:VAL:HG23	2.14	0.48
1:A:518:ASN:ND2	1:A:519:VAL:H	2.12	0.48
2:D:310:TYR:N	2:D:310:TYR:CD1	2.81	0.48
2:B:139:ALA:O	2:B:279:ARG:HD2	2.14	0.47
2:H:233:VAL:HG22	2:H:284:ARG:HD3	1.95	0.47
2:B:530:THR:HG22	2:B:546:LEU:HD12	1.96	0.47
1:G:373:TRP:CE2	5:G:533:NGT:HC81	2.48	0.47
1:C:36:ARG:HD3	3:C:12:NAG:H62	1.96	0.47
1:A:156:ILE:HG13	1:A:157:ASN:N	2.29	0.47
1:G:222:MET:HG2	1:G:233:ILE:HD12	1.96	0.47
1:G:259:THR:HB	1:G:355:TYR:OH	2.13	0.47
1:A:176:THR:HG22	1:A:181:LEU:HD12	1.97	0.47
1:A:115:ASN:ND2	3:A:1:NAG:N2	2.62	0.47
2:H:406:GLN:HE21	2:H:424:TRP:H	1.62	0.47
2:D:232:ASN:HA	2:D:283:ILE:HG13	1.96	0.47
1:A:377:PHE:HB2	1:A:389:ILE:CD1	2.44	0.47
1:E:237:GLN:HB2	2:H:92:THR:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:LEU:HG	1:A:517:LEU:HD11	1.96	0.47
1:C:157:ASN:O	1:C:159:THR:HG22	2.15	0.47
1:G:130:GLU:CG	4:G:21:NAG:H82	2.35	0.47
1:C:398:VAL:CG1	1:C:403:GLU:HG2	2.41	0.47
1:A:52:SER:HB2	1:A:97:VAL:HA	1.97	0.47
1:G:390:GLN:HG3	1:G:415:LEU:HB2	1.96	0.47
2:F:82:SER:HA	2:F:128:LEU:HD22	1.95	0.47
1:E:243:ILE:HA	1:E:253:VAL:HG21	1.97	0.47
2:D:354:ASP:OD1	2:D:405:TRP:CD1	2.67	0.47
1:G:120:ILE:HB	1:G:159:THR:HG22	1.95	0.47
1:A:99:VAL:HG23	1:A:100:VAL:N	2.29	0.47
1:G:113:VAL:HG12	1:G:115:ASN:H	1.80	0.47
1:E:36:ARG:N	4:E:17:NAG:C8	2.78	0.47
2:D:425:LYS:O	2:D:429:TYR:HB3	2.15	0.47
1:E:107:LEU:H	1:E:107:LEU:HD13	1.79	0.47
2:B:292:PRO:HA	2:B:322:ILE:HD12	1.96	0.47
1:G:356:ILE:O	1:G:360:LEU:HG	2.14	0.47
1:E:46:PHE:HD2	1:E:94:VAL:CG1	2.28	0.47
1:C:116:TYR:CZ	1:C:163:ASP:HB3	2.50	0.47
2:D:216:VAL:O	2:D:220:LEU:HG	2.14	0.47
1:G:131:THR:HG22	1:G:132:VAL:N	2.29	0.47
1:G:244:GLU:O	1:G:248:LEU:HG	2.15	0.47
2:F:222:THR:O	2:F:226:MET:HG3	2.15	0.47
1:C:364:SER:HB2	1:C:370:TYR:HE1	1.80	0.47
1:A:187:LEU:HD22	1:A:245:TYR:CG	2.50	0.47
1:G:424:ARG:HA	2:H:456:TYR:CD1	2.50	0.47
1:A:28:GLN:NE2	1:A:487:ASN:HD22	2.13	0.47
1:A:422:LEU:HD11	1:A:477:ALA:HB2	1.96	0.47
1:E:307:GLU:O	1:E:311:VAL:HG23	2.14	0.47
1:C:170:ARG:HG2	1:C:484:LEU:CB	2.45	0.46
2:F:388:ILE:HG12	2:F:408:VAL:HG11	1.96	0.46
2:H:490:GLY:HA2	2:H:493:VAL:HB	1.98	0.46
2:D:238:ILE:HG23	2:D:239:VAL:HG13	1.96	0.46
1:A:174:LEU:HB2	1:A:201:PHE:HE1	1.80	0.46
2:B:290:ASP:OD2	2:B:354:ASP:OD1	2.33	0.46
2:D:372:ARG:CG	2:D:372:ARG:NH1	2.75	0.46
1:C:302:SER:HA	1:C:362:ILE:HG21	1.96	0.46
1:C:176:THR:HG22	1:C:181:LEU:HD12	1.97	0.46
1:E:460:TRP:CH2	5:E:530:NGT:HC82	2.49	0.46
2:B:355:GLU:OE1	5:B:22:NGT:HC2	2.15	0.46
1:A:402:LYS:HD2	1:A:406:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:HG13	1:A:270:ILE:O	2.15	0.46
1:G:206:VAL:HG12	1:G:212:PRO:HD2	1.96	0.46
2:H:152:LEU:HB2	2:H:159:VAL:HB	1.97	0.46
1:C:290:VAL:O	1:C:292:PRO:HD3	2.15	0.46
2:F:330:TYR:CG	2:F:390:LYS:HE2	2.50	0.46
2:H:56:LEU:O	2:H:528:ARG:NH1	2.46	0.46
1:C:266:TRP:N	1:C:266:TRP:CD1	2.84	0.46
1:G:28:GLN:HE22	1:G:487:ASN:HD22	1.61	0.46
1:C:235:THR:HG22	1:C:236:ALA:N	2.31	0.46
1:E:175:ASP:HB3	1:E:461:GLY:N	2.30	0.46
1:E:210:SER:HB2	1:E:227:TYR:CE2	2.51	0.46
1:E:224:LYS:HB3	1:E:268:PRO:HB2	1.98	0.46
1:A:398:VAL:HG12	1:A:403:GLU:HG2	1.98	0.46
1:G:373:TRP:CZ2	5:G:533:NGT:HC82	2.50	0.46
1:E:424:ARG:HA	2:F:456:TYR:HD1	1.81	0.46
2:H:54:PRO:HB2	2:H:56:LEU:HG	1.97	0.46
1:G:392:TRP:HB2	1:G:421:TYR:OH	2.15	0.46
2:B:253:GLU:HA	2:B:256:ASN:HB2	1.97	0.46
1:E:404:LEU:HD11	1:E:416:LEU:HD13	1.97	0.46
2:B:140:PHE:CE1	2:B:279:ARG:HD3	2.51	0.46
1:A:270:ILE:HG13	1:A:273:LEU:HB2	1.98	0.46
2:F:261:SER:OG	2:F:264:HIS:CD2	2.68	0.46
1:C:519:VAL:HA	2:D:212:HIS:CE1	2.51	0.46
2:F:198:PRO:HB3	2:F:514:TRP:CE3	2.51	0.46
1:G:373:TRP:CZ2	5:G:533:NGT:C8	2.97	0.45
1:C:228:ASN:HD22	1:C:231:THR:H	1.65	0.45
1:C:232:HIS:O	1:C:233:ILE:HD13	2.16	0.45
1:E:216:PHE:CE2	1:E:307:GLU:HG3	2.51	0.45
2:F:244:PHE:N	2:F:258:GLY:O	2.42	0.45
2:B:388:ILE:HG12	2:B:408:VAL:HG21	1.97	0.45
2:F:533:ARG:HA	2:F:536:MET:HE3	1.98	0.45
1:C:100:VAL:HG12	1:C:102:PRO:CD	2.44	0.45
1:C:350:GLN:HA	1:C:353:SER:CB	2.46	0.45
1:C:462:GLU:CD	5:C:530:NGT:HC62	2.37	0.45
2:D:240:ASP:OD1	2:D:241:ASP:N	2.35	0.45
2:B:450:TYR:OH	5:B:22:NGT:S1	2.69	0.45
1:G:187:LEU:HA	1:G:190:LEU:HD12	1.97	0.45
2:H:307:THR:HG21	2:H:361:TRP:HD1	1.81	0.45
1:E:25:PRO:HB3	1:E:482:GLU:HA	1.97	0.45
1:A:373:TRP:CE2	5:A:21:NGT:C8	3.00	0.45
1:C:66:GLN:HE22	1:C:69:ARG:HD3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:HA	1:A:202:HIS:HB3	1.98	0.45
1:G:101:THR:N	1:G:102:PRO:CD	2.79	0.45
2:D:288:GLU:HG3	2:D:350:HIS:CD2	2.52	0.45
1:G:170:ARG:NH2	1:G:197:LYS:O	2.50	0.45
1:G:52:SER:OG	1:G:54:ALA:O	2.34	0.45
1:G:130:GLU:HG2	4:G:21:NAG:H81	1.92	0.45
1:E:322:ASP:HB3	1:E:373:TRP:CD1	2.51	0.45
1:A:100:VAL:CG1	1:A:102:PRO:CD	2.90	0.45
1:A:101:THR:O	1:A:102:PRO:C	2.54	0.45
2:H:499:THR:HB	2:H:500:PRO:HD3	1.99	0.45
2:F:376:PHE:CD1	2:F:382:LYS:HD3	2.52	0.45
1:G:482:GLU:HG3	1:G:486:SER:OG	2.16	0.45
2:H:82:SER:HA	2:H:128:LEU:HD22	1.98	0.45
1:E:188:ASP:O	1:E:192:VAL:HG23	2.17	0.45
1:E:171:GLY:HA2	1:E:200:VAL:O	2.17	0.45
2:B:429:TYR:N	2:B:430:PRO:CD	2.80	0.45
1:A:46:PHE:HD2	1:A:94:VAL:HG12	1.82	0.45
1:E:179:HIS:CE1	2:F:548:ALA:HA	2.52	0.45
2:B:65:MET:CE	2:B:190:ASN:HD22	2.30	0.45
2:H:204:GLY:HA2	2:H:233:VAL:O	2.16	0.45
1:E:464:VAL:HG21	1:E:472:ARG:HD2	1.99	0.45
1:E:116:TYR:CZ	1:E:163:ASP:HB3	2.52	0.45
1:A:475:PRO:HG3	1:A:504:ARG:HG3	1.98	0.45
2:F:175:PHE:HA	2:F:178:LEU:HD12	1.98	0.45
1:G:246:ALA:HB1	1:G:251:ILE:HB	1.98	0.45
1:A:131:THR:HG22	1:A:132:VAL:N	2.32	0.44
1:C:467:THR:CG2	2:D:544:GLN:HA	2.46	0.44
1:A:166:ARG:HH21	1:A:440:LEU:HD12	1.82	0.44
2:B:199:ARG:NH1	2:B:517:LYS:HA	2.32	0.44
1:A:393:ARG:O	1:A:400:TYR:HB3	2.17	0.44
1:A:258:ASP:OD2	1:A:322:ASP:OD1	2.35	0.44
1:G:69:ARG:HG3	1:G:70:ASP:N	2.32	0.44
1:E:179:HIS:HB3	1:E:465:ASP:HB3	2.00	0.44
1:A:140:GLU:O	1:A:141:THR:C	2.55	0.44
2:B:448:PRO:HB2	2:B:466:VAL:HG21	1.99	0.44
1:C:404:LEU:HD11	1:C:416:LEU:HD13	1.98	0.44
2:D:288:GLU:HB2	2:D:350:HIS:HB3	1.98	0.44
1:G:188:ASP:O	1:G:192:VAL:HG23	2.18	0.44
1:C:388:ILE:HG21	1:C:453:ILE:HD11	1.99	0.44
2:F:145:SER:HB3	2:F:166:TRP:CD1	2.53	0.44
2:F:376:PHE:HD1	2:F:382:LYS:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:TYR:HA	1:G:41:PRO:HD2	1.79	0.44
2:F:488:LEU:HD22	2:F:502:LEU:HG	1.99	0.44
2:H:453:LEU:HG	5:H:28:NGT:O6	2.18	0.44
2:H:403:ILE:HG12	2:H:420:ILE:HB	2.00	0.44
1:A:214:GLU:HA	1:A:222:MET:HB2	1.99	0.44
1:E:506:GLU:OE1	1:E:506:GLU:HA	2.18	0.44
1:C:36:ARG:HH11	3:C:12:NAG:H62	1.83	0.44
1:E:178:ARG:NE	1:E:462:GLU:OE2	2.51	0.44
2:D:215:PRO:HD2	2:D:495:ALA:HB2	1.99	0.44
2:F:151:LEU:HD13	2:F:160:LEU:HD13	1.99	0.44
1:E:237:GLN:HB2	2:H:92:THR:HG21	1.99	0.44
1:A:173:LEU:HB3	1:A:458:CYS:HA	2.00	0.44
1:E:168:PRO:HD2	1:E:453:ILE:O	2.18	0.44
1:G:118:LEU:HB3	1:G:161:ILE:HD12	1.99	0.44
2:D:429:TYR:O	2:D:432:GLU:HB2	2.17	0.44
1:C:41:PRO:HB3	1:C:73:PHE:HB3	1.99	0.44
2:H:464:TYR:HB2	2:H:508:ALA:HB1	2.00	0.44
2:B:502:LEU:HD13	2:B:503:TRP:CE2	2.52	0.44
2:B:200:PHE:CE1	2:B:481:PHE:CD1	3.06	0.44
1:E:445:THR:HB	1:E:446:PRO:HD2	2.00	0.44
1:G:120:ILE:HB	1:G:159:THR:CG2	2.48	0.43
1:A:215:SER:O	1:A:219:PRO:HA	2.17	0.43
1:A:339:MET:SD	1:A:351:LEU:HD22	2.58	0.43
1:E:520:GLY:O	2:F:212:HIS:HD2	2.00	0.43
2:D:199:ARG:HH21	2:D:469:LEU:HD12	1.82	0.43
1:C:392:TRP:HB2	1:C:421:TYR:OH	2.18	0.43
1:E:36:ARG:CB	4:E:17:NAG:H81	2.49	0.43
1:G:140:GLU:OE1	1:G:195:TYR:HD1	2.01	0.43
1:A:435:TYR:HE2	1:A:491:SER:HA	1.82	0.43
1:G:122:ASP:N	1:G:122:ASP:OD1	2.49	0.43
1:G:205:LEU:HD12	1:G:205:LEU:H	1.83	0.43
2:B:206:LEU:HB3	2:B:487:CYS:HA	1.99	0.43
1:E:460:TRP:CH2	5:E:530:NGT:C8	3.01	0.43
1:C:229:PRO:HA	1:C:233:ILE:HD11	2.00	0.43
2:D:302:GLN:HA	2:D:302:GLN:NE2	2.34	0.43
1:E:40:TYR:HA	1:E:41:PRO:HD2	1.79	0.43
2:B:149:TYR:CZ	2:B:196:ASP:HB3	2.53	0.43
1:G:55:GLN:HG3	1:G:56:PRO:HD3	1.95	0.43
1:G:373:TRP:CE3	5:G:533:NGT:HC81	2.54	0.43
1:E:52:SER:O	1:E:55:GLN:NE2	2.51	0.43
1:E:171:GLY:HA3	1:E:456:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:TYR:HE1	2:D:547:TYR:HD1	1.64	0.43
1:G:513:GLN:HG3	1:G:526:PHE:CZ	2.54	0.43
2:F:57:TRP:HA	2:F:58:PRO:C	2.38	0.43
2:F:63:VAL:HG12	2:F:65:MET:HG2	2.01	0.43
1:G:97:VAL:HG12	1:G:126:LEU:HD21	2.01	0.43
1:G:99:VAL:CG2	1:G:130:GLU:HA	2.47	0.43
1:G:356:ILE:HD13	1:G:376:VAL:HG22	2.01	0.43
1:C:59:SER:O	1:C:63:GLU:HG2	2.19	0.43
1:A:357:GLN:OE1	1:A:382:LYS:HB3	2.18	0.43
2:D:139:ALA:O	2:D:279:ARG:NH2	2.46	0.43
2:B:105:ILE:HG12	2:B:176:SER:HA	2.01	0.43
2:D:467:GLU:HA	2:D:468:PRO:HD2	1.88	0.43
2:B:200:PHE:HE1	2:B:481:PHE:HD1	1.67	0.43
1:A:356:ILE:HD13	1:A:376:VAL:HG22	2.00	0.43
2:F:153:VAL:HB	2:F:192:SER:H	1.84	0.43
1:C:332:ASN:HA	1:C:333:PRO:HD3	1.80	0.43
2:D:202:HIS:CE1	2:D:444:ILE:HD13	2.54	0.43
2:F:134:GLN:O	2:F:164:ARG:NH1	2.41	0.43
1:A:107:LEU:H	1:A:107:LEU:HD22	1.84	0.43
2:F:516:SER:HB2	2:F:519:VAL:HG23	2.00	0.43
1:A:95:LEU:HB2	1:A:126:LEU:HD23	2.00	0.43
1:C:235:THR:HG22	1:C:236:ALA:H	1.83	0.43
2:B:200:PHE:CE1	2:B:481:PHE:HD1	2.36	0.43
1:A:177:SER:O	1:A:210:SER:HB3	2.18	0.43
1:E:370:TYR:HD2	1:E:387:THR:HG23	1.84	0.43
1:G:171:GLY:HA2	1:G:200:VAL:O	2.18	0.43
2:F:54:PRO:HB2	2:F:56:LEU:HG	1.99	0.43
1:A:40:TYR:HA	1:A:41:PRO:HD2	1.88	0.43
2:F:468:PRO:HB2	2:F:481:PHE:CZ	2.54	0.43
2:H:206:LEU:HA	2:H:235:HIS:O	2.19	0.43
2:H:154:LYS:HD2	2:H:155:GLU:O	2.18	0.43
2:F:215:PRO:O	2:F:218:ILE:HG22	2.18	0.43
2:B:208:ASP:OD1	2:B:208:ASP:C	2.56	0.43
2:D:237:HIS:CD2	2:D:288:GLU:OE1	2.72	0.43
1:A:384:GLN:HG3	1:A:385:PRO:HD2	2.00	0.43
2:H:63:VAL:HA	2:H:194:ILE:HG13	2.01	0.43
1:E:101:THR:O	1:E:103:GLY:N	2.52	0.42
1:G:192:VAL:HA	1:G:195:TYR:CD2	2.54	0.42
1:E:430:ASP:OD2	1:E:476:ARG:NH1	2.51	0.42
2:D:323:ASN:HA	2:D:324:PRO:HD3	1.94	0.42
1:A:387:THR:HG22	1:A:388:ILE:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:VAL:HG23	1:G:100:VAL:H	1.83	0.42
1:C:316:TYR:CE2	1:C:388:ILE:HD11	2.53	0.42
1:E:469:LEU:HG	1:E:473:LEU:HD12	2.00	0.42
1:A:42:ASN:H	1:A:42:ASN:ND2	2.17	0.42
1:G:183:LEU:O	1:G:187:LEU:HG	2.19	0.42
2:H:55:ALA:CB	2:H:531:ARG:HG3	2.48	0.42
2:F:287:PRO:HB3	2:F:344:PHE:CZ	2.54	0.42
2:B:73:ALA:HB3	2:B:76:ASN:HB3	2.01	0.42
1:A:69:ARG:CZ	1:A:69:ARG:HB2	2.50	0.42
1:E:33:SER:HB3	1:E:158:LYS:O	2.19	0.42
2:F:74:PRO:HD2	2:H:183:SER:O	2.19	0.42
1:E:36:ARG:CG	4:E:17:NAG:H81	2.50	0.42
2:F:142:ASN:HB2	2:F:347:GLN:CD	2.38	0.42
2:D:211:ARG:HD3	2:D:211:ARG:N	2.34	0.42
1:G:69:ARG:CZ	1:G:69:ARG:HB2	2.48	0.42
2:F:182:ASP:OD1	2:F:186:THR:N	2.52	0.42
2:B:72:LEU:HD11	2:B:189:ILE:HG22	2.02	0.42
1:E:485:TRP:C	1:E:485:TRP:CD1	2.91	0.42
1:A:63:GLU:OE2	1:A:63:GLU:HA	2.20	0.42
1:C:353:SER:HA	1:C:381:VAL:HG13	2.00	0.42
1:G:169:HIS:CE1	1:G:456:GLU:OE2	2.73	0.42
1:E:167:PHE:HA	1:E:168:PRO:HD3	1.94	0.42
2:D:422:GLU:HA	2:D:444:ILE:O	2.19	0.42
1:A:388:ILE:CG2	1:A:415:LEU:HD22	2.49	0.42
2:H:93:LEU:HD21	2:H:169:LEU:HD11	1.99	0.42
2:F:239:VAL:HG12	2:F:245:PRO:HD2	2.02	0.42
2:D:237:HIS:HD2	2:D:288:GLU:OE1	2.01	0.42
2:D:429:TYR:HA	2:D:432:GLU:HB2	2.02	0.42
1:E:30:PHE:HE2	1:E:159:THR:OG1	2.01	0.42
1:A:381:VAL:O	1:A:383:ILE:HG22	2.20	0.42
1:G:45:GLN:HG2	1:G:93:ASN:OD1	2.19	0.42
2:D:129:VAL:HG22	2:D:160:LEU:HD23	2.02	0.42
1:E:172:LEU:CD1	1:E:174:LEU:HD13	2.50	0.42
2:H:98:PHE:CE1	2:H:129:VAL:HG21	2.55	0.42
2:F:205:ILE:CD1	2:F:486:ALA:HB3	2.44	0.42
1:C:121:ASN:HD21	1:C:124:GLN:HG2	1.84	0.42
1:E:176:THR:HG22	1:E:181:LEU:HD12	2.00	0.42
2:F:279:ARG:C	2:F:281:ARG:H	2.22	0.42
4:F:20:NAG:O7	4:F:20:NAG:H3	2.19	0.42
2:D:205:ILE:HG21	2:D:502:LEU:HD11	2.02	0.42
1:G:379:ASN:O	1:G:380:LYS:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:PRO:CG	2:B:54:PRO:N	2.81	0.42
1:G:256:GLU:HB2	1:G:318:HIS:HB3	2.01	0.42
2:H:253:GLU:HA	2:H:256:ASN:HB2	2.02	0.42
1:C:26:TRP:HA	1:C:27:PRO:HD3	1.95	0.42
1:C:459:MET:HE3	1:C:464:VAL:HG11	2.02	0.42
1:C:148:LYS:HA	1:C:153:THR:O	2.20	0.41
1:G:188:ASP:O	1:G:191:ASP:HB2	2.20	0.41
1:C:40:TYR:HA	1:C:41:PRO:HD2	1.94	0.41
2:F:168:ALA:O	2:F:172:LEU:HG	2.20	0.41
1:C:33:SER:CB	1:C:158:LYS:HG2	2.49	0.41
1:E:28:GLN:HE22	1:E:487:ASN:HD22	1.67	0.41
1:G:165:PRO:HB3	1:G:485:TRP:CE3	2.55	0.41
2:H:452:ASP:OD2	2:H:489:TRP:HB2	2.20	0.41
1:C:121:ASN:HD22	1:C:123:ASP:H	1.67	0.41
2:B:126:GLN:HE21	2:B:126:GLN:HB2	1.71	0.41
1:E:28:GLN:HG3	1:E:164:PHE:O	2.19	0.41
2:H:68:ASN:HB3	2:H:191:GLU:HG2	2.02	0.41
1:G:384:GLN:HG3	1:G:385:PRO:HD2	2.01	0.41
1:G:145:LEU:HD23	1:G:145:LEU:HA	1.95	0.41
2:D:350:HIS:HD2	2:D:352:GLY:H	1.68	0.41
2:D:350:HIS:HA	2:D:403:ILE:O	2.20	0.41
2:B:424:TRP:HB2	2:B:450:TYR:OH	2.20	0.41
1:A:323:GLU:OE1	5:A:21:NGT:HC2	2.19	0.41
2:H:66:THR:HA	2:H:67:PRO:HD3	1.95	0.41
1:E:386:ASP:O	1:E:413:ARG:NH1	2.54	0.41
1:G:350:GLN:HA	1:G:353:SER:HB3	2.02	0.41
1:E:131:THR:HG22	1:E:132:VAL:H	1.85	0.41
1:E:359:LEU:HA	1:E:362:ILE:HD12	2.02	0.41
1:G:55:GLN:CG	1:G:56:PRO:CD	2.84	0.41
1:C:38:VAL:HG22	1:C:155:PHE:CE1	2.55	0.41
1:C:292:PRO:HG3	1:C:329:TRP:CZ2	2.55	0.41
1:A:202:HIS:CE1	1:A:318:HIS:CD2	3.09	0.41
1:A:337:ASP:O	1:A:341:LYS:HG2	2.20	0.41
1:G:433:ASP:O	1:G:437:VAL:HG23	2.20	0.41
2:D:449:TRP:CD1	2:D:509:VAL:HG22	2.55	0.41
1:C:160:GLU:OE2	1:C:160:GLU:HA	2.19	0.41
1:G:524:GLN:HG2	1:G:524:GLN:O	2.20	0.41
1:A:164:PHE:CD2	3:A:1:NAG:H62	2.55	0.41
1:A:66:GLN:HE22	1:A:69:ARG:HD3	1.84	0.41
1:A:99:VAL:HG22	1:A:130:GLU:HA	2.02	0.41
2:D:532:HIS:HD2	2:D:535:ARG:NH2	2.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ILE:HD11	1:A:387:THR:HG21	2.03	0.41
2:F:131:ILE:HA	2:F:162:ALA:O	2.20	0.41
2:F:133:LEU:HD12	2:F:163:ASN:HB3	2.02	0.41
2:F:504:PRO:HD3	2:F:544:GLN:O	2.20	0.41
2:D:350:HIS:CD2	2:D:352:GLY:H	2.38	0.41
1:A:52:SER:HA	1:A:97:VAL:HG23	2.02	0.41
2:D:54:PRO:HB2	2:D:531:ARG:NH2	2.36	0.41
2:D:371:MET:H	2:D:371:MET:HG2	1.70	0.41
2:B:84:ASN:C	2:B:84:ASN:HD22	2.24	0.41
2:H:414:LYS:HD3	2:H:414:LYS:HA	1.97	0.41
1:C:228:ASN:ND2	1:C:230:VAL:H	2.16	0.41
1:C:26:TRP:HB2	1:C:499:ARG:NH1	2.36	0.41
1:E:59:SER:O	1:E:63:GLU:HG2	2.21	0.41
1:A:26:TRP:HA	1:A:27:PRO:HD3	1.95	0.41
1:E:278:TYR:CD1	1:E:332:ASN:HA	2.55	0.41
2:D:68:ASN:HB3	2:D:191:GLU:HG2	2.01	0.41
1:A:374:GLN:HA	1:A:389:ILE:HG23	2.03	0.41
1:G:464:VAL:HG22	1:G:472:ARG:NH1	2.36	0.41
1:A:61:LEU:HD11	1:A:135:ALA:HB3	2.02	0.41
1:E:475:PRO:HD3	1:E:515:GLN:O	2.20	0.41
1:C:425:ILE:HB	2:D:454:ILE:HD12	2.03	0.41
1:A:60:VAL:HG12	1:A:61:LEU:HD23	2.02	0.41
2:D:160:LEU:HD21	2:D:168:ALA:HA	2.02	0.41
1:C:120:ILE:O	1:C:158:LYS:HA	2.20	0.41
1:C:31:GLN:HB3	1:C:160:GLU:HB3	2.02	0.41
1:A:523:GLU:HG3	1:C:42:ASN:ND2	2.36	0.41
1:E:431:TRP:HA	1:E:434:PHE:CD2	2.55	0.41
2:F:295:THR:O	2:F:306:LEU:HD21	2.21	0.41
2:F:223:LEU:HD21	2:F:234:LEU:HD22	2.02	0.41
1:E:290:VAL:HG12	1:E:291:ASN:N	2.36	0.41
2:D:237:HIS:HE1	2:D:240:ASP:OD2	2.04	0.41
2:D:290:ASP:HA	2:D:352:GLY:HA3	2.03	0.41
2:H:532:HIS:CD2	2:H:535:ARG:HH21	2.39	0.41
1:G:428:GLY:HA2	2:H:492:TYR:CZ	2.56	0.41
1:A:90:LEU:HD13	1:A:92:LYS:HD2	2.02	0.40
1:C:459:MET:CE	1:C:464:VAL:HG11	2.51	0.40
2:B:186:THR:HA	2:D:184:TYR:O	2.21	0.40
1:G:232:HIS:NE2	2:H:550:TYR:HB2	2.36	0.40
1:G:401:MET:HA	1:G:404:LEU:HD12	2.02	0.40
1:C:270:ILE:HA	1:C:271:PRO:HD2	1.99	0.40
1:A:266:TRP:N	1:A:266:TRP:CD1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:229:ASN:OD1	2:D:532:HIS:HE1	2.03	0.40
1:G:465:ASP:C	1:G:467:THR:H	2.24	0.40
1:A:46:PHE:CD2	1:A:94:VAL:HG12	2.55	0.40
2:F:209:THR:O	2:F:245:PRO:HG2	2.21	0.40
2:H:347:GLN:O	2:H:401:GLY:N	2.43	0.40
1:E:423:ASN:OD1	1:E:460:TRP:HD1	2.05	0.40
1:C:228:ASN:HA	1:C:229:PRO:HD3	1.77	0.40
2:F:382:LYS:HA	2:F:385:SER:HB2	2.04	0.40
1:G:26:TRP:HA	1:G:27:PRO:HD3	1.85	0.40
2:F:70:LEU:HD21	2:F:155:GLU:HB3	2.04	0.40
1:C:100:VAL:HG23	1:C:130:GLU:HG3	2.04	0.40
2:B:437:THR:O	2:B:477:GLN:HG2	2.21	0.40
1:C:67:ARG:HD2	1:C:249:ARG:NH2	2.36	0.40
2:H:147:GLU:HB3	2:H:170:ARG:HG3	2.02	0.40
2:F:64:LYS:HE3	2:F:193:THR:O	2.21	0.40
2:F:150:THR:HG22	2:F:195:ILE:HG12	2.02	0.40
1:A:179:HIS:HE1	1:A:462:GLU:O	2.05	0.40
2:D:460:TRP:CD1	2:D:546:LEU:HD22	2.56	0.40
1:C:447:GLU:OE2	1:C:447:GLU:N	2.50	0.40
2:B:291:THR:HG22	2:B:322:ILE:CD1	2.51	0.40
2:B:235:HIS:NE2	2:B:288:GLU:OE1	2.42	0.40
2:F:219:ILE:O	2:F:222:THR:HB	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:424:ARG:NH2	2:H:369:ASP:OD1[2_456]	1.93	0.27

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	488/507 (96%)	446 (91%)	33 (7%)	9 (2%)	11	49
1	C	488/507 (96%)	450 (92%)	31 (6%)	7 (1%)	14	54
1	E	488/507 (96%)	450 (92%)	33 (7%)	5 (1%)	19	62
1	G	488/507 (96%)	448 (92%)	30 (6%)	10 (2%)	9	46
2	B	474/503 (94%)	434 (92%)	37 (8%)	3 (1%)	30	72
2	D	473/503 (94%)	430 (91%)	38 (8%)	5 (1%)	17	60
2	F	474/503 (94%)	425 (90%)	43 (9%)	6 (1%)	15	56
2	H	474/503 (94%)	440 (93%)	31 (6%)	3 (1%)	30	72
All	All	3847/4040 (95%)	3523 (92%)	276 (7%)	48 (1%)	16	58

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	GLY
2	B	55	ALA
1	C	102	PRO
1	C	103	GLY
1	E	102	PRO
2	F	458	GLN
1	G	102	PRO
1	G	380	LYS
1	G	462	GLU
1	C	466	ASN
2	D	427	SER
1	E	103	GLY
1	E	104	CYS
1	E	229	PRO
2	F	427	SER
1	A	488	LYS
2	B	237	HIS
2	D	458	GLN
2	D	495	ALA
2	F	76	ASN
1	A	102	PRO
1	A	280	GLY
1	G	41	PRO
1	G	490	THR
2	H	74	PRO
1	A	41	PRO
1	A	285	GLY

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Mol	Chain	Res	Type
1	A	490	THR
2	B	76	ASN
1	C	229	PRO
1	C	283	PRO
1	E	280	GLY
2	F	182	ASP
1	G	267	GLY
1	G	466	ASN
2	H	417	PRO
2	H	458	GLN
1	C	437	VAL
2	D	519	VAL
2	F	67	PRO
1	G	103	GLY
1	G	465	ASP
2	D	418	GLY
2	F	74	PRO
1	G	280	GLY
1	A	229	PRO
1	A	101	THR
1	C	267	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	440/454 (97%)	403 (92%)	37 (8%)	14 47
1	C	440/454 (97%)	401 (91%)	39 (9%)	12 43
1	E	440/454 (97%)	412 (94%)	28 (6%)	22 61
1	G	440/454 (97%)	405 (92%)	35 (8%)	15 50
2	B	426/445 (96%)	405 (95%)	21 (5%)	31 70
2	D	425/445 (96%)	394 (93%)	31 (7%)	17 55
2	F	426/445 (96%)	404 (95%)	22 (5%)	29 68
2	H	426/445 (96%)	408 (96%)	18 (4%)	36 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3463/3596 (96%)	3232 (93%)	231 (7%)	20 59

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	35	GLN
1	A	42	ASN
1	A	45	GLN
1	A	47	GLN
1	A	66	GLN
1	A	69	ARG
1	A	72	LEU
1	A	94	VAL
1	A	95	LEU
1	A	105	ASN
1	A	106	GLN
1	A	107	LEU
1	A	121	ASN
1	A	122	ASP
1	A	126	LEU
1	A	127	LEU
1	A	153	THR
1	A	178	ARG
1	A	198	LEU
1	A	270	ILE
1	A	299	GLU
1	A	306	LEU
1	A	372	VAL
1	A	382	LYS
1	A	396	ILE
1	A	398	VAL
1	A	402	LYS
1	A	409	LYS
1	A	415	LEU
1	A	416	LEU
1	A	466	ASN
1	A	489	LEU
1	A	507	LEU
1	A	518	ASN
1	A	521	PHE
1	A	528	GLN

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Mol	Chain	Res	Type
2	B	84	ASN
2	B	93	LEU
2	B	169	LEU
2	B	191	GLU
2	B	206	LEU
2	B	211	ARG
2	B	250	THR
2	B	257	LYS
2	B	328	THR
2	B	338	LYS
2	B	356	VAL
2	B	364	ASN
2	B	384	GLU
2	B	414	LYS
2	B	426	ASP
2	B	431	GLU
2	B	462	LYS
2	B	502	LEU
2	B	512	ARG
2	B	516	SER
2	B	522	MET
1	C	32	THR
1	C	35	GLN
1	C	55	GLN
1	C	72	LEU
1	C	73	PHE
1	C	90	LEU
1	C	92	LYS
1	C	93	ASN
1	C	94	VAL
1	C	98	SER
1	C	101	THR
1	C	106	GLN
1	C	107	LEU
1	C	121	ASN
1	C	126	LEU
1	C	131	THR
1	C	158	LYS
1	C	159	THR
1	C	162	GLU
1	C	172	LEU
1	C	178	ARG

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Mol	Chain	Res	Type
1	C	228	ASN
1	C	240	LYS
1	C	263	THR
1	C	296	ASN
1	C	299	GLU
1	C	336	GLN
1	C	339	MET
1	C	358	THR
1	C	370	TYR
1	C	372	VAL
1	C	382	LYS
1	C	399	ASN
1	C	403	GLU
1	C	406	LEU
1	C	465	ASP
1	C	523	GLU
1	C	525	GLU
1	C	528	GLN
2	D	66	THR
2	D	84	ASN
2	D	154	LYS
2	D	165	VAL
2	D	174	THR
2	D	183	SER
2	D	211	ARG
2	D	217	LYS
2	D	250	THR
2	D	257	LYS
2	D	267	THR
2	D	291	THR
2	D	307	THR
2	D	310	TYR
2	D	317	ASP
2	D	338	LYS
2	D	341	SER
2	D	359	LYS
2	D	360	CYS
2	D	362	GLU
2	D	369	ASP
2	D	372	ARG
2	D	384	GLU
2	D	390	LYS

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Mol	Chain	Res	Type
2	D	393	ASP
2	D	431	GLU
2	D	451	LEU
2	D	455	SER
2	D	476	LYS
2	D	502	LEU
2	D	522	MET
1	E	23	LEU
1	E	28	GLN
1	E	47	GLN
1	E	55	GLN
1	E	66	GLN
1	E	69	ARG
1	E	89	THR
1	E	92	LYS
1	E	106	GLN
1	E	107	LEU
1	E	121	ASN
1	E	126	LEU
1	E	127	LEU
1	E	131	THR
1	E	153	THR
1	E	162	GLU
1	E	174	LEU
1	E	189	THR
1	E	228	ASN
1	E	295	ASN
1	E	370	TYR
1	E	382	LYS
1	E	395	ASP
1	E	396	ILE
1	E	399	ASN
1	E	466	ASN
1	E	515	GLN
1	E	518	ASN
2	F	68	ASN
2	F	79	ILE
2	F	80	SER
2	F	130	SER
2	F	155	GLU
2	F	211	ARG
2	F	250	THR

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Mol	Chain	Res	Type
2	F	311	SER
2	F	338	LYS
2	F	341	SER
2	F	351	LEU
2	F	359	LYS
2	F	385	SER
2	F	390	LYS
2	F	403	ILE
2	F	414	LYS
2	F	431	GLU
2	F	451	LEU
2	F	476	LYS
2	F	502	LEU
2	F	522	MET
2	F	550	TYR
1	G	47	GLN
1	G	51	SER
1	G	69	ARG
1	G	72	LEU
1	G	90	LEU
1	G	92	LYS
1	G	95	LEU
1	G	98	SER
1	G	106	GLN
1	G	107	LEU
1	G	121	ASN
1	G	122	ASP
1	G	126	LEU
1	G	162	GLU
1	G	172	LEU
1	G	198	LEU
1	G	235	THR
1	G	270	ILE
1	G	299	GLU
1	G	311	VAL
1	G	322	ASP
1	G	336	GLN
1	G	370	TYR
1	G	382	LYS
1	G	398	VAL
1	G	399	ASN
1	G	406	LEU

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Mol	Chain	Res	Type
1	G	415	LEU
1	G	443	GLU
1	G	463	TYR
1	G	467	THR
1	G	518	ASN
1	G	521	PHE
1	G	523	GLU
1	G	528	GLN
2	H	65	MET
2	H	84	ASN
2	H	154	LYS
2	H	211	ARG
2	H	216	VAL
2	H	257	LYS
2	H	309	CYS
2	H	311	SER
2	H	338	LYS
2	H	359	LYS
2	H	364	ASN
2	H	369	ASP
2	H	379	ASP
2	H	414	LYS
2	H	431	GLU
2	H	502	LEU
2	H	518	ASP
2	H	522	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	42	ASN
1	A	47	GLN
1	A	55	GLN
1	A	66	GLN
1	A	93	ASN
1	A	115	ASN
1	A	121	ASN
1	A	157	ASN
1	A	204	HIS
1	A	228	ASN
1	A	262	HIS

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Mol	Chain	Res	Type
1	A	336	GLN
1	A	384	GLN
1	A	466	ASN
1	A	518	ASN
1	A	528	GLN
2	B	76	ASN
2	B	84	ASN
2	B	102	HIS
2	B	123	GLN
2	B	126	GLN
2	B	190	ASN
2	B	237	HIS
2	B	264	HIS
2	B	302	GLN
2	B	347	GLN
2	B	350	HIS
2	B	364	ASN
2	B	406	GLN
2	B	532	HIS
1	C	28	GLN
1	C	55	GLN
1	C	66	GLN
1	C	106	GLN
1	C	121	ASN
1	C	124	GLN
1	C	204	HIS
1	C	228	ASN
1	C	336	GLN
1	C	350	GLN
1	C	466	ASN
1	C	518	ASN
2	D	76	ASN
2	D	81	HIS
2	D	84	ASN
2	D	102	HIS
2	D	123	GLN
2	D	126	GLN
2	D	237	HIS
2	D	302	GLN
2	D	373	GLN
2	D	406	GLN
2	D	477	GLN

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Mol	Chain	Res	Type
2	D	532	HIS
1	E	28	GLN
1	E	43	ASN
1	E	47	GLN
1	E	55	GLN
1	E	106	GLN
1	E	121	ASN
1	E	124	GLN
1	E	228	ASN
1	E	336	GLN
1	E	399	ASN
1	E	448	GLN
1	E	515	GLN
1	E	518	ASN
2	F	76	ASN
2	F	84	ASN
2	F	123	GLN
2	F	126	GLN
2	F	237	HIS
2	F	264	HIS
2	F	350	HIS
2	F	406	GLN
2	F	477	GLN
2	F	532	HIS
1	G	28	GLN
1	G	29	ASN
1	G	43	ASN
1	G	55	GLN
1	G	105	ASN
1	G	121	ASN
1	G	169	HIS
1	G	204	HIS
1	G	228	ASN
1	G	336	GLN
1	G	350	GLN
1	G	384	GLN
1	G	399	ASN
1	G	466	ASN
1	G	518	ASN
2	H	76	ASN
2	H	81	HIS
2	H	84	ASN

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Mol	Chain	Res	Type
2	H	123	GLN
2	H	237	HIS
2	H	264	HIS
2	H	302	GLN
2	H	364	ASN
2	H	406	GLN
2	H	532	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

27 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	NAG	A	1	1,3	14,14,15	0.72	0	15,19,21	0.59	0
3	NAG	A	2	3	14,14,15	0.56	0	15,19,21	1.25	1 (6%)
3	BMA	A	3	3	11,11,12	0.61	0	14,15,17	1.54	3 (21%)
3	NAG	A	4	1,3	14,14,15	0.48	0	15,19,21	0.59	0
3	NAG	A	5	3	14,14,15	0.56	0	15,19,21	1.21	2 (13%)
3	BMA	A	6	3	11,11,12	0.74	0	14,15,17	2.54	2 (14%)
3	NAG	B	7	3	14,14,15	0.55	0	15,19,21	0.59	0
3	NAG	B	8	3	14,14,15	0.61	0	15,19,21	1.16	1 (6%)
3	BMA	B	9	3	11,11,12	2.16	2 (18%)	14,15,17	3.55	6 (42%)
4	NAG	C	10	1,4	14,14,15	0.63	0	15,19,21	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	11	4	14,14,15	0.51	0	15,19,21	0.79	0
3	NAG	C	12	1,3	14,14,15	0.96	1 (7%)	15,19,21	0.61	0
3	NAG	C	13	3	14,14,15	1.10	2 (14%)	15,19,21	3.11	4 (26%)
3	BMA	C	14	3	11,11,12	0.60	0	14,15,17	1.81	2 (14%)
4	NAG	D	15	2,4	14,14,15	0.45	0	15,19,21	0.59	0
4	NAG	D	16	4	14,14,15	0.57	0	15,19,21	0.98	0
4	NAG	E	17	1,4	14,14,15	2.77	5 (35%)	15,19,21	0.75	0
4	NAG	E	18	4	14,14,15	1.15	1 (7%)	15,19,21	2.08	3 (20%)
4	NAG	F	19	2,4	14,14,15	0.59	0	15,19,21	0.58	0
4	NAG	F	20	4	14,14,15	0.65	0	15,19,21	1.17	2 (13%)
4	NAG	G	21	1,4	14,14,15	1.90	2 (14%)	15,19,21	0.62	0
4	NAG	G	22	4	14,14,15	0.62	0	15,19,21	1.31	3 (20%)
3	NAG	G	530	1,3	14,14,15	0.55	0	15,19,21	0.59	0
3	NAG	G	531	3	14,14,15	0.60	0	15,19,21	1.14	1 (6%)
3	BMA	G	532	3	11,11,12	0.61	0	14,15,17	1.06	1 (7%)
4	NAG	H	26	2,4	14,14,15	1.00	1 (7%)	15,19,21	0.59	0
4	NAG	H	27	4	14,14,15	0.61	0	15,19,21	1.21	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	BMA	A	3	3	-	0/2/19/22	0/1/1/1
3	NAG	A	4	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	5	3	-	0/6/23/26	0/1/1/1
3	BMA	A	6	3	-	0/2/19/22	0/1/1/1
3	NAG	B	7	3	-	0/6/23/26	0/1/1/1
3	NAG	B	8	3	-	0/6/23/26	0/1/1/1
3	BMA	B	9	3	-	0/2/19/22	0/1/1/1
4	NAG	C	10	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	11	4	-	0/6/23/26	0/1/1/1
3	NAG	C	12	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	13	3	1/1/5/7	0/6/23/26	0/1/1/1
3	BMA	C	14	3	-	0/2/19/22	0/1/1/1
4	NAG	D	15	2,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	D	16	4	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	17	1,4	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	E	18	4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	F	19	2,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	F	20	4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	G	21	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	22	4	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	G	530	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	531	3	1/1/5/7	0/6/23/26	0/1/1/1
3	BMA	G	532	3	-	0/2/19/22	0/1/1/1
4	NAG	H	26	2,4	-	0/6/23/26	0/1/1/1
4	NAG	H	27	4	1/1/5/7	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	17	NAG	O4-C4	-6.43	1.27	1.43
4	E	17	NAG	O5-C1	-4.40	1.36	1.43
4	E	17	NAG	C4-C5	-4.34	1.43	1.53
3	C	13	NAG	O5-C1	-3.14	1.38	1.43
4	G	21	NAG	C1-C2	-2.76	1.48	1.52
4	E	17	NAG	C2-N2	-2.28	1.42	1.46
3	C	13	NAG	O5-C5	-2.01	1.39	1.43
3	C	12	NAG	C1-C2	2.17	1.55	1.52
4	H	26	NAG	C2-N2	2.34	1.50	1.46
3	B	9	BMA	C2-C3	2.88	1.56	1.52
4	E	18	NAG	C1-C2	3.47	1.57	1.52
4	E	17	NAG	C1-C2	4.32	1.58	1.52
4	G	21	NAG	C2-N2	5.73	1.56	1.46
3	B	9	BMA	O2-C2	6.15	1.57	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	6	BMA	C1-C2-C3	-6.94	101.33	109.54
3	B	9	BMA	C1-O5-C5	-6.37	104.16	112.25
3	A	6	BMA	C1-O5-C5	-5.05	105.84	112.25
3	C	14	BMA	C1-O5-C5	-3.93	107.26	112.25
3	G	532	BMA	C1-O5-C5	-2.76	108.75	112.25
3	B	9	BMA	C2-C3-C4	-2.23	107.25	111.04
3	A	5	NAG	O4-C4-C3	-2.06	105.71	110.34
4	E	18	NAG	C3-C4-C5	-2.03	106.66	110.20
4	C	10	NAG	C1-O5-C5	2.22	115.06	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	22	NAG	C1-O5-C5	2.27	115.12	112.25
4	F	20	NAG	C4-C3-C2	2.28	114.77	111.23
4	F	20	NAG	C2-N2-C7	2.34	126.04	123.04
3	G	531	NAG	C4-C3-C2	2.40	114.96	111.23
3	A	5	NAG	C4-C3-C2	2.44	115.02	111.23
4	G	22	NAG	C2-N2-C7	2.45	126.18	123.04
3	B	8	NAG	C2-N2-C7	2.52	126.28	123.04
3	A	3	BMA	O5-C1-C2	2.65	115.15	110.86
4	G	22	NAG	C4-C3-C2	2.79	115.57	111.23
3	A	3	BMA	C1-C2-C3	3.00	113.09	109.54
4	E	18	NAG	C2-N2-C7	3.04	126.94	123.04
3	C	13	NAG	C4-C3-C2	3.18	116.18	111.23
4	H	27	NAG	C2-N2-C7	3.31	127.29	123.04
3	A	3	BMA	C1-O5-C5	3.64	116.87	112.25
3	C	13	NAG	C2-N2-C7	3.67	127.76	123.04
3	A	2	NAG	C2-N2-C7	3.85	127.98	123.04
3	B	9	BMA	O5-C5-C6	4.11	116.23	107.35
3	C	13	NAG	C3-C4-C5	4.20	117.52	110.20
3	B	9	BMA	O2-C2-C3	4.32	118.81	110.12
3	C	14	BMA	O5-C5-C6	4.65	117.40	107.35
3	B	9	BMA	O2-C2-C1	4.87	118.98	109.21
4	E	18	NAG	C1-O5-C5	6.21	120.13	112.25
3	B	9	BMA	C1-C2-C3	8.10	119.12	109.54
3	C	13	NAG	O5-C5-C6	9.59	128.11	107.35

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	13	NAG	C5
4	H	27	NAG	C1
4	G	22	NAG	C1
3	G	531	NAG	C1
4	E	18	NAG	C1
4	F	20	NAG	C1
4	F	19	NAG	C1
4	D	16	NAG	C1
4	E	17	NAG	C1
4	D	15	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	17	NAG	O7-C7-N2-C2
3	C	12	NAG	C8-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NAG	5	0
3	A	4	NAG	1	0
3	B	7	NAG	1	0
4	C	10	NAG	1	0
3	C	12	NAG	7	0
3	C	13	NAG	1	0
4	D	15	NAG	2	0
4	E	17	NAG	9	0
4	F	19	NAG	1	0
4	F	20	NAG	1	0
4	G	21	NAG	7	0
3	G	530	NAG	1	0
3	G	531	NAG	1	0
4	H	26	NAG	3	0
4	H	27	NAG	1	0

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	$\#\|Z\| > 2$
5	NGT	A	21	-	13,15,15	1.19	2 (15%)	11,22,22	0.77	1 (9%)
5	NGT	B	22	-	13,15,15	1.22	2 (15%)	11,22,22	0.77	1 (9%)
5	NGT	C	530	-	13,15,15	1.34	2 (15%)	11,22,22	0.77	1 (9%)
5	NGT	D	24	-	13,15,15	1.32	2 (15%)	11,22,22	0.76	1 (9%)
5	NGT	E	530	-	13,15,15	1.32	3 (23%)	11,22,22	0.77	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NGT	F	26	-	13,15,15	1.25	2 (15%)	11,22,22	0.77	1 (9%)
5	NGT	G	533	-	13,15,15	1.28	2 (15%)	11,22,22	0.76	1 (9%)
5	NGT	H	28	-	13,15,15	1.35	4 (30%)	11,22,22	0.76	1 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NGT	A	21	-	-	0/2/30/30	0/2/2/2
5	NGT	B	22	-	-	0/2/30/30	0/2/2/2
5	NGT	C	530	-	-	0/2/30/30	0/2/2/2
5	NGT	D	24	-	-	0/2/30/30	0/2/2/2
5	NGT	E	530	-	-	0/2/30/30	0/2/2/2
5	NGT	F	26	-	-	0/2/30/30	0/2/2/2
5	NGT	G	533	-	-	0/2/30/30	0/2/2/2
5	NGT	H	28	-	-	0/2/30/30	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	24	NGT	C2-N2	-2.74	1.45	1.47
5	F	26	NGT	C2-N2	-2.50	1.45	1.47
5	B	22	NGT	C2-N2	-2.45	1.45	1.47
5	C	530	NGT	C2-N2	-2.44	1.45	1.47
5	H	28	NGT	C2-N2	-2.17	1.45	1.47
5	G	533	NGT	C2-N2	-2.17	1.45	1.47
5	E	530	NGT	C2-N2	-2.15	1.45	1.47
5	H	28	NGT	O5-C1	-2.11	1.38	1.42
5	H	28	NGT	C7-S1	2.06	1.78	1.77
5	A	21	NGT	C7-N2	2.12	1.29	1.27
5	E	530	NGT	C7-S1	2.20	1.78	1.77
5	H	28	NGT	C3-C2	2.53	1.58	1.53
5	D	24	NGT	C3-C2	2.58	1.58	1.53
5	E	530	NGT	C3-C2	2.66	1.58	1.53
5	F	26	NGT	C3-C2	2.74	1.58	1.53
5	A	21	NGT	C3-C2	2.79	1.58	1.53
5	B	22	NGT	C3-C2	2.81	1.59	1.53
5	G	533	NGT	C3-C2	2.89	1.59	1.53
5	C	530	NGT	C3-C2	3.14	1.59	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	24	NGT	C1-O5-C5	2.11	116.76	112.74
5	G	533	NGT	C1-O5-C5	2.11	116.76	112.74
5	H	28	NGT	C1-O5-C5	2.12	116.77	112.74
5	E	530	NGT	C1-O5-C5	2.12	116.77	112.74
5	F	26	NGT	C1-O5-C5	2.12	116.77	112.74
5	A	21	NGT	C1-O5-C5	2.13	116.79	112.74
5	C	530	NGT	C1-O5-C5	2.13	116.80	112.74
5	B	22	NGT	C1-O5-C5	2.13	116.80	112.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	21	NGT	6	0
5	B	22	NGT	3	0
5	C	530	NGT	12	0
5	D	24	NGT	4	0
5	E	530	NGT	6	0
5	F	26	NGT	2	0
5	G	533	NGT	8	0
5	H	28	NGT	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	492/507 (97%)	0.35	11 (2%) 65 55	31, 53, 60, 66	0
1	C	492/507 (97%)	0.35	21 (4%) 39 29	31, 57, 62, 66	0
1	E	492/507 (97%)	0.69	58 (11%) 6 4	32, 57, 62, 64	0
1	G	492/507 (97%)	0.79	78 (15%) 3 2	31, 56, 60, 61	0
2	B	480/503 (95%)	0.44	24 (5%) 32 24	21, 56, 60, 63	0
2	D	479/503 (95%)	0.46	22 (4%) 36 28	21, 56, 60, 62	0
2	F	480/503 (95%)	0.90	71 (14%) 3 2	21, 58, 62, 64	0
2	H	480/503 (95%)	1.44	129 (26%) 1 1	21, 57, 59, 61	0
All	All	3887/4040 (96%)	0.68	414 (10%) 8 5	21, 56, 61, 66	0

All (414) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	107	GLY	10.4
1	G	279	SER	9.7
2	H	54	PRO	7.7
2	H	480	LEU	6.8
2	H	483	GLY	6.7
2	H	484	GLY	6.5
2	F	362	GLU	6.5
2	F	548	ALA	6.3
1	G	327	THR	6.1
2	F	67	PRO	6.0
2	H	482	ILE	6.0
1	G	328	CYS	5.6
1	G	382	LYS	5.6
1	E	344	PHE	5.5
2	H	552	ASN	5.5
2	F	479	GLN	5.5

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Mol	Chain	Res	Type	RSRZ
2	F	122	THR	5.5
2	F	68	ASN	5.3
1	G	280	GLY	5.3
2	F	311	SER	5.3
2	H	90	SER	5.1
2	H	106	PHE	5.1
2	F	140	PHE	5.0
2	H	361	TRP	5.0
2	H	122	THR	5.0
2	H	380	PHE	5.0
2	H	84	ASN	4.8
1	E	115	ASN	4.7
1	E	367	GLY	4.7
2	F	399	ASN	4.6
2	B	204	GLY	4.5
2	H	418	GLY	4.5
1	G	331	SER	4.4
1	G	362	ILE	4.4
2	H	383	LEU	4.4
2	H	397	THR	4.4
2	F	154	LYS	4.4
1	E	89	THR	4.3
1	G	107	LEU	4.3
2	F	542	ALA	4.3
1	G	396	ILE	4.2
2	H	409	PHE	4.2
2	H	135	SER	4.2
2	H	193	THR	4.2
2	D	317	ASP	4.1
2	H	250	THR	4.1
1	G	347	ASP	4.1
2	H	85	SER	4.1
2	F	325	THR	4.1
2	F	181	GLN	4.0
2	F	204	GLY	3.9
1	G	349	LYS	3.9
2	H	507	SER	3.9
1	E	489	LEU	3.9
2	H	136	GLU	3.9
2	D	382	LYS	3.9
2	H	402	SER	3.9
2	F	69	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	344	PHE	3.8
2	H	356	VAL	3.8
2	H	547	TYR	3.8
2	H	411	ASP	3.8
1	G	180	TYR	3.8
2	H	137	CYS	3.7
2	H	479	GLN	3.7
2	H	140	PHE	3.7
2	H	317	ASP	3.7
1	G	395	ASP	3.6
1	C	43	ASN	3.6
1	G	303	THR	3.6
2	H	379	ASP	3.6
2	H	288	GLU	3.6
2	H	370	PHE	3.6
1	G	381	VAL	3.6
2	H	542	ALA	3.6
2	F	552	ASN	3.6
2	H	146	ASP	3.6
2	H	436	VAL	3.6
2	H	175	PHE	3.6
2	B	412	LYS	3.5
1	E	98	SER	3.5
1	E	293	SER	3.5
2	H	328	THR	3.5
2	H	350	HIS	3.5
2	H	429	TYR	3.5
2	H	83	PRO	3.5
2	H	235	HIS	3.5
1	C	344	PHE	3.5
2	H	62	SER	3.5
2	F	184	TYR	3.5
1	E	43	ASN	3.4
2	H	86	THR	3.4
2	H	134	GLN	3.4
2	H	398	ILE	3.4
2	H	472	GLY	3.4
1	E	285	GLY	3.4
1	A	258	ASP	3.4
2	H	138	ASP	3.4
2	H	132	THR	3.4
2	H	474	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	113	VAL	3.4
1	G	285	GLY	3.4
2	F	303	LYS	3.4
2	H	69	LEU	3.4
2	H	188	THR	3.4
2	F	379	ASP	3.4
1	E	270	ILE	3.3
2	H	372	ARG	3.3
2	H	417	PRO	3.3
2	H	471	PHE	3.3
2	B	325	THR	3.3
2	H	460	TRP	3.3
2	F	66	THR	3.3
1	G	284	SER	3.3
2	H	91	CYS	3.3
2	H	468	PRO	3.3
1	E	444	GLY	3.3
1	G	348	PHE	3.3
2	H	546	LEU	3.3
2	H	68	ASN	3.3
1	G	43	ASN	3.2
1	G	384	GLN	3.2
2	H	345	PRO	3.2
1	E	130	GLU	3.2
2	H	357	GLU	3.2
1	E	338	PHE	3.2
1	E	350	GLN	3.2
2	F	182	ASP	3.2
1	C	284	SER	3.2
2	F	530	THR	3.2
1	E	369	GLY	3.2
2	F	130	SER	3.2
1	G	293	SER	3.2
2	H	374	LYS	3.2
1	G	281	SER	3.2
2	H	325	THR	3.1
2	F	551	CYS	3.1
2	H	156	PRO	3.1
2	H	387	TYR	3.1
2	F	382	LYS	3.1
1	E	162	GLU	3.1
2	H	386	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	183	SER	3.1
1	G	228	ASN	3.1
2	F	305	LEU	3.1
1	E	396	ILE	3.1
1	E	101	THR	3.0
1	G	259	THR	3.0
2	F	402	SER	3.0
2	H	373	GLN	3.0
2	F	527	ASP	3.0
1	E	287	PHE	3.0
2	H	524	ASP	3.0
1	E	271	PRO	3.0
2	F	445	LEU	3.0
1	G	363	VAL	3.0
2	D	426	ASP	3.0
2	H	541	ILE	3.0
1	G	353	SER	3.0
2	H	443	VAL	3.0
1	A	458	CYS	3.0
1	C	346	GLU	3.0
2	F	83	PRO	2.9
1	G	379	ASN	2.9
2	H	148	SER	2.9
2	F	290	ASP	2.9
2	D	235	HIS	2.9
1	E	347	ASP	2.9
2	F	153	VAL	2.9
1	C	89	THR	2.9
2	F	158	ALA	2.9
2	H	516	SER	2.9
2	F	526	TYR	2.9
2	H	355	GLU	2.9
2	F	82	SER	2.9
1	G	412	PHE	2.9
2	B	411	ASP	2.9
2	H	464	TYR	2.9
2	F	226	MET	2.8
1	C	385	PRO	2.8
1	G	258	ASP	2.8
2	H	412	LYS	2.8
1	G	282	GLU	2.8
2	H	187	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	394	ILE	2.8
1	G	330	LYS	2.8
2	H	450	TYR	2.8
1	C	285	GLY	2.7
1	G	343	GLY	2.7
1	E	213	TYR	2.7
2	H	125	GLN	2.7
1	G	286	THR	2.7
2	H	477	GLN	2.7
2	H	133	LEU	2.7
2	F	132	THR	2.7
1	A	320	GLY	2.7
2	D	325	THR	2.7
2	H	342	GLU	2.7
1	G	314	ASP	2.7
2	B	311	SER	2.7
2	F	376	PHE	2.7
1	G	393	ARG	2.7
1	E	443	GLU	2.7
2	H	487	CYS	2.7
2	D	428	ALA	2.7
1	E	225	GLY	2.6
1	G	295	ASN	2.6
2	H	229	ASN	2.6
1	C	446	PRO	2.6
2	F	326	LEU	2.6
2	H	87	ALA	2.6
1	E	73	PHE	2.6
2	H	231	PHE	2.6
2	B	229	ASN	2.6
2	D	287	PRO	2.6
1	G	89	THR	2.6
1	A	256	GLU	2.6
1	E	276	PRO	2.6
2	B	552	ASN	2.6
2	H	360	CYS	2.6
1	G	387	THR	2.6
2	H	378	THR	2.6
2	H	382	LYS	2.6
1	A	204	HIS	2.6
1	E	211	PHE	2.6
1	G	229	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	527	ASP	2.6
1	G	256	GLU	2.6
1	C	458	CYS	2.6
2	H	102	HIS	2.6
2	F	523	ASP	2.5
2	F	475	GLN	2.5
1	G	264	LEU	2.5
2	D	288	GLU	2.5
1	E	29	ASN	2.5
2	B	232	ASN	2.5
1	E	50	VAL	2.5
1	E	234	TYR	2.5
2	B	170	ARG	2.5
2	F	156	PRO	2.5
2	F	304	ASP	2.5
1	G	45	GLN	2.5
2	H	438	ALA	2.5
1	E	267	GLY	2.5
1	E	354	PHE	2.5
2	F	513	LEU	2.5
1	G	468	ASN	2.5
2	F	135	SER	2.5
2	H	189	ILE	2.5
1	E	99	VAL	2.5
1	E	330	LYS	2.5
2	H	419	THR	2.5
1	E	345	GLY	2.5
1	G	123	ASP	2.5
2	H	290	ASP	2.5
1	G	268	PRO	2.5
1	C	524	GLN	2.5
1	G	386	ASP	2.5
1	E	240	LYS	2.5
1	G	106	GLN	2.4
2	H	475	GLN	2.4
2	D	472	GLY	2.4
2	H	347	GLN	2.4
2	H	540	GLY	2.4
1	E	181	LEU	2.4
1	E	521	PHE	2.4
2	F	370	PHE	2.4
2	H	88	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	481	PHE	2.4
2	D	378	THR	2.4
1	G	383	ILE	2.4
2	H	421	VAL	2.4
2	F	139	ALA	2.4
2	F	518	ASP	2.4
1	E	294	LEU	2.4
2	D	362	GLU	2.4
2	H	89	PRO	2.4
2	B	237	HIS	2.4
2	B	487	CYS	2.4
1	G	528	GLN	2.4
2	F	310	TYR	2.4
2	B	195	ILE	2.4
2	F	233	VAL	2.4
2	F	58	PRO	2.4
1	C	409	LYS	2.4
1	E	281	SER	2.3
1	G	93	ASN	2.3
1	E	290	VAL	2.3
2	H	469	LEU	2.3
1	A	171	GLY	2.3
1	E	368	LYS	2.3
1	E	51	SER	2.3
2	D	473	GLY	2.3
2	F	141	PRO	2.3
2	H	144	SER	2.3
2	F	236	TRP	2.3
2	H	399	ASN	2.3
2	H	543	ALA	2.3
1	C	348	PHE	2.3
2	F	106	PHE	2.3
2	H	499	THR	2.3
2	F	76	ASN	2.3
1	G	255	ALA	2.3
2	B	486	ALA	2.3
2	F	192	SER	2.3
2	B	484	GLY	2.3
1	C	256	GLU	2.3
1	C	299	GLU	2.3
1	G	370	TYR	2.3
1	G	319	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	449	TRP	2.3
2	H	366	LYS	2.3
2	F	137	CYS	2.3
2	F	65	MET	2.3
2	H	428	ALA	2.3
1	E	279	SER	2.3
2	D	122	THR	2.3
2	B	372	ARG	2.2
2	H	435	ARG	2.2
1	G	269	GLY	2.2
1	E	327	THR	2.2
2	B	86	THR	2.2
1	C	258	ASP	2.2
1	E	272	GLY	2.2
1	G	312	PHE	2.2
1	G	397	PRO	2.2
2	B	133	LEU	2.2
2	F	107	GLY	2.2
2	H	367	ILE	2.2
1	C	286	THR	2.2
2	H	403	ILE	2.2
1	A	255	ALA	2.2
2	D	237	HIS	2.2
1	E	299	GLU	2.2
2	D	132	THR	2.2
2	H	197	SER	2.2
1	C	338	PHE	2.2
2	F	547	TYR	2.2
1	C	457	ALA	2.2
1	E	269	GLY	2.2
1	C	204	HIS	2.2
1	C	318	HIS	2.2
2	H	139	ALA	2.2
1	G	225	GLY	2.2
2	H	517	LYS	2.2
2	F	531	ARG	2.2
2	H	369	ASP	2.2
1	E	524	GLN	2.2
2	H	158	ALA	2.2
1	G	277	CYS	2.2
1	G	452	VAL	2.2
2	D	291	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	466	ASN	2.2
2	H	308	PRO	2.2
1	E	315	PHE	2.2
2	B	235	HIS	2.2
2	H	307	THR	2.2
2	D	231	PHE	2.2
2	H	510	GLY	2.2
1	C	202	HIS	2.2
1	G	350	GLN	2.1
2	F	185	GLY	2.1
1	E	346	GLU	2.1
1	A	93	ASN	2.1
2	B	184	TYR	2.1
2	D	310	TYR	2.1
1	A	455	GLY	2.1
2	B	171	GLY	2.1
2	H	358	PHE	2.1
2	F	375	GLY	2.1
2	H	408	VAL	2.1
1	G	304	PHE	2.1
1	G	321	GLY	2.1
2	H	279	ARG	2.1
1	G	223	ARG	2.1
2	F	193	THR	2.1
1	G	133	TRP	2.1
1	G	421	TYR	2.1
1	E	335	ILE	2.1
2	H	195	ILE	2.1
1	A	208	ASP	2.1
1	G	263	THR	2.1
2	D	208	ASP	2.1
2	F	506	ALA	2.1
1	E	277	CYS	2.0
1	E	298	TYR	2.0
2	D	107	GLY	2.0
1	E	97	VAL	2.0
1	G	283	PRO	2.0
2	H	61	LEU	2.0
2	F	361	TRP	2.0
2	F	366	LYS	2.0
1	A	162	GLU	2.0
2	H	67	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	394	GLU	2.0
1	E	494	THR	2.0
1	G	458	CYS	2.0
1	G	340	ARG	2.0
1	G	477	ALA	2.0
2	B	128	LEU	2.0
2	F	77	PHE	2.0
1	E	297	THR	2.0
2	B	226	MET	2.0
2	D	65	MET	2.0
2	F	438	ALA	2.0
1	G	102	PRO	2.0
1	G	385	PRO	2.0
2	H	206	LEU	2.0
1	G	336	GLN	2.0
1	G	230	VAL	2.0
2	B	317	ASP	2.0
2	D	290	ASP	2.0
2	F	217	LYS	2.0
1	G	445	THR	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	E	17	14/15	0.81	0.31	1.67	58,59,62,64	0
3	NAG	B	7	14/15	0.83	0.30	0.61	47,50,53,56	0
4	NAG	D	15	14/15	0.74	0.32	0.41	60,62,67,67	0
3	NAG	A	4	14/15	0.87	0.24	0.05	54,55,58,60	0
3	NAG	C	12	14/15	0.83	0.21	-0.29	45,47,48,51	0
3	NAG	G	530	14/15	0.91	0.17	-0.76	52,54,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	H	26	14/15	0.81	0.26	-0.98	61,62,63,66	0
4	NAG	F	19	14/15	0.78	0.32	-1.29	61,62,62,66	0
3	BMA	B	9	11/12	0.83	0.18	-	48,54,56,57	0
3	BMA	A	6	11/12	0.82	0.26	-	52,53,55,56	0
3	NAG	G	531	14/15	0.84	0.35	-	57,63,64,65	0
3	NAG	B	8	14/15	0.83	0.34	-	61,66,68,68	0
3	NAG	A	2	14/15	0.91	0.31	-	58,61,63,63	0
4	NAG	E	18	14/15	0.49	0.46	-	73,76,78,79	0
3	NAG	A	1	14/15	0.86	0.21	-	45,47,50,51	0
3	NAG	C	13	14/15	0.70	0.33	-	55,59,63,63	0
4	NAG	H	27	14/15	0.82	0.27	-	73,76,76,76	0
4	NAG	F	20	14/15	0.75	0.38	-	73,76,77,77	0
4	NAG	G	21	14/15	0.80	0.55	-	59,60,63,65	0
4	NAG	D	16	14/15	0.86	0.46	-	74,76,78,78	0
3	BMA	G	532	11/12	0.86	0.20	-	48,48,50,52	0
3	BMA	C	14	11/12	0.65	0.41	-	46,49,51,51	0
4	NAG	C	11	14/15	0.68	0.49	-	65,68,69,69	0
3	NAG	A	5	14/15	0.81	0.45	-	61,66,71,71	0
4	NAG	C	10	14/15	0.73	0.42	-	51,56,60,62	0
4	NAG	G	22	14/15	0.65	0.46	-	72,75,76,76	0
3	BMA	A	3	11/12	0.88	0.29	-	50,52,54,55	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NGT	G	533	14/14	0.76	0.34	-0.30	47,47,49,50	0
5	NGT	H	28	14/14	0.74	0.33	-0.33	48,50,53,54	0
5	NGT	E	530	14/14	0.76	0.26	-0.33	47,49,52,53	0
5	NGT	F	26	14/14	0.84	0.23	-0.79	40,41,42,43	0
5	NGT	B	22	14/14	0.90	0.24	-0.88	38,39,41,44	0
5	NGT	C	530	14/14	0.81	0.25	-1.31	44,46,49,50	0
5	NGT	A	21	14/14	0.94	0.17	-2.36	33,35,37,37	0
5	NGT	D	24	14/14	0.93	0.18	-2.36	39,41,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.