Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 02:48 PM BST

PDB ID	:	4M7E
Title	:	Structural insight into BL-induced activation of the BRI1-BAK1 complex
Authors	:	Chai, J.; Han, Z.; Sun, Y.
Deposited on	:	2013-08-12
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

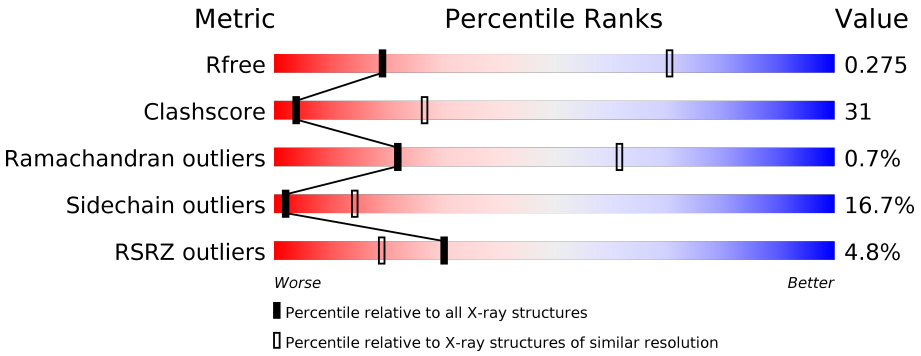
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	767	4% 43% 44% 8%
1	B	767	4% 44% 44% 8%
2	C	201	5% 32% 37% 18% 13%
2	D	201	7% 28% 42% 16% 13%
3	E	2	100%
3	F	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	G	2	100%
3	H	2	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13926 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 Protein BRASSINOSTEROID INSENSITIVE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	733	Total	C	N	O	S	0	0	0
			5542	3499	919	1093	31			
1	B	734	Total	C	N	O	S	0	0	0
			5554	3506	921	1096	31			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	785	HIS	-	expression tag	UNP O22476
A	786	HIS	-	expression tag	UNP O22476
A	787	HIS	-	expression tag	UNP O22476
A	788	HIS	-	expression tag	UNP O22476
A	789	HIS	-	expression tag	UNP O22476
A	790	HIS	-	expression tag	UNP O22476
B	785	HIS	-	expression tag	UNP O22476
B	786	HIS	-	expression tag	UNP O22476
B	787	HIS	-	expression tag	UNP O22476
B	788	HIS	-	expression tag	UNP O22476
B	789	HIS	-	expression tag	UNP O22476
B	790	HIS	-	expression tag	UNP O22476

- Molecule 2 is a protein called BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	175	Total	C	N	O	S	0	0	0
			1299	821	221	254	3			
2	C	175	Total	C	N	O	S	0	0	0
			1299	821	221	254	3			

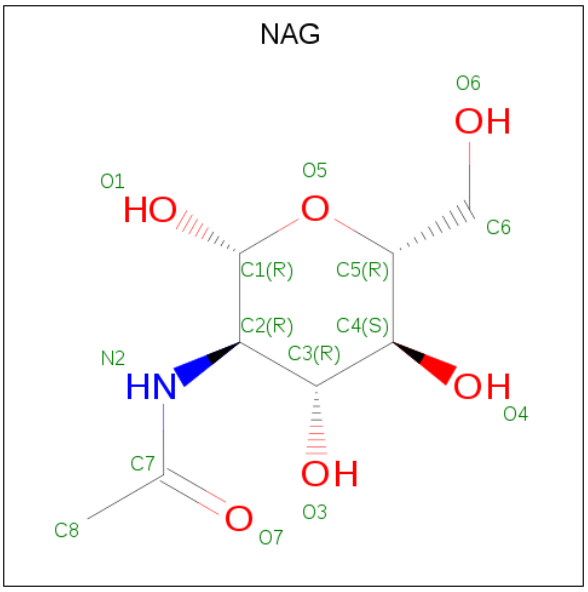
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	221	HIS	-	expression tag	UNP Q94F62
D	222	HIS	-	expression tag	UNP Q94F62
D	223	HIS	-	expression tag	UNP Q94F62
D	224	HIS	-	expression tag	UNP Q94F62
D	225	HIS	-	expression tag	UNP Q94F62
D	226	HIS	-	expression tag	UNP Q94F62
C	221	HIS	-	expression tag	UNP Q94F62
C	222	HIS	-	expression tag	UNP Q94F62
C	223	HIS	-	expression tag	UNP Q94F62
C	224	HIS	-	expression tag	UNP Q94F62
C	225	HIS	-	expression tag	UNP Q94F62
C	226	HIS	-	expression tag	UNP Q94F62

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

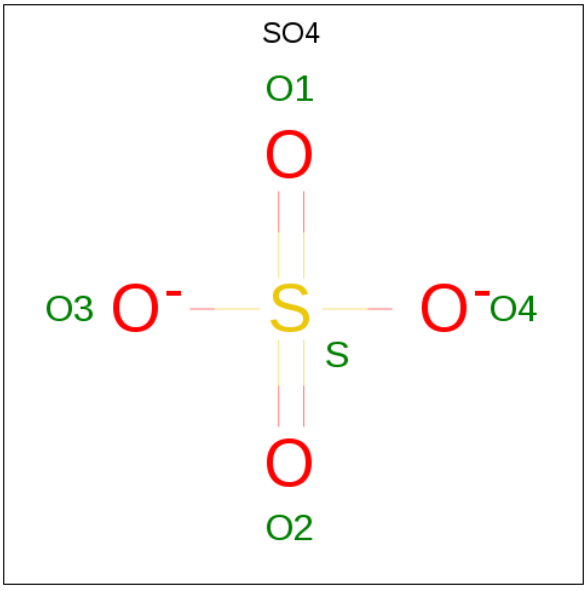
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

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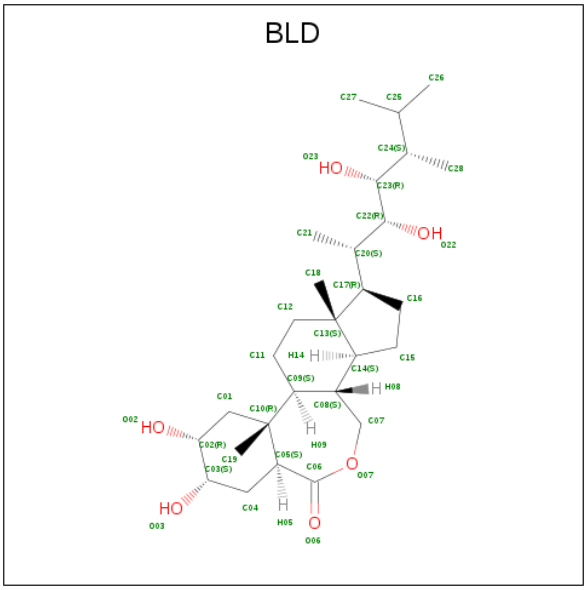
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is Brassinolide (three-letter code: BLD) (formula: $C_{28}H_{48}O_6$).



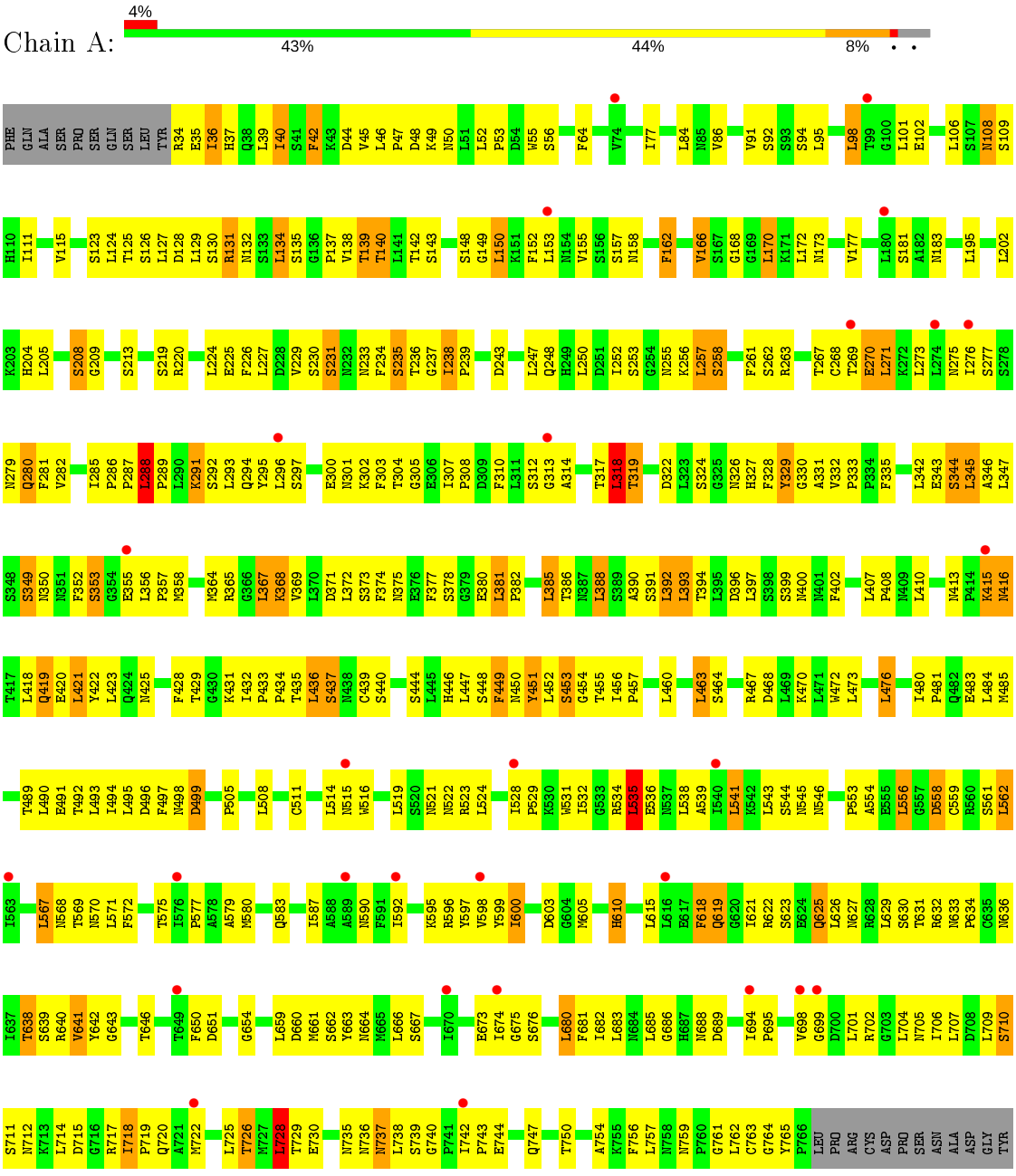
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 34 28 6	0	0
6	B	1	Total C O 34 28 6	0	0

3 Residue-property plots (i)

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

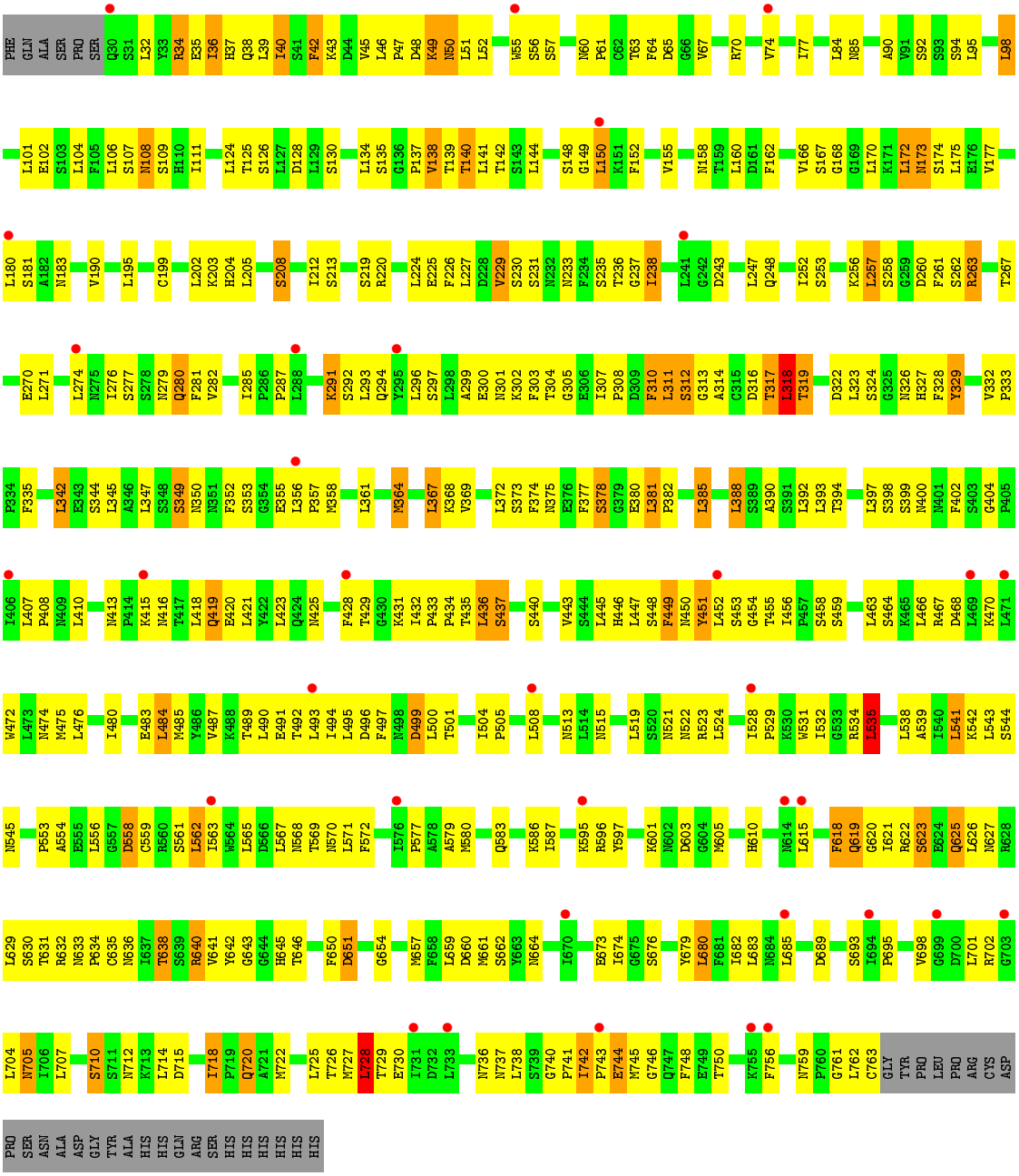
- Molecule 1: Protein BRASSINOSTEROID INSENSITIVE 1

Chain A:



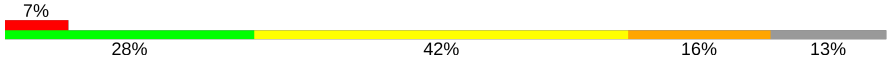
• Molecule 1: Protein BRASSINOSTEROID INSENSITIVE 1

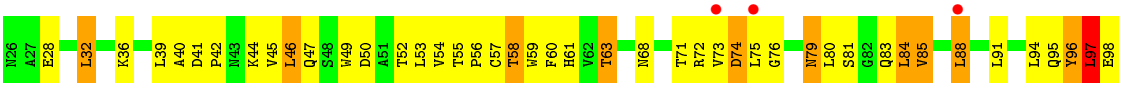
Chain B:

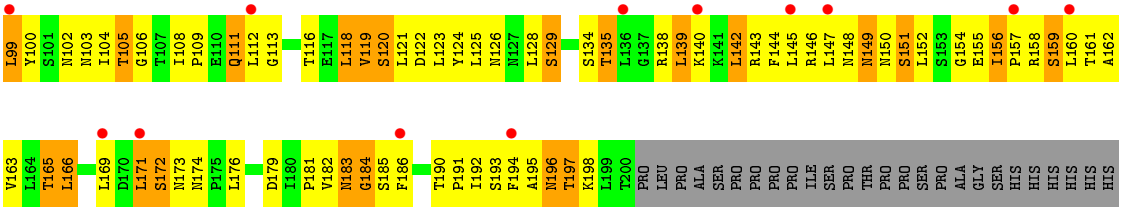


• Molecule 2: BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1

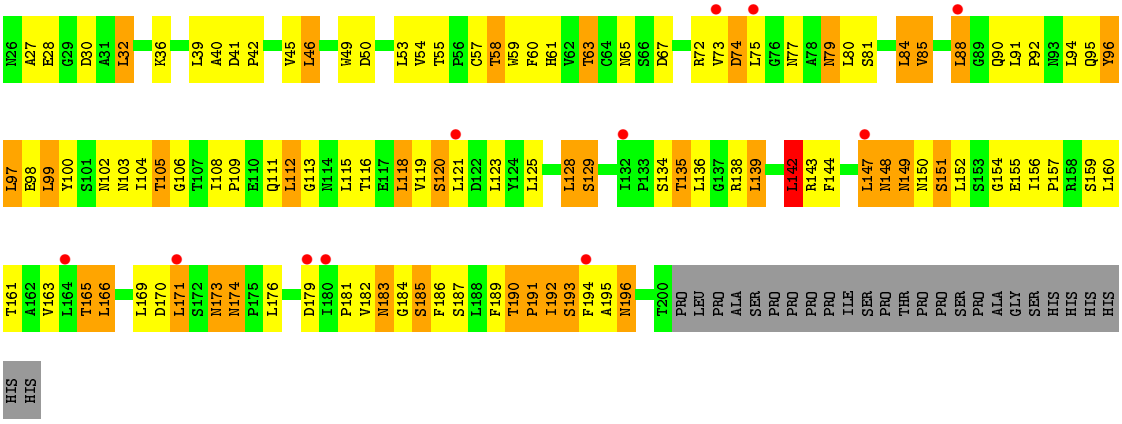
Chain D:



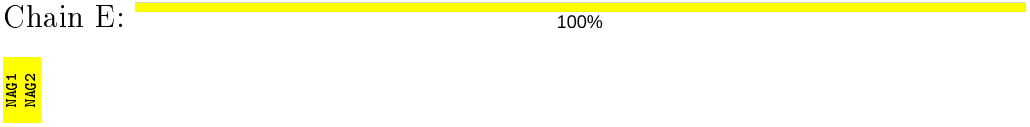




• Molecule 2: BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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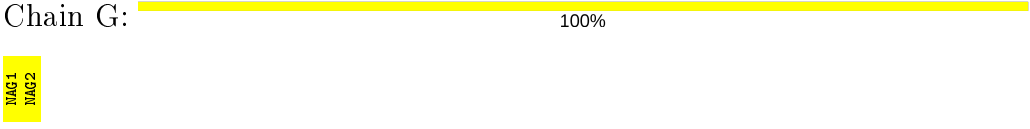
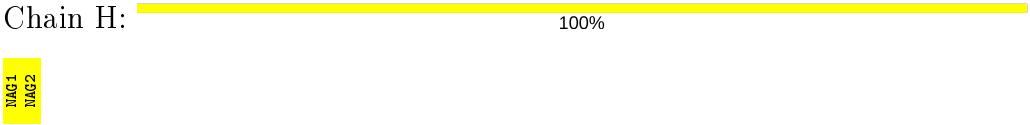


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	145.91Å 145.91Å 166.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.90 – 3.60 47.76 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (45.90-3.60) 98.3 (47.76-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.220 , 0.275 0.221 , 0.275	Depositor DCC
R_{free} test set	2269 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	85.6	Xtriage
Anisotropy	0.873	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 0.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.310 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13926	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: BLD, NAG, SO4

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	0.65	1/5648 (0.0%)	0.96	14/7664 (0.2%)
1	B	0.61	0/5659	0.93	5/7678 (0.1%)
2	C	0.75	0/1321	1.05	4/1810 (0.2%)
2	D	0.74	0/1321	1.05	4/1810 (0.2%)
All	All	0.65	1/13949 (0.0%)	0.97	27/18962 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
2	C	0	1
2	D	0	3
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	ARG	CG-CD	5.02	1.64	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	131	ARG	NE-CZ-NH2	8.67	124.63	120.30
1	A	288	LEU	CA-CB-CG	8.40	134.62	115.30
2	D	142	LEU	CA-CB-CG	7.16	131.76	115.30
2	C	142	LEU	CA-CB-CG	7.03	131.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	535	LEU	CA-CB-CG	6.52	130.30	115.30
1	B	728	LEU	CB-CG-CD2	-6.47	100.00	111.00
1	A	535	LEU	CA-CB-CG	6.18	129.53	115.30
1	A	153	LEU	CA-CB-CG	6.08	129.30	115.30
1	A	567	LEU	CB-CG-CD2	-5.79	101.15	111.00
2	C	147	LEU	CA-CB-CG	-5.67	102.26	115.30
1	A	718	ILE	CB-CA-C	-5.65	100.31	111.60
1	A	421	LEU	CA-CB-CG	5.56	128.09	115.30
2	D	119	VAL	N-CA-C	-5.46	96.26	111.00
2	D	184	GLY	N-CA-C	5.46	126.75	113.10
1	A	271	LEU	CA-CB-CG	5.46	127.85	115.30
2	C	128	LEU	CA-CB-CG	5.45	127.83	115.30
1	A	728	LEU	CB-CG-CD2	-5.40	101.83	111.00
1	A	476	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	170	LEU	CA-CB-CG	5.22	127.31	115.30
2	D	97	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	168	GLY	N-CA-C	-5.14	100.25	113.10
1	B	318	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	764	GLY	N-CA-C	5.13	125.93	113.10
1	B	342	LEU	CA-CB-CG	5.11	127.06	115.30
2	C	183	ASN	N-CA-C	-5.05	97.38	111.00
1	B	311	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	393	LEU	CA-CB-CG	-5.03	103.72	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	PHE	Peptide
1	A	415	LYS	Peptide
1	B	172	LEU	Peptide
1	B	312	SER	Peptide
2	C	155	GLU	Peptide
2	D	155	GLU	Peptide
2	D	172	SER	Mainchain,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	5542	0	5503	326	0
1	B	5554	0	5517	297	0
2	C	1299	0	1272	122	0
2	D	1299	0	1270	116	0
3	E	28	0	25	0	0
3	F	28	0	25	1	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
4	A	28	0	26	3	0
4	B	14	0	13	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	34	0	48	8	0
6	B	34	0	48	4	0
All	All	13926	0	13797	846	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 31.

All (846) 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)
2:D:190:THR:HG22	2:D:191:PRO:CD	1.46	1.42
2:D:196:ASN:O	2:D:198:LYS:N	1.58	1.35
2:D:190:THR:CG2	2:D:191:PRO:HD2	1.70	1.21
2:D:190:THR:CG2	2:D:191:PRO:CD	2.30	1.06
2:C:163:VAL:HG23	2:C:166:LEU:HD11	1.41	1.02
2:C:190:THR:HG22	2:C:191:PRO:HD2	1.43	1.01
1:B:577:PRO:HG2	1:B:580:MET:HB2	1.41	1.00
2:C:190:THR:HG22	2:C:191:PRO:CD	1.94	0.96
2:C:182:VAL:O	2:C:182:VAL:HG12	1.68	0.91
1:A:519:LEU:O	1:A:522:ASN:ND2	2.05	0.90
2:D:163:VAL:HG23	2:D:166:LEU:HD11	1.55	0.88
1:B:640:ARG:NH1	2:D:68:ASN:OD1	2.06	0.88
1:B:52:LEU:HD23	1:B:55:TRP:CE2	2.10	0.87
1:A:577:PRO:HG2	1:A:580:MET:HB2	1.58	0.86
1:B:519:LEU:O	1:B:522:ASN:ND2	2.12	0.82
2:C:152:LEU:H	2:C:174:ASN:HB2	1.45	0.81
1:B:385:LEU:HD12	1:B:388:LEU:HD23	1.64	0.80
1:B:515:ASN:HA	1:B:538:LEU:HA	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:195:ALA:O	2:D:196:ASN:CB	2.29	0.80
4:A:805:NAG:O4	4:A:806:NAG:O7	1.99	0.80
1:A:128:ASP:OD1	1:A:130:SER:OG	1.99	0.79
1:A:661:MET:O	1:A:664:ASN:ND2	2.16	0.79
2:C:195:ALA:O	2:C:196:ASN:CB	2.29	0.78
2:C:161:THR:O	2:C:185:SER:HB3	1.83	0.78
1:B:434:PRO:O	1:B:437:SER:OG	2.02	0.77
2:D:134:SER:HA	2:D:157:PRO:HB3	1.66	0.77
1:A:356:LEU:HD12	1:A:357:PRO:HD2	1.67	0.76
2:C:182:VAL:C	2:C:184:GLY:N	2.34	0.76
1:A:717:ARG:HG2	1:A:740:GLY:HA3	1.68	0.76
2:D:96:TYR:N	2:D:96:TYR:HD2	1.83	0.76
1:B:125:THR:HA	1:B:150:LEU:HA	1.68	0.76
1:A:497:PHE:O	1:A:632:ARG:NH1	2.19	0.76
2:C:136:LEU:HB2	2:C:160:LEU:HD11	1.67	0.76
2:C:161:THR:O	2:C:185:SER:CB	2.34	0.76
2:D:45:VAL:HG12	2:D:46:LEU:HD23	1.67	0.75
1:B:742:ILE:HB	1:B:744:GLU:OE1	1.86	0.75
2:D:96:TYR:N	2:D:96:TYR:CD2	2.54	0.75
1:A:125:THR:HA	1:A:150:LEU:HA	1.67	0.75
1:B:408:PRO:O	1:B:435:THR:OG1	2.05	0.75
1:A:132:ASN:H	1:A:158:ASN:HD21	1.31	0.75
2:C:149:ASN:HA	2:C:173:ASN:HB2	1.67	0.74
1:A:686:GLY:O	1:A:688:ASN:ND2	2.20	0.74
1:A:293:LEU:HD21	1:A:296:LEU:HB2	1.70	0.74
2:D:196:ASN:C	2:D:198:LYS:N	2.41	0.74
1:B:722:MET:HE2	1:B:748:PHE:HZ	1.52	0.73
1:A:659:LEU:HD11	1:A:661:MET:HG3	1.70	0.73
2:D:41:ASP:OD2	2:D:46:LEU:N	2.14	0.73
2:C:169:LEU:O	2:C:193:SER:OG	2.07	0.72
1:A:49:LYS:HB3	1:B:49:LYS:HD3	1.70	0.72
2:C:96:TYR:N	2:C:96:TYR:HD2	1.86	0.72
1:B:312:SER:O	1:B:314:ALA:N	2.18	0.72
1:A:569:THR:HG23	1:A:610:HIS:CD2	2.24	0.72
1:B:42:PHE:CE1	1:B:95:LEU:HD11	2.25	0.72
2:C:96:TYR:N	2:C:96:TYR:CD2	2.56	0.72
1:B:521:ASN:HA	1:B:545:ASN:HB3	1.72	0.71
2:C:191:PRO:C	2:C:193:SER:N	2.40	0.71
2:D:190:THR:HG22	2:D:191:PRO:HD2	0.73	0.71
1:B:303:PHE:HB2	1:B:326:ASN:OD1	1.89	0.71
2:D:190:THR:CG2	2:D:191:PRO:HD3	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:128:LEU:HB2	2:C:150:ASN:OD1	1.91	0.70
1:B:42:PHE:HE1	1:B:95:LEU:HD11	1.56	0.70
1:A:109:SER:HB2	1:A:111:ILE:HG12	1.72	0.70
1:A:515:ASN:HA	1:A:538:LEU:HA	1.74	0.69
2:D:152:LEU:H	2:D:174:ASN:HB2	1.56	0.69
2:D:97:LEU:HD11	2:D:99:LEU:HD22	1.73	0.69
1:B:142:THR:HG23	1:B:170:LEU:O	1.93	0.69
1:B:45:VAL:HG21	1:B:90:ALA:HB1	1.75	0.69
1:A:303:PHE:HB2	1:A:326:ASN:OD1	1.93	0.69
1:B:128:ASP:OD1	1:B:130:SER:OG	2.11	0.69
1:A:756:PHE:O	1:A:759:ASN:ND2	2.26	0.68
2:D:190:THR:HG22	2:D:191:PRO:HD3	1.67	0.68
1:A:368:LYS:HG3	1:A:393:LEU:HD12	1.75	0.68
2:C:169:LEU:HD12	2:C:171:LEU:H	1.59	0.68
1:B:394:THR:HG23	1:B:420:GLU:HB2	1.75	0.68
1:B:308:PRO:HB2	1:B:310:PHE:HD2	1.58	0.68
1:B:673:GLU:O	1:B:676:SER:OG	2.11	0.68
2:C:182:VAL:CG1	2:C:182:VAL:O	2.42	0.68
2:D:135:THR:HG22	2:D:138:ARG:HD2	1.75	0.67
1:A:77:ILE:HD13	1:A:95:LEU:HD22	1.77	0.67
1:B:42:PHE:HD1	1:B:95:LEU:HD21	1.59	0.67
2:C:193:SER:O	2:C:194:PHE:CD1	2.47	0.67
1:B:134:LEU:HB2	1:B:158:ASN:ND2	2.09	0.67
1:A:382:PRO:O	1:A:385:LEU:HB3	1.94	0.67
1:A:569:THR:HG21	4:A:805:NAG:H82	1.76	0.67
1:B:399:SER:O	1:B:622:ARG:NH2	2.28	0.67
1:B:661:MET:O	1:B:664:ASN:ND2	2.28	0.67
2:C:161:THR:CB	2:C:183:ASN:HB3	2.25	0.67
2:C:184:GLY:O	2:C:187:SER:CB	2.42	0.67
2:C:190:THR:HG22	2:C:191:PRO:HD3	1.74	0.67
2:D:149:ASN:HA	2:D:173:ASN:HB2	1.76	0.67
1:B:626:LEU:O	1:B:629:LEU:HB2	1.95	0.67
2:C:45:VAL:HG12	2:C:46:LEU:HD23	1.76	0.67
1:A:170:LEU:HD11	1:A:172:LEU:HD12	1.77	0.67
1:B:109:SER:HB2	1:B:111:ILE:HG12	1.77	0.66
1:A:142:THR:HG23	1:A:170:LEU:O	1.95	0.66
2:C:191:PRO:C	2:C:193:SER:H	1.98	0.66
1:A:718:ILE:HD11	1:A:762:LEU:HD11	1.78	0.66
1:B:368:LYS:HG3	1:B:393:LEU:HD12	1.76	0.66
1:B:70:ARG:NH2	1:B:102:GLU:OE1	2.29	0.66
1:A:705:ASN:ND2	6:A:808:BLD:O02	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ILE:HD11	1:B:352:PHE:CZ	2.30	0.66
1:B:36:ILE:HB	1:B:61:PRO:HG3	1.76	0.66
1:B:277:SER:O	1:B:279:ASN:ND2	2.29	0.66
1:A:554:ALA:HB1	1:A:579:ALA:HB3	1.79	0.65
1:B:369:VAL:HG22	1:B:394:THR:HB	1.78	0.65
1:A:262:SER:OG	1:A:287:PRO:O	2.14	0.65
1:B:636:ASN:HB3	1:B:638:THR:HG22	1.79	0.65
2:C:97:LEU:HD11	2:C:99:LEU:HD22	1.77	0.65
1:A:529:PRO:HB3	1:A:531:TRP:CE2	2.32	0.65
1:A:282:VAL:HG12	1:A:302:LYS:HB2	1.80	0.64
1:A:546:ASN:H	1:A:570:ASN:HD21	1.45	0.64
1:A:636:ASN:HB3	1:A:638:THR:HG22	1.80	0.64
2:C:191:PRO:HD2	2:C:192:ILE:H	1.62	0.64
1:A:567:LEU:HD22	1:A:572:PHE:CZ	2.32	0.64
2:C:50:ASP:HB3	2:C:53:LEU:HD12	1.79	0.64
2:D:50:ASP:HB3	2:D:53:LEU:HD12	1.79	0.64
1:A:314:ALA:O	1:A:318:LEU:HB2	1.98	0.64
1:B:659:LEU:HD11	1:B:661:MET:HG3	1.79	0.64
1:A:747:GLN:O	1:A:750:THR:OG1	2.16	0.64
1:A:425:ASN:ND2	1:A:625:GLN:OE1	2.29	0.64
1:A:709:LEU:O	1:A:712:ASN:ND2	2.31	0.64
1:A:307:ILE:HD11	1:A:352:PHE:CZ	2.33	0.64
1:A:35:GLU:HG3	1:A:98:LEU:HD11	1.79	0.63
2:C:184:GLY:O	2:C:187:SER:N	2.29	0.63
1:A:650:PHE:CD1	1:A:654:GLY:HA3	2.34	0.63
2:C:190:THR:CG2	2:C:191:PRO:HD2	2.25	0.63
1:A:277:SER:O	1:A:279:ASN:ND2	2.32	0.63
2:C:182:VAL:O	2:C:184:GLY:N	2.30	0.63
1:A:181:SER:OG	1:A:208:SER:N	2.32	0.63
6:B:807:BLD:H212	2:D:60:PHE:CZ	2.34	0.63
1:A:472:TRP:HB3	1:A:494:ILE:HG22	1.81	0.62
2:D:99:LEU:O	2:D:102:ASN:ND2	2.32	0.62
1:A:256:LYS:O	1:A:280:GLN:HG3	1.98	0.62
1:B:150:LEU:HD23	1:B:175:LEU:HD21	1.81	0.62
2:D:182:VAL:O	2:D:184:GLY:N	2.32	0.62
2:D:63:THR:HG23	2:D:72:ARG:HB2	1.80	0.62
1:A:397:LEU:HD22	1:A:402:PHE:HE2	1.64	0.62
1:B:455:THR:OG1	1:B:456:ILE:N	2.33	0.62
1:A:50:ASN:O	1:A:53:PRO:HG3	1.99	0.62
2:C:169:LEU:HD11	2:C:171:LEU:HB3	1.82	0.62
2:D:150:ASN:O	2:D:174:ASN:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:HG13	1:A:394:THR:HB	1.79	0.62
2:C:184:GLY:C	2:C:186:PHE:N	2.47	0.62
1:B:225:GLU:HA	1:B:247:LEU:HA	1.82	0.62
1:A:49:LYS:NZ	1:B:46:LEU:O	2.31	0.62
1:B:125:THR:HG22	1:B:149:GLY:O	1.99	0.61
1:B:399:SER:HA	1:B:425:ASN:HD22	1.66	0.61
2:C:191:PRO:CD	2:C:192:ILE:H	2.14	0.61
1:B:285:ILE:HD11	1:B:328:PHE:CZ	2.35	0.61
1:A:236:THR:OG1	1:A:237:GLY:N	2.33	0.61
2:D:150:ASN:C	2:D:174:ASN:HB3	2.21	0.61
1:B:36:ILE:HD11	1:B:57:SER:HA	1.81	0.61
1:B:497:PHE:O	1:B:632:ARG:NH1	2.32	0.61
1:A:124:LEU:HD21	1:A:127:LEU:HD13	1.81	0.61
1:A:640:ARG:HD2	2:C:57:CYS:HB3	1.81	0.61
2:C:45:VAL:HG13	2:C:61:HIS:CD2	2.36	0.61
2:D:85:VAL:O	2:D:88:LEU:HB2	2.01	0.61
2:C:91:LEU:O	2:C:94:LEU:HB2	2.01	0.60
1:B:248:GLN:HA	1:B:271:LEU:HA	1.82	0.60
1:B:390:ALA:HA	1:B:416:ASN:HA	1.83	0.60
1:B:449:PHE:HE2	1:B:472:TRP:CH2	2.19	0.60
2:C:84:LEU:HD13	2:C:104:ILE:HG21	1.83	0.60
1:A:449:PHE:HE2	1:A:472:TRP:CH2	2.19	0.60
1:A:455:THR:OG1	1:A:456:ILE:N	2.34	0.60
1:A:52:LEU:HD22	1:A:55:TRP:NE1	2.17	0.60
2:C:85:VAL:O	2:C:88:LEU:HB2	2.02	0.60
1:B:448:SER:HA	1:B:474:ASN:HD21	1.67	0.60
1:A:36:ILE:HG12	1:A:40:ILE:HD11	1.84	0.60
1:A:125:THR:HG22	1:A:149:GLY:O	2.02	0.59
1:A:322:ASP:OD1	1:A:324:SER:OG	2.16	0.59
1:B:568:ASN:OD1	1:B:569:THR:OG1	2.15	0.59
2:C:150:ASN:O	2:C:174:ASN:HB3	2.01	0.59
1:B:390:ALA:HB1	1:B:415:LYS:HB3	1.82	0.59
1:B:710:SER:O	1:B:712:ASN:ND2	2.34	0.59
1:A:308:PRO:HB2	1:A:310:PHE:HD1	1.67	0.59
1:B:181:SER:OG	1:B:208:SER:N	2.34	0.59
2:D:128:LEU:HB2	2:D:150:ASN:OD1	2.01	0.59
1:B:50:ASN:O	1:B:50:ASN:ND2	2.29	0.59
1:A:553:PRO:HG2	1:A:556:LEU:HD12	1.83	0.59
1:B:522:ASN:HB2	1:B:524:LEU:HG	1.83	0.59
2:C:184:GLY:C	2:C:186:PHE:H	2.04	0.59
2:C:98:GLU:HB3	2:C:100:TYR:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PHE:CE2	1:A:166:VAL:HG13	2.38	0.59
1:B:501:THR:HG22	1:B:523:ARG:HB2	1.84	0.59
2:D:169:LEU:HD11	2:D:171:LEU:HB3	1.85	0.59
1:A:132:ASN:H	1:A:158:ASN:ND2	2.01	0.59
2:C:191:PRO:CD	2:C:192:ILE:N	2.63	0.59
1:A:285:ILE:HD11	1:A:328:PHE:CZ	2.37	0.59
1:B:67:VAL:HG13	1:B:74:VAL:HG13	1.85	0.58
2:C:98:GLU:HB3	2:C:100:TYR:HD2	1.67	0.58
1:A:177:VAL:HG22	1:A:204:HIS:HB3	1.86	0.58
6:B:807:BLD:O02	2:D:61:HIS:N	2.27	0.58
1:A:332:VAL:HG21	1:A:357:PRO:HG3	1.85	0.58
1:A:380:GLU:O	1:A:382:PRO:HD3	2.03	0.58
1:A:399:SER:O	1:A:622:ARG:NH2	2.36	0.58
1:A:408:PRO:O	1:A:435:THR:OG1	2.19	0.58
1:B:468:ASP:HA	1:B:492:THR:HB	1.84	0.58
2:C:95:GLN:O	2:C:118:LEU:HD13	2.04	0.58
1:B:407:LEU:HB2	1:B:410:LEU:HB2	1.85	0.58
1:B:633:ASN:ND2	1:B:635:CYS:SG	2.76	0.58
1:B:202:LEU:HD21	1:B:205:LEU:HB2	1.85	0.58
1:A:52:LEU:N	1:A:53:PRO:HD3	2.19	0.57
1:A:521:ASN:HA	1:A:545:ASN:HB3	1.86	0.57
2:C:113:GLY:HA2	2:C:139:LEU:HD21	1.85	0.57
2:C:63:THR:HG23	2:C:72:ARG:HB2	1.86	0.57
1:B:349:SER:HA	1:B:374:PHE:O	2.03	0.57
1:B:554:ALA:HB1	1:B:579:ALA:HB3	1.85	0.57
2:C:41:ASP:OD2	2:C:46:LEU:N	2.27	0.57
1:A:480:ILE:HG22	1:A:505:PRO:HG3	1.86	0.57
1:A:725:LEU:HB2	1:A:728:LEU:HD12	1.85	0.57
1:B:567:LEU:HD22	1:B:572:PHE:CZ	2.40	0.57
2:D:169:LEU:HD12	2:D:171:LEU:H	1.69	0.57
1:A:538:LEU:HD11	1:A:541:LEU:HB2	1.86	0.57
1:B:282:VAL:HG12	1:B:302:LYS:HD2	1.87	0.57
1:B:425:ASN:ND2	1:B:625:GLN:OE1	2.36	0.57
1:B:322:ASP:OD1	1:B:324:SER:OG	2.14	0.57
1:B:382:PRO:O	1:B:385:LEU:HB3	2.04	0.57
1:A:599:TYR:HB3	1:A:642:TYR:HB2	1.87	0.57
2:D:145:LEU:HB3	2:D:169:LEU:HD13	1.86	0.57
1:A:344:SER:OG	1:A:369:VAL:HB	2.04	0.57
1:A:390:ALA:HB1	1:A:415:LYS:HB3	1.86	0.57
1:B:500:LEU:HB2	1:B:524:LEU:HD21	1.87	0.57
2:D:150:ASN:H	2:D:174:ASN:HD22	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ALA:HA	1:A:416:ASN:HA	1.86	0.56
1:A:394:THR:HG23	1:A:420:GLU:HB2	1.87	0.56
1:A:268:CYS:C	1:A:270:GLU:H	2.06	0.56
1:A:626:LEU:O	1:A:629:LEU:HB2	2.06	0.56
2:D:148:ASN:OD1	2:D:149:ASN:N	2.38	0.56
1:B:467:ARG:HG2	1:B:489:THR:HB	1.87	0.56
1:A:329:TYR:HD2	1:A:329:TYR:H	1.53	0.56
1:A:377:PHE:HB3	1:A:402:PHE:HE1	1.71	0.56
1:A:42:PHE:HB2	1:A:94:SER:OG	2.05	0.56
2:D:46:LEU:HD22	2:D:49:TRP:CE2	2.40	0.56
1:A:662:SER:O	1:A:664:ASN:ND2	2.39	0.56
1:B:372:LEU:HD22	1:B:377:PHE:CE2	2.41	0.56
1:B:431:LYS:HE2	1:B:454:GLY:HA3	1.85	0.56
1:B:39:LEU:HB3	1:B:55:TRP:CZ3	2.41	0.56
1:B:662:SER:O	1:B:664:ASN:ND2	2.38	0.56
2:C:74:ASP:OD2	2:C:74:ASP:N	2.39	0.56
1:A:252:ILE:HD12	1:A:257:LEU:HD13	1.88	0.56
1:A:213:SER:HB3	1:A:233:ASN:HB3	1.86	0.56
1:A:425:ASN:HA	1:A:449:PHE:HB3	1.88	0.56
1:A:715:ASP:HB3	1:A:737:ASN:HB3	1.88	0.56
1:A:98:LEU:HB3	1:A:101:LEU:HB2	1.88	0.56
1:A:49:LYS:HB3	1:B:49:LYS:CD	2.35	0.56
1:B:541:LEU:HD11	1:B:543:LEU:HD11	1.88	0.56
1:A:258:SER:HB3	1:A:280:GLN:HB2	1.88	0.56
1:A:381:LEU:HD22	1:A:385:LEU:HD22	1.88	0.56
1:B:152:PHE:HD1	1:B:177:VAL:HB	1.71	0.55
2:D:74:ASP:N	2:D:74:ASP:OD2	2.39	0.55
1:A:261:PHE:CE1	1:A:276:ILE:HD13	2.41	0.55
1:B:374:PHE:HE1	1:B:622:ARG:HA	1.70	0.55
1:A:642:TYR:CD1	2:C:58:THR:HG22	2.41	0.55
1:A:680:LEU:HD12	1:A:681:PHE:N	2.21	0.55
1:A:372:LEU:HD22	1:A:377:PHE:CE2	2.41	0.55
1:A:46:LEU:HB3	1:A:48:ASP:O	2.06	0.55
1:A:710:SER:O	1:A:712:ASN:ND2	2.39	0.55
2:D:102:ASN:HB2	2:D:104:ILE:HG13	1.89	0.55
2:D:79:ASN:ND2	2:D:79:ASN:O	2.27	0.55
1:A:399:SER:HA	1:A:425:ASN:HD22	1.71	0.55
1:B:569:THR:HG21	4:B:805:NAG:H82	1.88	0.55
1:B:55:TRP:NE1	1:B:64:PHE:HB3	2.22	0.55
1:B:742:ILE:HB	1:B:744:GLU:CD	2.27	0.55
1:A:162:PHE:HE2	1:A:166:VAL:HG13	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PHE:HD2	1:B:301:ASN:OD1	1.89	0.55
1:B:356:LEU:HD23	1:B:382:PRO:HD2	1.89	0.55
1:B:493:LEU:HD11	1:B:495:LEU:HD11	1.89	0.55
2:C:182:VAL:C	2:C:184:GLY:H	2.09	0.55
1:A:52:LEU:HD13	1:A:55:TRP:CD2	2.42	0.55
1:A:328:PHE:O	1:A:350:ASN:HB3	2.06	0.55
1:A:434:PRO:O	1:A:437:SER:OG	2.24	0.55
1:B:451:TYR:N	1:B:451:TYR:HD2	2.04	0.55
2:D:119:VAL:HG13	2:D:143:ARG:HB2	1.88	0.55
1:A:673:GLU:O	1:A:676:SER:OG	2.15	0.54
1:A:680:LEU:HD11	1:A:682:ILE:O	2.07	0.54
1:B:52:LEU:HD23	1:B:55:TRP:CD2	2.42	0.54
1:B:195:LEU:HD22	1:B:199:CYS:HB3	1.90	0.54
2:D:160:LEU:O	2:D:186:PHE:HE2	1.91	0.54
1:A:659:LEU:HD12	1:A:660:ASP:N	2.22	0.54
1:B:740:GLY:N	1:B:761:GLY:O	2.40	0.54
2:C:91:LEU:HD12	2:C:94:LEU:HD12	1.88	0.54
1:B:356:LEU:O	1:B:358:MET:N	2.38	0.54
2:C:186:PHE:HA	2:C:189:PHE:CD2	2.43	0.54
2:C:79:ASN:O	2:C:79:ASN:ND2	2.30	0.54
2:C:90:GLN:O	2:C:92:PRO:HD3	2.07	0.54
1:A:101:LEU:HD23	1:A:124:LEU:HD12	1.90	0.54
1:A:569:THR:HG23	1:A:610:HIS:HD2	1.73	0.54
1:B:759:ASN:HB2	1:B:762:LEU:HB2	1.90	0.54
2:D:98:GLU:HB3	2:D:100:TYR:HD2	1.72	0.54
1:A:546:ASN:H	1:A:570:ASN:ND2	2.06	0.54
2:D:124:TYR:HB3	2:D:146:ARG:HB3	1.89	0.54
1:A:195:LEU:HD21	1:A:205:LEU:HD22	1.88	0.54
2:C:102:ASN:HB2	2:C:104:ILE:HG13	1.90	0.54
2:C:190:THR:CG2	2:C:191:PRO:CD	2.78	0.54
1:B:532:ILE:HD12	1:B:535:LEU:HD21	1.89	0.54
1:A:433:PRO:O	1:A:436:LEU:HB2	2.07	0.54
1:A:451:TYR:CD2	1:A:451:TYR:N	2.75	0.54
1:A:483:GLU:H	1:A:483:GLU:CD	2.09	0.54
1:B:355:GLU:HG3	1:B:378:SER:O	2.07	0.54
1:B:640:ARG:NE	2:D:57:CYS:HB3	2.23	0.54
1:B:674:ILE:HD11	1:B:683:LEU:HD21	1.89	0.53
1:A:432:ILE:HG12	1:A:452:LEU:HD13	1.89	0.53
2:D:40:ALA:O	2:D:42:PRO:HD3	2.09	0.53
1:A:42:PHE:CE2	1:A:46:LEU:HD11	2.43	0.53
1:A:369:VAL:HG22	1:A:394:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:TRP:HB2	1:A:496:ASP:HB2	1.90	0.53
1:A:646:THR:HG22	6:A:808:BLD:H228	1.89	0.53
1:B:137:PRO:O	1:B:140:THR:OG1	2.23	0.53
2:D:36:LYS:HD2	2:D:49:TRP:HB2	1.91	0.53
2:D:192:ILE:O	2:D:192:ILE:HG23	2.09	0.53
1:B:529:PRO:HB3	1:B:531:TRP:CE2	2.44	0.53
2:C:120:SER:HA	2:C:144:PHE:HB2	1.91	0.53
2:C:161:THR:O	2:C:185:SER:HB2	2.08	0.53
1:A:202:LEU:HD21	1:A:205:LEU:HB2	1.89	0.53
1:A:347:LEU:HB3	1:A:352:PHE:CE2	2.44	0.53
1:B:738:LEU:O	1:B:759:ASN:HB3	2.09	0.53
1:A:238:ILE:HB	1:A:257:LEU:HD21	1.89	0.52
1:A:659:LEU:HD21	1:A:661:MET:HE1	1.91	0.52
1:A:451:TYR:HD2	1:A:451:TYR:N	2.07	0.52
1:A:515:ASN:OD1	1:A:516:TRP:N	2.42	0.52
1:B:451:TYR:N	1:B:451:TYR:CD2	2.74	0.52
1:B:446:HIS:CD2	1:B:470:LYS:HD2	2.45	0.52
1:B:224:LEU:HD21	1:B:227:LEU:HB2	1.91	0.52
1:B:282:VAL:HG12	1:B:302:LYS:HB2	1.91	0.52
1:B:314:ALA:O	1:B:318:LEU:HB2	2.09	0.52
1:B:433:PRO:O	1:B:436:LEU:HB2	2.09	0.52
1:B:48:ASP:C	1:B:50:ASN:H	2.13	0.52
1:B:727:MET:HE1	2:D:75:LEU:C	2.29	0.52
1:B:597:TYR:CE1	1:B:643:GLY:HA2	2.44	0.52
1:B:633:ASN:OD1	1:B:634:PRO:HD2	2.09	0.52
2:C:109:PRO:O	2:C:112:LEU:HB2	2.10	0.52
2:D:172:SER:O	2:D:174:ASN:N	2.43	0.52
1:A:382:PRO:O	1:A:407:LEU:HD11	2.09	0.52
1:A:597:TYR:CE1	1:A:643:GLY:HA2	2.43	0.52
1:A:84:LEU:O	1:A:86:VAL:HG13	2.09	0.52
1:B:77:ILE:HD13	1:B:95:LEU:HD22	1.92	0.52
2:C:191:PRO:O	2:C:193:SER:N	2.42	0.52
2:D:28:GLU:O	2:D:32:LEU:HD12	2.10	0.52
1:A:367:LEU:HD23	1:A:392:LEU:HD11	1.91	0.52
1:B:299:ALA:O	1:B:301:ASN:ND2	2.42	0.52
1:B:659:LEU:HD21	1:B:661:MET:HE2	1.91	0.52
2:D:196:ASN:O	2:D:197:THR:C	2.32	0.52
1:A:397:LEU:HD22	1:A:402:PHE:CE2	2.43	0.52
1:A:531:TRP:HB2	1:A:534:ARG:HD3	1.90	0.52
1:B:539:ALA:HA	1:B:562:LEU:HA	1.92	0.52
2:D:111:GLN:H	2:D:111:GLN:CD	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:LEU:HG	2:D:123:LEU:HD23	1.92	0.52
1:A:711:SER:HA	1:A:735:ASN:HB2	1.91	0.51
1:B:364:MET:SD	1:B:367:LEU:HD13	2.50	0.51
1:B:372:LEU:HD22	1:B:377:PHE:HE2	1.75	0.51
2:C:108:ILE:HG13	2:C:128:LEU:HD22	1.92	0.51
1:B:42:PHE:HB2	1:B:94:SER:OG	2.09	0.51
2:C:156:ILE:HG22	2:C:157:PRO:O	2.10	0.51
1:B:84:LEU:HD12	1:B:109:SER:HB3	1.93	0.51
1:B:293:LEU:HD21	1:B:296:LEU:HB2	1.91	0.51
1:B:318:LEU:HD22	1:B:342:LEU:HD12	1.91	0.51
1:B:583:GLN:OE1	1:B:586:LYS:HB2	2.10	0.51
1:A:714:LEU:HB2	1:A:736:ASN:OD1	2.10	0.51
1:B:333:PRO:HB2	1:B:335:PHE:CD2	2.45	0.51
1:B:368:LYS:HG3	1:B:393:LEU:CD1	2.41	0.51
1:A:754:ALA:O	1:A:757:LEU:HB2	2.10	0.51
1:A:333:PRO:HB2	1:A:335:PHE:CD2	2.46	0.51
1:A:42:PHE:CE1	1:A:95:LEU:HD11	2.45	0.51
1:A:714:LEU:O	1:A:736:ASN:HB3	2.10	0.51
1:B:303:PHE:O	1:B:326:ASN:HB3	2.11	0.51
2:D:44:LYS:HE3	2:D:47:GLN:OE1	2.10	0.51
1:A:699:GLY:HA2	1:A:725:LEU:HD21	1.93	0.51
2:D:157:PRO:C	2:D:159:SER:H	2.14	0.51
1:A:102:GLU:HA	1:A:123:SER:O	2.10	0.51
1:A:132:ASN:N	1:A:158:ASN:HD21	2.05	0.51
2:C:96:TYR:H	2:C:96:TYR:HD2	1.57	0.51
1:A:225:GLU:HA	1:A:247:LEU:HA	1.92	0.51
1:A:300:GLU:O	1:A:301:ASN:ND2	2.44	0.51
1:A:456:ILE:HD12	1:A:481:PRO:HD3	1.93	0.51
1:A:532:ILE:HD12	1:A:535:LEU:HD21	1.91	0.51
1:A:705:ASN:HD21	2:C:61:HIS:CE1	2.29	0.51
1:B:380:GLU:O	1:B:382:PRO:HD3	2.11	0.51
1:B:467:ARG:O	1:B:490:LEU:HD12	2.11	0.51
1:B:596:ARG:HG2	1:B:597:TYR:N	2.26	0.51
1:A:747:GLN:HE22	2:C:74:ASP:HB3	1.75	0.51
1:A:355:GLU:HG3	1:A:378:SER:O	2.11	0.51
1:A:489:THR:O	1:A:491:GLU:HG3	2.11	0.51
1:A:522:ASN:HB2	1:A:524:LEU:HG	1.92	0.51
1:B:51:LEU:C	1:B:52:LEU:HD12	2.30	0.50
1:B:583:GLN:HB3	1:B:587:ILE:HD11	1.91	0.50
1:B:651:ASP:OD1	1:B:651:ASP:N	2.40	0.50
1:B:36:ILE:HG12	1:B:40:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:134:SER:HA	2:C:157:PRO:CG	2.41	0.50
2:D:97:LEU:CD1	2:D:99:LEU:HD13	2.41	0.50
2:C:192:ILE:HG23	2:C:192:ILE:O	2.12	0.50
1:A:157:SER:C	1:A:158:ASN:HD22	2.14	0.50
1:A:377:PHE:HB3	1:A:402:PHE:CE1	2.46	0.50
1:A:610:HIS:CD2	1:A:663:TYR:CD1	2.99	0.50
1:B:32:LEU:O	1:B:36:ILE:HG22	2.11	0.50
2:D:120:SER:HA	2:D:144:PHE:HB2	1.93	0.50
1:A:423:LEU:HD22	1:A:428:PHE:HE2	1.76	0.50
1:A:140:THR:O	1:A:143:SER:OG	2.23	0.50
1:A:42:PHE:HE2	1:A:46:LEU:HD11	1.77	0.50
1:A:603:ASP:C	1:A:605:MET:H	2.14	0.50
1:A:737:ASN:O	1:A:737:ASN:ND2	2.36	0.50
1:B:458:SER:OG	1:B:483:GLU:OE1	2.23	0.50
2:C:73:VAL:HG12	2:C:75:LEU:HG	1.94	0.50
1:A:493:LEU:HD11	1:A:495:LEU:HD11	1.94	0.49
1:A:704:LEU:HD21	1:A:707:LEU:HD22	1.94	0.49
6:A:808:BLD:H17	2:C:60:PHE:CZ	2.47	0.49
1:B:238:ILE:HD12	1:B:238:ILE:H	1.78	0.49
1:B:294:GLN:HB3	1:B:319:THR:HG23	1.94	0.49
1:B:447:LEU:O	1:B:450:ASN:ND2	2.39	0.49
1:B:642:TYR:CD1	2:D:58:THR:HG22	2.47	0.49
1:A:152:PHE:HD1	1:A:177:VAL:HB	1.76	0.49
1:A:447:LEU:O	1:A:450:ASN:ND2	2.35	0.49
1:A:431:LYS:HE2	1:A:454:GLY:HA3	1.95	0.49
1:A:508:LEU:HD22	1:A:514:LEU:HD11	1.94	0.49
2:C:135:THR:HG22	2:C:138:ARG:HD2	1.93	0.49
1:B:292:SER:HA	1:B:317:THR:HG21	1.94	0.49
1:B:456:ILE:HG12	1:B:476:LEU:HD13	1.95	0.49
2:C:191:PRO:O	2:C:192:ILE:C	2.51	0.49
1:A:473:LEU:N	1:A:496:ASP:O	2.32	0.49
1:A:740:GLY:O	1:A:763:CYS:N	2.29	0.49
1:A:681:PHE:CD1	6:A:808:BLD:H112	2.47	0.49
1:B:177:VAL:HG13	1:B:204:HIS:HB3	1.94	0.49
2:C:72:ARG:NH2	2:C:74:ASP:OD1	2.42	0.49
2:D:129:SER:HA	2:D:151:SER:O	2.13	0.49
1:A:235:SER:O	1:A:235:SER:OG	2.29	0.49
1:A:47:PRO:N	1:A:48:ASP:HB3	2.28	0.49
1:B:715:ASP:HB3	1:B:737:ASN:HB3	1.94	0.49
2:C:191:PRO:HD2	2:C:192:ILE:N	2.26	0.49
1:A:137:PRO:O	1:A:140:THR:OG1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:TYR:N	1:A:329:TYR:HD2	2.10	0.49
1:B:261:PHE:CE1	1:B:276:ILE:HD13	2.47	0.49
2:D:105:THR:OG1	2:D:106:GLY:N	2.40	0.49
1:B:456:ILE:HG12	1:B:476:LEU:CD1	2.43	0.49
2:D:32:LEU:HB3	2:D:49:TRP:CZ3	2.48	0.49
1:A:248:GLN:HA	1:A:271:LEU:HA	1.95	0.49
1:A:374:PHE:O	1:A:375:ASN:ND2	2.46	0.49
1:A:42:PHE:CD2	1:A:42:PHE:C	2.86	0.49
1:A:456:ILE:HG12	1:A:476:LEU:HD13	1.95	0.49
1:A:332:VAL:CG2	1:A:357:PRO:HG3	2.43	0.48
1:A:444:SER:OG	1:A:468:ASP:HB2	2.12	0.48
1:A:467:ARG:O	1:A:490:LEU:HD12	2.12	0.48
1:B:368:LYS:HB3	1:B:393:LEU:HD12	1.95	0.48
1:B:596:ARG:HB2	1:B:645:HIS:CD2	2.48	0.48
1:B:60:ASN:O	1:B:63:THR:HG23	2.12	0.48
2:D:91:LEU:HD12	2:D:94:LEU:HD12	1.95	0.48
1:B:294:GLN:O	1:B:318:LEU:HD23	2.13	0.48
1:B:293:LEU:HD11	1:B:296:LEU:HD13	1.95	0.48
2:C:151:SER:O	2:C:151:SER:OG	2.27	0.48
1:B:377:PHE:HB3	1:B:402:PHE:HE1	1.78	0.48
1:B:404:GLY:O	1:B:428:PHE:HA	2.14	0.48
1:B:595:LYS:O	1:B:646:THR:HG23	2.13	0.48
1:B:714:LEU:HB2	1:B:736:ASN:OD1	2.12	0.48
2:D:73:VAL:HG12	2:D:75:LEU:HG	1.96	0.48
1:A:460:LEU:HD23	1:A:463:LEU:CD1	2.43	0.48
1:B:304:THR:HG22	1:B:327:HIS:HB2	1.95	0.48
1:B:553:PRO:O	1:B:556:LEU:HB2	2.13	0.48
1:B:603:ASP:C	1:B:605:MET:H	2.15	0.48
2:C:36:LYS:HD2	2:C:49:TRP:HB2	1.95	0.48
1:A:268:CYS:O	1:A:269:THR:OG1	2.28	0.48
1:A:294:GLN:HB3	1:A:319:THR:HG23	1.95	0.48
1:A:627:ASN:C	1:A:629:LEU:N	2.67	0.48
1:B:236:THR:OG1	1:B:237:GLY:N	2.47	0.48
1:B:542:LYS:HZ3	1:B:615:LEU:H	1.59	0.48
2:D:39:LEU:HD13	2:D:80:LEU:CD1	2.43	0.48
1:A:108:ASN:HA	1:A:131:ARG:O	2.13	0.48
2:D:41:ASP:OD2	2:D:45:VAL:N	2.46	0.48
1:A:386:THR:HG23	1:A:410:LEU:O	2.12	0.48
1:B:369:VAL:HG13	1:B:394:THR:HB	1.96	0.48
2:D:123:LEU:HB2	2:D:147:LEU:HD23	1.95	0.48
1:B:167:SER:OG	1:B:168:GLY:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:PRO:O	1:A:556:LEU:HB2	2.14	0.48
1:B:484:LEU:O	1:B:487:VAL:HG23	2.13	0.48
1:B:705:ASN:HD22	1:B:705:ASN:N	2.12	0.48
1:A:304:THR:HG22	1:A:327:HIS:HB2	1.96	0.48
1:A:358:MET:HE1	1:A:388:LEU:HD22	1.96	0.48
1:A:639:SER:OG	1:A:640:ARG:N	2.47	0.48
1:B:650:PHE:CD1	1:B:654:GLY:HA3	2.49	0.48
1:B:260:ASP:CG	1:B:263:ARG:HB3	2.35	0.47
1:B:282:VAL:CG1	1:B:302:LYS:HD2	2.44	0.47
1:B:432:ILE:HG12	1:B:452:LEU:HD13	1.96	0.47
2:C:186:PHE:HA	2:C:189:PHE:CE2	2.49	0.47
2:D:98:GLU:HB3	2:D:100:TYR:CD2	2.47	0.47
2:D:160:LEU:O	2:D:186:PHE:CE2	2.67	0.47
2:D:96:TYR:HB3	2:D:98:GLU:OE2	2.14	0.47
1:A:287:PRO:HA	1:A:310:PHE:CE2	2.50	0.47
1:B:361:LEU:HD23	1:B:364:MET:HE1	1.96	0.47
1:B:601:LYS:HD2	6:B:807:BLD:O06	2.13	0.47
1:A:52:LEU:HD13	1:A:55:TRP:CE3	2.49	0.47
1:A:650:PHE:CE1	1:A:654:GLY:HA3	2.49	0.47
1:A:738:LEU:HB2	1:A:759:ASN:OD1	2.14	0.47
1:B:108:ASN:ND2	1:B:108:ASN:O	2.43	0.47
1:B:499:ASP:O	1:B:501:THR:HG23	2.14	0.47
1:A:682:ILE:HG12	1:A:706:ILE:HG13	1.96	0.47
1:A:269:THR:HA	1:A:289:PRO:HB2	1.96	0.47
1:A:529:PRO:HB3	1:A:531:TRP:NE1	2.28	0.47
1:A:706:ILE:HD13	1:A:730:GLU:HB2	1.95	0.47
1:B:252:ILE:HD12	1:B:257:LEU:HD13	1.97	0.47
1:B:674:ILE:O	1:B:701:LEU:HD21	2.15	0.47
1:B:328:PHE:O	1:B:350:ASN:HB3	2.15	0.47
1:A:37:HIS:HB3	1:B:37:HIS:CG	2.49	0.47
1:B:467:ARG:HD2	1:B:491:GLU:CD	2.35	0.47
2:D:108:ILE:HG13	2:D:128:LEU:HD22	1.95	0.47
2:C:105:THR:OG1	2:C:106:GLY:N	2.47	0.47
2:D:163:VAL:CG2	2:D:166:LEU:HD11	2.35	0.47
1:A:368:LYS:HG3	1:A:393:LEU:CD1	2.42	0.47
1:A:52:LEU:O	1:A:55:TRP:HB2	2.14	0.47
1:A:598:VAL:O	1:A:615:LEU:HD12	2.15	0.47
1:B:347:LEU:HB3	1:B:352:PHE:CE2	2.49	0.47
1:B:718:ILE:HG21	1:B:742:ILE:HG22	1.96	0.47
2:D:96:TYR:H	2:D:96:TYR:HD2	1.61	0.47
1:A:329:TYR:CD2	1:A:329:TYR:N	2.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:HD21	1:A:421:LEU:HD13	1.96	0.47
1:A:55:TRP:NE1	1:A:64:PHE:HB3	2.29	0.47
1:B:101:LEU:HD23	1:B:124:LEU:HD12	1.97	0.47
2:D:49:TRP:HA	2:D:59:TRP:CD2	2.50	0.47
1:A:268:CYS:C	1:A:270:GLU:N	2.68	0.47
1:B:489:THR:O	1:B:491:GLU:HG3	2.15	0.47
1:B:553:PRO:HG2	1:B:556:LEU:HD12	1.97	0.47
2:C:97:LEU:CD1	2:C:99:LEU:HD13	2.45	0.47
2:C:96:TYR:HB3	2:C:98:GLU:OE2	2.15	0.47
1:B:727:MET:HE1	2:D:76:GLY:N	2.30	0.47
1:A:137:PRO:HB2	1:A:139:THR:OG1	2.14	0.46
1:A:204:HIS:CD2	1:A:226:PHE:CG	3.03	0.46
1:B:349:SER:N	1:B:373:SER:O	2.47	0.46
1:B:627:ASN:C	1:B:629:LEU:N	2.68	0.46
2:C:150:ASN:C	2:C:174:ASN:HB3	2.35	0.46
2:D:193:SER:O	2:D:194:PHE:CD1	2.68	0.46
1:B:419:GLN:HB2	1:B:420:GLU:HG3	1.96	0.46
1:B:683:LEU:HD11	1:B:685:LEU:HD21	1.97	0.46
1:A:289:PRO:O	1:A:293:LEU:HD12	2.15	0.46
1:A:528:ILE:CG2	1:A:553:PRO:HG3	2.46	0.46
1:B:329:TYR:HD2	1:B:329:TYR:N	2.13	0.46
1:B:745:MET:HG3	1:B:746:GLY:N	2.31	0.46
2:C:123:LEU:HB2	2:C:147:LEU:HD23	1.96	0.46
2:D:83:GLN:HG2	2:D:106:GLY:HA3	1.97	0.46
2:D:95:GLN:HB3	2:D:96:TYR:CD2	2.51	0.46
1:A:349:SER:HA	1:A:374:PHE:O	2.16	0.46
1:B:141:LEU:HD11	1:B:160:LEU:CD1	2.45	0.46
1:B:138:VAL:HG12	1:B:162:PHE:CD1	2.50	0.46
1:B:569:THR:HG23	1:B:610:HIS:ND1	2.31	0.46
2:C:112:LEU:HA	2:C:112:LEU:HD23	1.69	0.46
2:C:191:PRO:O	2:C:194:PHE:N	2.30	0.46
2:C:46:LEU:HD22	2:C:49:TRP:CE2	2.51	0.46
2:D:126:ASN:O	2:D:150:ASN:HA	2.15	0.46
1:A:295:TYR:CZ	3:F:1:NAG:H82	2.51	0.46
1:A:162:PHE:HE2	1:A:166:VAL:HA	1.81	0.46
1:A:177:VAL:HG13	1:A:204:HIS:HB3	1.98	0.46
1:A:373:SER:HB3	1:A:396:ASP:OD1	2.16	0.46
6:A:808:BLD:H17	2:C:60:PHE:HZ	1.79	0.46
1:B:397:LEU:HD22	1:B:402:PHE:HE2	1.80	0.46
2:C:182:VAL:O	2:C:183:ASN:C	2.53	0.46
2:C:192:ILE:HA	2:C:192:ILE:HD13	1.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:SER:OG	1:A:313:GLY:N	2.46	0.46
1:A:343:GLU:O	1:A:368:LYS:N	2.43	0.46
1:A:420:GLU:OE2	1:A:422:TYR:OH	2.25	0.46
1:A:456:ILE:HG12	1:A:476:LEU:CD1	2.46	0.46
1:A:596:ARG:HD2	1:A:618:PHE:O	2.15	0.46
1:B:480:ILE:HG22	1:B:505:PRO:HG3	1.97	0.46
2:D:182:VAL:C	2:D:184:GLY:N	2.68	0.46
2:D:49:TRP:HA	2:D:59:TRP:CG	2.49	0.46
1:B:203:LYS:O	1:B:224:LEU:HD12	2.16	0.46
1:B:260:ASP:OD2	1:B:263:ARG:HB3	2.15	0.46
4:A:805:NAG:O6	4:A:805:NAG:O4	2.22	0.46
1:B:443:VAL:HA	1:B:466:LEU:HA	1.98	0.46
1:A:209:GLY:HA2	1:A:231:SER:HB2	1.97	0.45
1:A:495:LEU:O	1:A:498:ASN:ND2	2.43	0.45
1:A:633:ASN:OD1	1:A:634:PRO:HD2	2.15	0.45
2:D:121:LEU:HB3	2:D:145:LEU:HD12	1.97	0.45
1:A:674:ILE:HD11	1:A:683:LEU:HD21	1.97	0.45
1:A:292:SER:O	1:A:294:GLN:HG3	2.17	0.45
1:A:392:LEU:HD12	1:A:392:LEU:HA	1.76	0.45
1:A:539:ALA:HA	1:A:562:LEU:HA	1.98	0.45
1:A:642:TYR:OH	6:A:808:BLD:H104	2.16	0.45
1:B:618:PHE:HE2	1:B:623:SER:HA	1.80	0.45
2:C:108:ILE:HA	2:C:109:PRO:HD3	1.78	0.45
2:D:95:GLN:HB3	2:D:96:TYR:CE2	2.51	0.45
1:A:393:LEU:O	1:A:419:GLN:N	2.42	0.45
1:A:627:ASN:C	1:A:629:LEU:H	2.20	0.45
1:A:675:GLY:HA2	1:A:701:LEU:HD21	1.99	0.45
1:B:472:TRP:HB2	1:B:496:ASP:HB2	1.97	0.45
1:A:619:GLN:HB3	1:A:619:GLN:HE21	1.65	0.45
2:D:154:GLY:O	2:D:176:LEU:HB3	2.16	0.45
1:A:711:SER:HA	1:A:735:ASN:CB	2.45	0.45
1:B:472:TRP:HB3	1:B:494:ILE:HG22	1.99	0.45
1:B:659:LEU:HD12	1:B:660:ASP:N	2.32	0.45
2:C:49:TRP:HA	2:C:59:TRP:CD2	2.52	0.45
2:D:161:THR:HA	2:D:185:SER:CB	2.46	0.45
1:A:407:LEU:HB2	1:A:410:LEU:HB2	1.98	0.45
1:B:741:PRO:HA	1:B:763:CYS:CB	2.47	0.45
1:A:134:LEU:HB2	1:A:158:ASN:OD1	2.17	0.45
1:A:742:ILE:HA	1:A:743:PRO:HD3	1.75	0.45
1:B:329:TYR:H	1:B:329:TYR:HD2	1.64	0.45
1:B:373:SER:HA	1:B:398:SER:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:147:LEU:HD23	2:C:147:LEU:HA	1.66	0.45
1:A:492:THR:CG2	1:A:494:ILE:HG12	2.47	0.45
1:A:590:ASN:HD21	1:A:651:ASP:HA	1.82	0.45
1:B:204:HIS:CD2	1:B:226:PHE:CG	3.05	0.45
1:B:329:TYR:CD2	1:B:329:TYR:N	2.84	0.45
1:B:650:PHE:CE1	1:B:654:GLY:HA3	2.51	0.45
1:A:305:GLY:O	1:A:328:PHE:HA	2.17	0.45
1:A:42:PHE:HD2	1:A:42:PHE:C	2.19	0.45
1:B:144:LEU:HB2	1:B:172:LEU:HD21	1.99	0.45
1:B:368:LYS:CG	1:B:393:LEU:HD12	2.44	0.45
1:A:558:ASP:N	1:A:558:ASP:OD1	2.50	0.44
1:B:36:ILE:HA	1:B:39:LEU:HD12	1.99	0.44
2:C:84:LEU:CD1	2:C:104:ILE:HG21	2.47	0.44
1:A:375:ASN:O	1:A:400:ASN:HA	2.17	0.44
1:B:483:GLU:H	1:B:483:GLU:CD	2.21	0.44
1:B:55:TRP:CD1	1:B:64:PHE:HB3	2.51	0.44
2:C:148:ASN:OD1	2:C:149:ASN:N	2.50	0.44
1:A:129:LEU:O	1:A:132:ASN:ND2	2.51	0.44
1:A:281:PHE:HB2	1:A:301:ASN:OD1	2.18	0.44
1:A:291:LYS:HA	1:A:291:LYS:HD2	1.67	0.44
1:A:35:GLU:O	1:A:39:LEU:HD12	2.18	0.44
1:A:48:ASP:HA	1:A:50:ASN:OD1	2.17	0.44
1:B:281:PHE:HB2	1:B:301:ASN:OD1	2.17	0.44
1:A:508:LEU:HD23	1:A:511:CYS:SG	2.57	0.44
1:A:610:HIS:CD2	1:A:663:TYR:CG	3.05	0.44
1:B:627:ASN:C	1:B:629:LEU:H	2.20	0.44
2:C:148:ASN:HB2	2:C:170:ASP:O	2.17	0.44
1:A:247:LEU:HD21	1:A:250:LEU:HD13	1.99	0.44
1:B:162:PHE:HE2	1:B:166:VAL:HB	1.82	0.44
1:B:531:TRP:HB2	1:B:534:ARG:HD3	1.99	0.44
1:B:543:LEU:HB2	1:B:567:LEU:HD23	1.99	0.44
1:A:750:THR:HG22	2:C:96:TYR:HD1	1.83	0.44
1:A:499:ASP:OD1	1:A:523:ARG:NH2	2.51	0.44
1:A:449:PHE:CD2	1:A:621:ILE:HD13	2.52	0.44
1:B:425:ASN:HA	1:B:449:PHE:HB3	1.99	0.44
1:B:35:GLU:HG3	1:B:98:LEU:HD11	1.98	0.44
2:C:32:LEU:HB3	2:C:49:TRP:CZ3	2.53	0.44
2:C:39:LEU:HD13	2:C:80:LEU:HD13	1.99	0.44
2:D:95:GLN:O	2:D:118:LEU:HD13	2.17	0.44
2:D:165:THR:HB	2:D:166:LEU:H	1.64	0.44
1:A:204:HIS:CD2	1:A:226:PHE:CD2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:THR:OG1	2:C:77:ASN:HB3	2.17	0.44
2:C:99:LEU:O	2:C:102:ASN:ND2	2.48	0.44
1:B:155:VAL:HG22	1:B:180:LEU:HD23	2.00	0.44
1:B:355:GLU:HG2	1:B:356:LEU:H	1.83	0.44
2:D:147:LEU:HA	2:D:147:LEU:HD23	1.79	0.44
1:A:367:LEU:O	1:A:368:LYS:HD2	2.18	0.44
2:C:40:ALA:O	2:C:42:PRO:HD3	2.18	0.44
1:A:385:LEU:HG	1:A:385:LEU:O	2.19	0.43
1:A:483:GLU:C	1:A:485:MET:N	2.72	0.43
1:A:91:VAL:HG11	1:A:106:LEU:HD11	2.00	0.43
1:B:229:VAL:O	1:B:229:VAL:HG23	2.18	0.43
1:B:402:PHE:HB3	1:B:428:PHE:HE1	1.83	0.43
1:B:725:LEU:HB2	1:B:728:LEU:HD12	2.00	0.43
2:C:95:GLN:HB3	2:C:96:TYR:CD2	2.53	0.43
1:B:256:LYS:O	1:B:280:GLN:HG3	2.18	0.43
1:B:312:SER:HA	1:B:335:PHE:CE1	2.53	0.43
1:B:368:LYS:O	1:B:393:LEU:HB2	2.18	0.43
1:B:680:LEU:HD11	1:B:682:ILE:O	2.18	0.43
1:B:744:GLU:N	1:B:744:GLU:OE2	2.50	0.43
2:D:169:LEU:CD1	2:D:171:LEU:H	2.29	0.43
1:A:342:LEU:HD21	1:A:345:LEU:HB2	2.00	0.43
1:A:719:PRO:O	1:A:722:MET:HB2	2.18	0.43
1:A:42:PHE:HE1	1:A:95:LEU:HD11	1.83	0.43
1:B:230:SER:HA	1:B:253:SER:O	2.17	0.43
1:B:300:GLU:C	1:B:301:ASN:HD22	2.22	0.43
2:D:157:PRO:HG2	2:D:160:LEU:HD13	2.00	0.43
1:A:286:PRO:O	1:A:288:LEU:HD13	2.18	0.43
1:B:291:LYS:HD2	1:B:291:LYS:HA	1.58	0.43
1:B:307:ILE:HD11	1:B:352:PHE:HZ	1.78	0.43
2:D:46:LEU:HD13	2:D:49:TRP:CD2	2.53	0.43
2:D:45:VAL:HG13	2:D:61:HIS:CD2	2.52	0.43
1:A:308:PRO:HB2	1:A:310:PHE:CD1	2.51	0.43
1:A:333:PRO:HB2	1:A:335:PHE:CE2	2.53	0.43
1:A:468:ASP:HA	1:A:492:THR:HB	2.01	0.43
1:A:505:PRO:HG2	1:A:508:LEU:CD1	2.47	0.43
1:A:707:LEU:HA	1:A:707:LEU:HD12	1.70	0.43
2:D:113:GLY:HA2	2:D:139:LEU:HD21	2.00	0.43
1:A:115:VAL:O	1:A:140:THR:HG22	2.19	0.43
1:A:595:LYS:O	1:A:646:THR:HG23	2.19	0.43
1:B:47:PRO:HG2	1:B:85:ASN:HB2	2.00	0.43
1:A:505:PRO:HG2	1:A:508:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PHE:O	1:B:302:LYS:N	2.47	0.43
1:B:297:SER:OG	1:B:322:ASP:HB3	2.18	0.43
2:C:115:LEU:HB3	2:C:118:LEU:HD23	2.00	0.43
2:C:121:LEU:HG	2:C:123:LEU:HD23	2.00	0.43
2:D:80:LEU:HD12	2:D:80:LEU:C	2.39	0.43
1:B:42:PHE:C	1:B:42:PHE:CD2	2.92	0.43
1:A:84:LEU:HD12	1:A:109:SER:HB3	2.00	0.43
1:A:155:VAL:HG23	1:A:183:ASN:HD21	1.84	0.43
1:B:657:MET:HE3	1:B:657:MET:HB3	1.84	0.43
2:C:65:ASN:ND2	2:C:67:ASP:HB2	2.33	0.43
1:A:600:ILE:HG23	1:A:641:VAL:HG13	1.99	0.43
1:A:717:ARG:CG	1:A:740:GLY:HA3	2.42	0.43
1:B:381:LEU:HD22	1:B:385:LEU:HD22	2.00	0.43
1:B:558:ASP:OD1	1:B:558:ASP:N	2.52	0.43
1:B:718:ILE:HG23	1:B:743:PRO:HD2	2.01	0.43
2:C:27:ALA:O	2:C:30:ASP:HB2	2.18	0.43
1:A:372:LEU:HD22	1:A:377:PHE:HE2	1.84	0.42
1:B:563:ILE:HB	1:B:657:MET:HG3	2.01	0.42
2:C:36:LYS:HA	2:C:46:LEU:HD12	2.00	0.42
1:A:158:ASN:O	1:A:183:ASN:HA	2.19	0.42
1:A:330:GLY:O	1:A:352:PHE:HA	2.19	0.42
1:A:432:ILE:HB	1:A:457:PRO:HD3	2.00	0.42
1:A:528:ILE:HG21	1:A:553:PRO:HG3	2.01	0.42
2:C:152:LEU:HD12	2:C:174:ASN:OD1	2.19	0.42
2:D:80:LEU:O	2:D:102:ASN:HB3	2.19	0.42
1:A:562:LEU:HG	1:A:562:LEU:O	2.19	0.42
1:A:592:ILE:O	1:A:592:ILE:HG13	2.19	0.42
1:A:659:LEU:HD21	1:A:661:MET:CE	2.49	0.42
1:A:680:LEU:HD12	1:A:680:LEU:C	2.40	0.42
1:A:720:GLN:HB2	1:A:743:PRO:HB3	2.01	0.42
1:B:728:LEU:HD21	1:B:730:GLU:O	2.19	0.42
2:C:169:LEU:CD1	2:C:171:LEU:H	2.29	0.42
2:D:39:LEU:HD13	2:D:80:LEU:HD11	2.00	0.42
1:B:43:LYS:HA	1:B:46:LEU:HD13	2.01	0.42
2:C:143:ARG:HG2	2:C:165:THR:HG21	2.01	0.42
1:A:388:LEU:O	1:A:391:SER:N	2.53	0.42
1:B:277:SER:HA	1:B:299:ALA:O	2.20	0.42
1:B:528:ILE:CG2	1:B:553:PRO:HG3	2.49	0.42
1:B:756:PHE:O	1:B:759:ASN:ND2	2.52	0.42
1:B:522:ASN:HD22	1:B:524:LEU:HD11	1.85	0.42
1:B:640:ARG:HB2	1:B:640:ARG:NH2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:ILE:HG22	2:D:158:ARG:H	1.84	0.42
1:A:630:SER:OG	1:A:631:THR:N	2.52	0.42
1:B:104:LEU:HD11	1:B:106:LEU:HD21	2.02	0.42
1:B:305:GLY:O	1:B:328:PHE:HA	2.19	0.42
1:B:332:VAL:HG21	1:B:357:PRO:HG3	2.02	0.42
2:C:119:VAL:HG12	2:C:120:SER:N	2.33	0.42
2:C:28:GLU:O	2:C:32:LEU:HD12	2.19	0.42
2:D:145:LEU:HD12	2:D:145:LEU:HA	1.79	0.42
1:A:346:ALA:HA	1:A:371:ASP:HB3	2.02	0.42
1:A:483:GLU:N	1:A:483:GLU:CD	2.72	0.42
1:B:570:ASN:HB3	1:B:572:PHE:CD2	2.54	0.42
1:B:682:ILE:HD11	6:B:807:BLD:H119	2.01	0.42
2:C:106:GLY:O	2:C:129:SER:N	2.50	0.42
1:A:448:SER:OG	1:A:470:LYS:O	2.36	0.42
1:A:683:LEU:HD11	1:A:685:LEU:HD21	2.02	0.42
1:A:666:LEU:O	1:A:688:ASN:HB3	2.20	0.42
1:B:34:ARG:O	1:B:38:GLN:HG3	2.20	0.42
1:A:129:LEU:O	1:A:132:ASN:HB2	2.20	0.42
1:A:738:LEU:O	1:A:759:ASN:HB3	2.20	0.42
1:B:505:PRO:HG2	1:B:508:LEU:HD12	2.01	0.42
1:B:374:PHE:CE2	1:B:620:GLY:HA2	2.55	0.42
1:B:630:SER:OG	1:B:631:THR:N	2.52	0.42
1:A:281:PHE:HD2	1:A:301:ASN:OD1	2.03	0.41
1:A:49:LYS:O	1:A:49:LYS:HG2	2.20	0.41
1:A:583:GLN:HB3	1:A:587:ILE:HD11	2.01	0.41
1:B:312:SER:HA	1:B:335:PHE:CD1	2.55	0.41
1:B:375:ASN:O	1:B:400:ASN:HA	2.20	0.41
1:B:640:ARG:HB2	1:B:640:ARG:HH21	1.85	0.41
1:B:741:PRO:HA	1:B:763:CYS:HB2	2.00	0.41
2:C:184:GLY:C	2:C:187:SER:H	2.20	0.41
2:D:122:ASP:HB3	2:D:124:TYR:CD2	2.55	0.41
1:A:173:ASN:N	1:A:173:ASN:OD1	2.53	0.41
1:A:230:SER:HA	1:A:253:SER:O	2.19	0.41
1:A:47:PRO:CD	1:A:48:ASP:HB3	2.50	0.41
1:A:694:ILE:HG23	1:A:698:VAL:HG21	2.02	0.41
1:A:740:GLY:O	1:A:762:LEU:HG	2.20	0.41
1:B:261:PHE:HB3	1:B:281:PHE:CE1	2.55	0.41
1:B:562:LEU:HD11	1:B:565:LEU:HB2	2.02	0.41
1:B:583:GLN:NE2	1:B:586:LYS:HD2	2.35	0.41
1:B:704:LEU:HD21	1:B:707:LEU:HD22	2.01	0.41
2:C:139:LEU:CD1	2:C:142:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:39:LEU:HA	2:C:39:LEU:HD23	1.81	0.41
2:D:84:LEU:HD11	2:D:104:ILE:HD13	2.02	0.41
1:A:431:LYS:HA	1:A:453:SER:O	2.19	0.41
1:B:428:PHE:O	1:B:452:LEU:HD23	2.21	0.41
1:B:720:GLN:HG3	1:B:720:GLN:H	1.41	0.41
1:A:331:ALA:HB2	1:A:353:SER:O	2.21	0.41
1:A:446:HIS:CD2	1:A:470:LYS:HD2	2.54	0.41
1:B:332:VAL:CG2	1:B:357:PRO:HG3	2.51	0.41
1:B:397:LEU:HD22	1:B:402:PHE:CE2	2.56	0.41
1:B:48:ASP:HB3	1:B:51:LEU:HG	2.02	0.41
2:C:149:ASN:HA	2:C:173:ASN:CB	2.41	0.41
2:D:140:LYS:NZ	2:D:162:ALA:HB1	2.35	0.41
1:A:238:ILE:HD12	1:A:239:PRO:HD2	2.02	0.41
1:B:323:LEU:HB2	1:B:347:LEU:HD23	2.02	0.41
1:B:695:PRO:O	1:B:698:VAL:HG23	2.21	0.41
1:B:727:MET:HA	1:B:727:MET:CE	2.50	0.41
2:C:46:LEU:HD13	2:C:49:TRP:CE3	2.56	0.41
1:A:98:LEU:HD23	1:A:101:LEU:HD13	2.02	0.41
1:A:108:ASN:O	1:A:108:ASN:ND2	2.48	0.41
1:A:423:LEU:HD22	1:A:428:PHE:CE2	2.56	0.41
1:A:568:ASN:OD1	1:A:569:THR:OG1	2.23	0.41
1:A:642:TYR:CE1	2:C:58:THR:HA	2.56	0.41
1:A:224:LEU:HD21	1:A:227:LEU:HB2	2.03	0.41
1:A:483:GLU:C	1:A:485:MET:H	2.24	0.41
1:A:695:PRO:O	1:A:698:VAL:HG23	2.20	0.41
1:B:158:ASN:O	1:B:183:ASN:HA	2.21	0.41
1:B:190:VAL:HB	1:B:212:ILE:HD13	2.02	0.41
1:B:619:GLN:O	1:B:621:ILE:N	2.54	0.41
2:D:121:LEU:HG	2:D:123:LEU:CD2	2.51	0.41
2:D:56:PRO:HB3	2:D:59:TRP:CZ2	2.55	0.41
1:A:402:PHE:HB3	1:A:428:PHE:HE1	1.85	0.41
6:A:808:BLD:H211	6:A:808:BLD:H101	1.75	0.41
1:B:448:SER:OG	1:B:470:LYS:O	2.36	0.41
2:C:99:LEU:HA	2:C:99:LEU:HD12	1.65	0.41
1:A:450:ASN:C	1:A:451:TYR:HD2	2.24	0.41
1:B:271:LEU:HD21	1:B:274:LEU:HD13	2.02	0.41
2:D:111:GLN:N	2:D:111:GLN:CD	2.74	0.41
2:D:171:LEU:HG	2:D:171:LEU:O	2.20	0.41
1:A:739:SER:HA	1:A:761:GLY:C	2.41	0.41
6:A:808:BLD:H121	6:A:808:BLD:H23	1.89	0.41
1:B:107:SER:HB2	1:B:128:ASP:CG	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:ILE:HA	2:D:109:PRO:HD3	1.88	0.41
2:D:152:LEU:HB2	2:D:174:ASN:OD1	2.21	0.41
1:A:273:LEU:C	1:A:273:LEU:HD23	2.42	0.41
1:A:273:LEU:HD21	1:A:275:ASN:HB2	2.02	0.41
1:A:371:ASP:HA	1:A:396:ASP:HB3	2.02	0.41
1:A:52:LEU:HD22	1:A:55:TRP:CD1	2.55	0.41
1:B:213:SER:HB3	1:B:233:ASN:HB3	2.03	0.41
1:B:368:LYS:CB	1:B:393:LEU:HD12	2.51	0.41
1:B:448:SER:HB3	1:B:472:TRP:O	2.21	0.41
1:B:650:PHE:HB3	1:B:679:TYR:CZ	2.56	0.41
2:C:154:GLY:O	2:C:176:LEU:HB3	2.21	0.41
2:D:120:SER:OG	2:D:122:ASP:OD1	2.38	0.41
1:B:750:THR:HG22	2:D:96:TYR:HD1	1.85	0.41
1:B:262:SER:OG	1:B:287:PRO:O	2.40	0.40
1:B:380:GLU:OE1	1:B:404:GLY:HA3	2.21	0.40
2:D:59:TRP:N	2:D:59:TRP:CD1	2.89	0.40
1:B:361:LEU:HA	1:B:364:MET:HE3	2.02	0.40
1:B:483:GLU:C	1:B:485:MET:N	2.74	0.40
1:B:491:GLU:HA	1:B:513:ASN:O	2.22	0.40
2:C:97:LEU:HD12	2:C:97:LEU:C	2.42	0.40
2:D:160:LEU:C	2:D:186:PHE:HE2	2.25	0.40
2:D:36:LYS:HG3	2:D:46:LEU:HB3	2.03	0.40
1:A:297:SER:OG	1:A:322:ASP:HB3	2.21	0.40
1:A:388:LEU:HA	1:A:388:LEU:HD12	1.87	0.40
1:A:575:THR:HG22	1:A:667:SER:O	2.21	0.40
1:B:300:GLU:O	1:B:301:ASN:ND2	2.54	0.40
1:B:399:SER:HA	1:B:425:ASN:ND2	2.35	0.40
1:B:418:LEU:HD21	1:B:421:LEU:HD13	2.03	0.40
1:B:421:LEU:HD23	1:B:445:LEU:HD13	2.03	0.40
1:A:49:LYS:HD2	1:B:49:LYS:HD3	2.03	0.40
2:C:49:TRP:CD1	2:C:59:TRP:HB3	2.56	0.40
1:B:640:ARG:HE	2:D:57:CYS:HB3	1.86	0.40
1:A:234:PHE:HD2	1:A:255:ASN:OD1	2.05	0.40
1:A:257:LEU:O	1:A:279:ASN:HB3	2.22	0.40
1:A:515:ASN:O	1:A:538:LEU:HD12	2.21	0.40
1:A:541:LEU:HD11	1:A:543:LEU:HD11	2.03	0.40
1:A:722:MET:HB3	1:A:722:MET:HE3	1.88	0.40
1:B:173:ASN:N	1:B:173:ASN:OD1	2.46	0.40
1:B:42:PHE:HD2	1:B:42:PHE:C	2.25	0.40
2:C:39:LEU:HD22	2:C:80:LEU:HD13	2.04	0.40
2:D:119:VAL:HG12	2:D:120:SER:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:GLU:H	1:A:536:GLU:HG2	1.72	0.40
1:B:385:LEU:O	1:B:385:LEU:HG	2.22	0.40
1:B:423:LEU:HD22	1:B:428:PHE:HE2	1.86	0.40
1:B:434:PRO:HB3	1:B:459:SER:HB2	2.02	0.40
1:B:707:LEU:HA	1:B:707:LEU:HD12	1.74	0.40
2:D:123:LEU:HD12	2:D:128:LEU:HD11	2.02	0.40
2:D:50:ASP:OD1	2:D:52:THR:OG1	2.35	0.40
2:D:71:THR:C	2:D:72:ARG:HG3	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	731/767 (95%)	695 (95%)	35 (5%)	1 (0%)	51 83
1	B	732/767 (95%)	699 (96%)	30 (4%)	3 (0%)	34 71
2	C	173/201 (86%)	146 (84%)	24 (14%)	3 (2%)	9 45
2	D	173/201 (86%)	147 (85%)	21 (12%)	5 (3%)	4 33
All	All	1809/1936 (93%)	1687 (93%)	110 (6%)	12 (1%)	22 61

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	197	THR
1	B	313	GLY
2	D	183	ASN
2	C	173	ASN
2	C	196	ASN
2	D	179	ASP
2	D	196	ASN

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Mol	Chain	Res	Type
2	C	179	ASP
1	B	65	ASP
1	A	318	LEU
1	B	311	LEU
2	D	156	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	645/676 (95%)	552 (86%)	93 (14%)	3 20
1	B	647/676 (96%)	552 (85%)	95 (15%)	3 20
2	C	144/179 (80%)	103 (72%)	41 (28%)	0 3
2	D	144/179 (80%)	109 (76%)	35 (24%)	0 4
All	All	1580/1710 (92%)	1316 (83%)	264 (17%)	2 14

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	36	ILE
1	A	40	ILE
1	A	42	PHE
1	A	44	ASP
1	A	45	VAL
1	A	56	SER
1	A	92	SER
1	A	98	LEU
1	A	108	ASN
1	A	126	SER
1	A	134	LEU
1	A	135	SER
1	A	138	VAL
1	A	139	THR
1	A	140	THR

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Mol	Chain	Res	Type
1	A	148	SER
1	A	150	LEU
1	A	166	VAL
1	A	208	SER
1	A	219	SER
1	A	220	ARG
1	A	229	VAL
1	A	231	SER
1	A	235	SER
1	A	238	ILE
1	A	243	ASP
1	A	257	LEU
1	A	258	SER
1	A	263	ARG
1	A	267	THR
1	A	270	GLU
1	A	280	GLN
1	A	288	LEU
1	A	291	LYS
1	A	317	THR
1	A	318	LEU
1	A	319	THR
1	A	329	TYR
1	A	344	SER
1	A	345	LEU
1	A	349	SER
1	A	353	SER
1	A	364	MET
1	A	365	ARG
1	A	367	LEU
1	A	368	LYS
1	A	381	LEU
1	A	385	LEU
1	A	388	LEU
1	A	392	LEU
1	A	413	ASN
1	A	416	ASN
1	A	419	GLN
1	A	429	THR
1	A	436	LEU
1	A	437	SER
1	A	439	CYS

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Mol	Chain	Res	Type
1	A	440	SER
1	A	449	PHE
1	A	451	TYR
1	A	453	SER
1	A	463	LEU
1	A	464	SER
1	A	484	LEU
1	A	499	ASP
1	A	535	LEU
1	A	541	LEU
1	A	544	SER
1	A	556	LEU
1	A	558	ASP
1	A	559	CYS
1	A	561	SER
1	A	562	LEU
1	A	571	LEU
1	A	600	ILE
1	A	610	HIS
1	A	618	PHE
1	A	619	GLN
1	A	623	SER
1	A	625	GLN
1	A	638	THR
1	A	641	VAL
1	A	680	LEU
1	A	689	ASP
1	A	702	ARG
1	A	710	SER
1	A	726	THR
1	A	728	LEU
1	A	729	THR
1	A	737	ASN
1	A	744	GLU
1	A	765	TYR
1	B	34	ARG
1	B	36	ILE
1	B	40	ILE
1	B	42	PHE
1	B	49	LYS
1	B	50	ASN
1	B	56	SER

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Mol	Chain	Res	Type
1	B	92	SER
1	B	98	LEU
1	B	108	ASN
1	B	126	SER
1	B	135	SER
1	B	138	VAL
1	B	139	THR
1	B	140	THR
1	B	148	SER
1	B	150	LEU
1	B	173	ASN
1	B	174	SER
1	B	208	SER
1	B	219	SER
1	B	220	ARG
1	B	229	VAL
1	B	231	SER
1	B	235	SER
1	B	238	ILE
1	B	243	ASP
1	B	257	LEU
1	B	258	SER
1	B	263	ARG
1	B	267	THR
1	B	270	GLU
1	B	280	GLN
1	B	291	LYS
1	B	310	PHE
1	B	316	ASP
1	B	317	THR
1	B	318	LEU
1	B	319	THR
1	B	329	TYR
1	B	344	SER
1	B	345	LEU
1	B	349	SER
1	B	353	SER
1	B	364	MET
1	B	367	LEU
1	B	378	SER
1	B	381	LEU
1	B	385	LEU

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Mol	Chain	Res	Type
1	B	388	LEU
1	B	392	LEU
1	B	413	ASN
1	B	419	GLN
1	B	429	THR
1	B	436	LEU
1	B	437	SER
1	B	440	SER
1	B	449	PHE
1	B	451	TYR
1	B	453	SER
1	B	463	LEU
1	B	464	SER
1	B	475	MET
1	B	484	LEU
1	B	499	ASP
1	B	504	ILE
1	B	535	LEU
1	B	541	LEU
1	B	544	SER
1	B	558	ASP
1	B	559	CYS
1	B	561	SER
1	B	562	LEU
1	B	571	LEU
1	B	618	PHE
1	B	619	GLN
1	B	623	SER
1	B	625	GLN
1	B	638	THR
1	B	640	ARG
1	B	641	VAL
1	B	651	ASP
1	B	680	LEU
1	B	689	ASP
1	B	693	SER
1	B	702	ARG
1	B	705	ASN
1	B	710	SER
1	B	718	ILE
1	B	720	GLN
1	B	726	THR

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Mol	Chain	Res	Type
1	B	728	LEU
1	B	729	THR
1	B	742	ILE
1	B	744	GLU
2	D	32	LEU
2	D	46	LEU
2	D	54	VAL
2	D	55	THR
2	D	58	THR
2	D	63	THR
2	D	74	ASP
2	D	79	ASN
2	D	81	SER
2	D	84	LEU
2	D	85	VAL
2	D	88	LEU
2	D	96	TYR
2	D	97	LEU
2	D	99	LEU
2	D	103	ASN
2	D	105	THR
2	D	111	GLN
2	D	112	LEU
2	D	116	THR
2	D	118	LEU
2	D	120	SER
2	D	125	LEU
2	D	129	SER
2	D	135	THR
2	D	139	LEU
2	D	142	LEU
2	D	149	ASN
2	D	151	SER
2	D	159	SER
2	D	165	THR
2	D	166	LEU
2	D	171	LEU
2	D	181	PRO
2	D	183	ASN
2	C	32	LEU
2	C	46	LEU
2	C	54	VAL

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Mol	Chain	Res	Type
2	C	55	THR
2	C	58	THR
2	C	63	THR
2	C	74	ASP
2	C	79	ASN
2	C	81	SER
2	C	84	LEU
2	C	85	VAL
2	C	88	LEU
2	C	96	TYR
2	C	97	LEU
2	C	99	LEU
2	C	103	ASN
2	C	105	THR
2	C	111	GLN
2	C	112	LEU
2	C	116	THR
2	C	118	LEU
2	C	120	SER
2	C	125	LEU
2	C	129	SER
2	C	135	THR
2	C	139	LEU
2	C	142	LEU
2	C	148	ASN
2	C	149	ASN
2	C	151	SER
2	C	159	SER
2	C	165	THR
2	C	166	LEU
2	C	171	LEU
2	C	174	ASN
2	C	181	PRO
2	C	185	SER
2	C	190	THR
2	C	191	PRO
2	C	192	ILE
2	C	193	SER

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

Mol	Chain	Res	Type
1	A	158	ASN
1	A	619	GLN
1	A	705	ASN
1	A	712	ASN
1	B	37	HIS
1	B	279	ASN
1	B	712	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

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.67	0	17,19,21	1.66	3 (17%)
3	NAG	E	2	3	14,14,15	0.63	0	17,19,21	2.07	7 (41%)
3	NAG	F	1	1,3	14,14,15	0.46	0	17,19,21	1.41	2 (11%)
3	NAG	F	2	3	14,14,15	0.65	0	17,19,21	1.56	3 (17%)
3	NAG	G	1	1,3	14,14,15	0.76	0	17,19,21	1.73	3 (17%)
3	NAG	G	2	3	14,14,15	0.47	0	17,19,21	1.87	3 (17%)
3	NAG	H	1	1,3	14,14,15	0.56	0	17,19,21	1.15	2 (11%)
3	NAG	H	2	3	14,14,15	0.52	0	17,19,21	1.80	3 (17%)

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	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2	NAG	C1-O5-C5	5.96	120.27	112.19
3	H	2	NAG	C1-O5-C5	5.87	120.14	112.19
3	G	1	NAG	O5-C1-C2	-5.20	103.07	111.29
3	E	1	NAG	O5-C1-C2	-5.16	103.14	111.29
3	F	2	NAG	C1-O5-C5	4.60	118.42	112.19
3	F	1	NAG	C1-O5-C5	3.60	117.06	112.19
3	E	2	NAG	C6-C5-C4	-3.32	105.23	113.00
3	E	2	NAG	C4-C3-C2	3.24	115.77	111.02
3	E	2	NAG	C2-N2-C7	-3.19	118.36	122.90
3	E	2	NAG	C1-O5-C5	3.10	116.39	112.19
3	E	1	NAG	C2-N2-C7	-2.95	118.70	122.90
3	G	1	NAG	C1-O5-C5	-2.54	108.74	112.19
3	E	2	NAG	O5-C5-C6	-2.46	103.35	107.20
3	F	2	NAG	O5-C1-C2	-2.40	107.50	111.29
3	H	2	NAG	O5-C5-C4	2.38	116.62	110.83
3	H	1	NAG	C1-O5-C5	2.30	115.31	112.19
3	F	1	NAG	O5-C5-C6	2.28	110.77	107.20
3	E	2	NAG	O7-C7-C8	-2.27	117.84	122.06
3	E	1	NAG	O5-C5-C4	-2.27	105.31	110.83
3	F	2	NAG	O4-C4-C5	2.23	114.83	109.30
3	G	1	NAG	O5-C5-C4	-2.23	105.40	110.83
3	H	2	NAG	C3-C4-C5	2.19	114.14	110.24
3	E	2	NAG	O6-C6-C5	-2.15	103.91	111.29
3	G	2	NAG	C2-N2-C7	-2.14	119.86	122.90
3	G	2	NAG	C6-C5-C4	-2.11	108.07	113.00
3	H	1	NAG	O5-C5-C6	2.10	110.50	107.20

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6

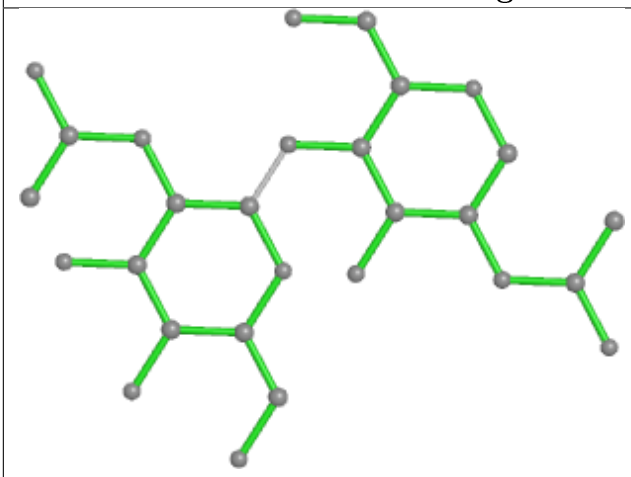
There are no ring outliers.

1 monomer is involved in 1 short contact:

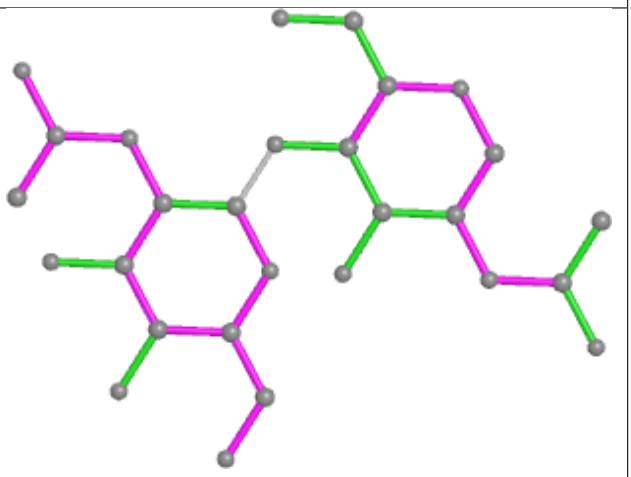
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0

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

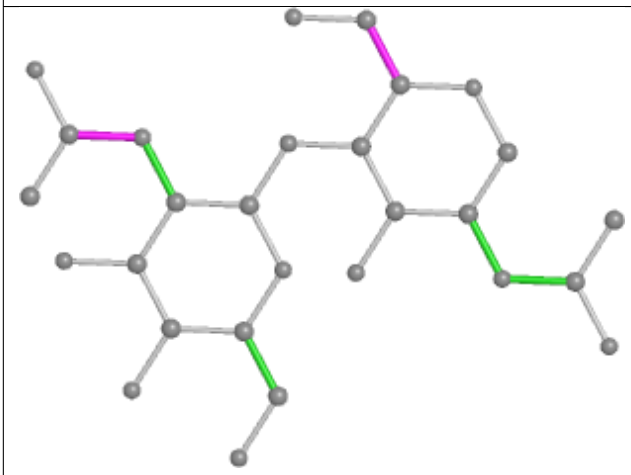
Oligosaccharide Chain E



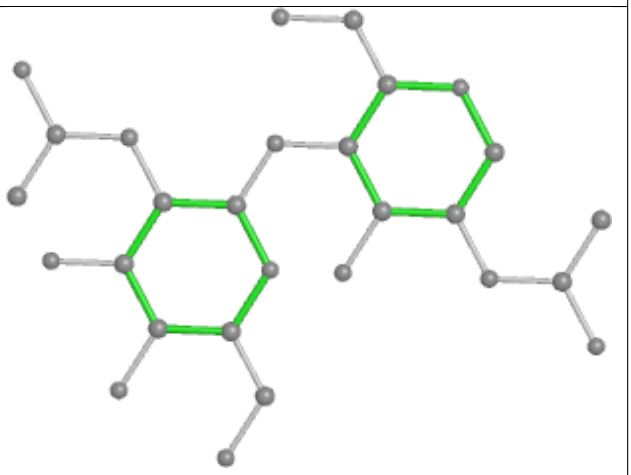
Bond lengths



Bond angles

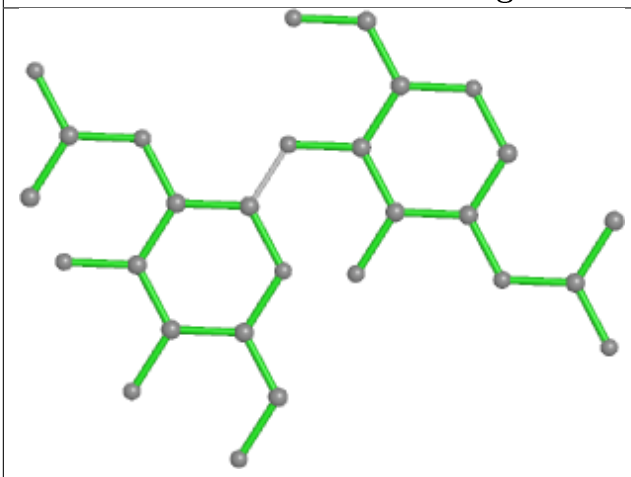


Torsions

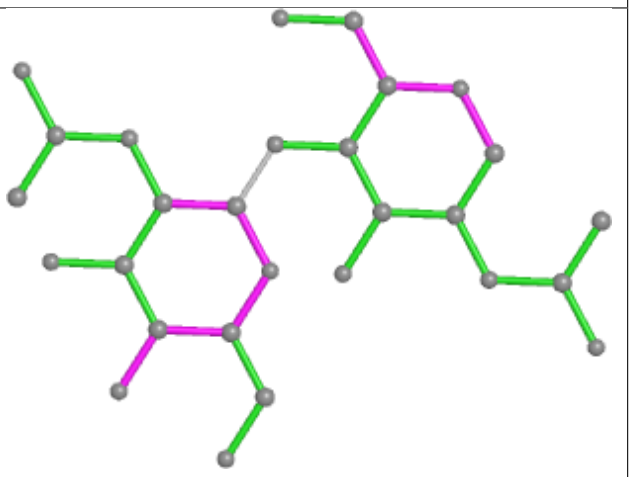


Rings

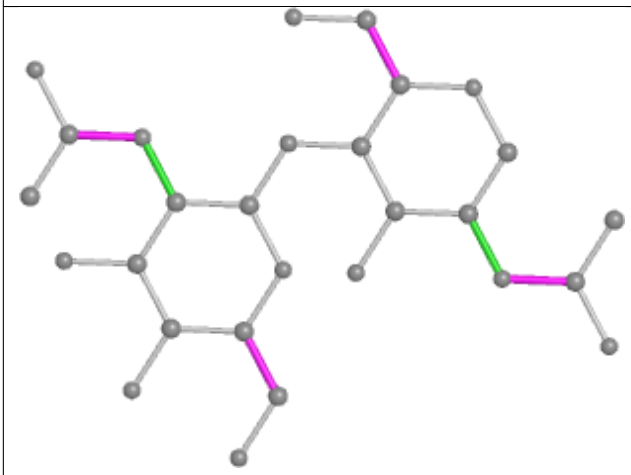
Oligosaccharide Chain F



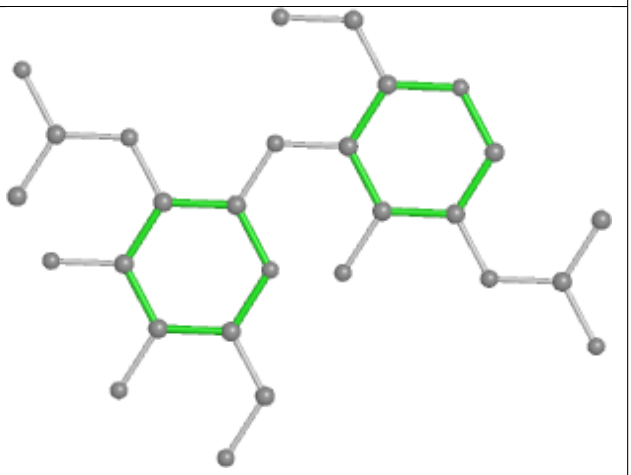
Bond lengths



Bond angles

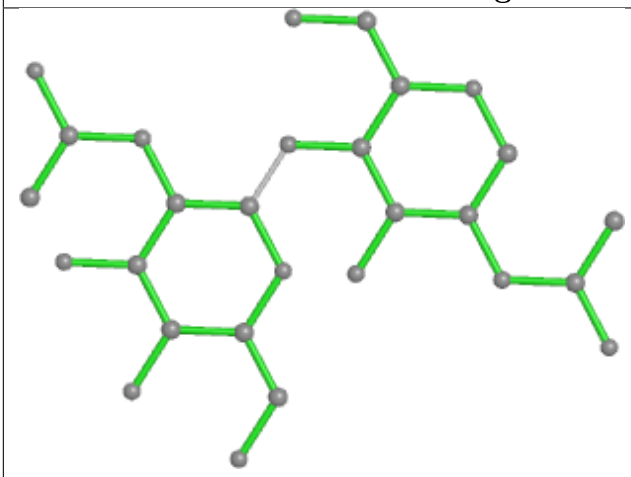


Torsions

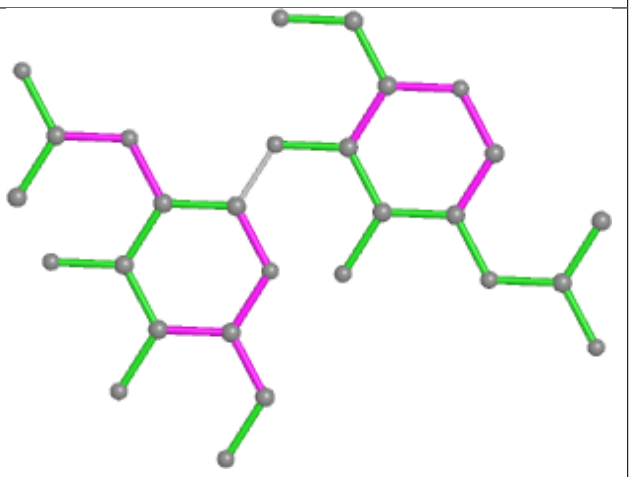


Rings

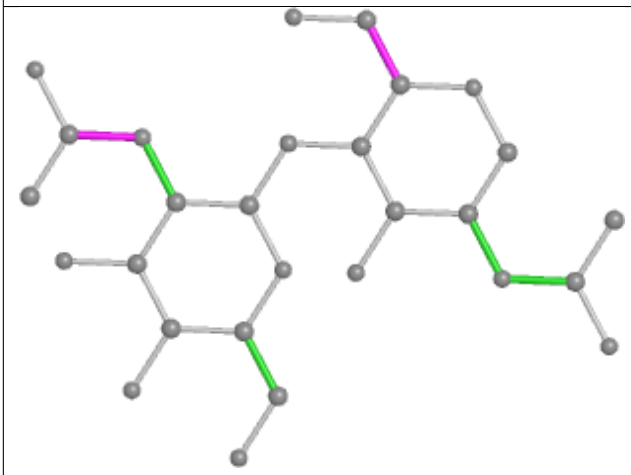
Oligosaccharide Chain G



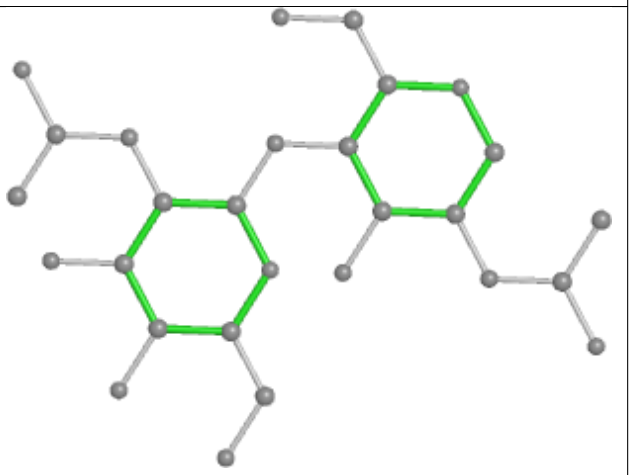
Bond lengths



Bond angles

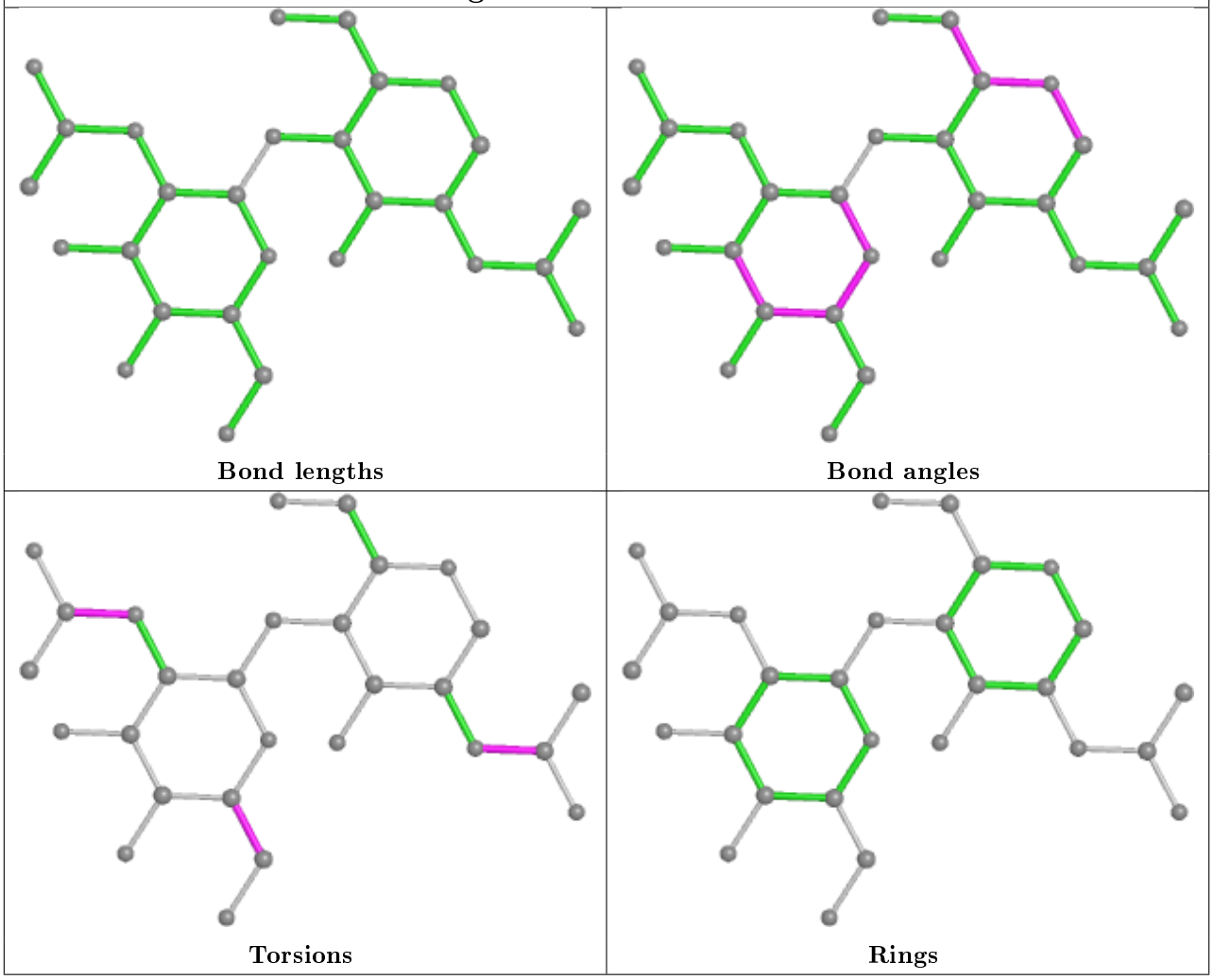


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	806	-	14,14,15	0.89	1 (7%)	17,19,21	1.54	3 (17%)
6	BLD	A	808	-	36,37,37	1.63	2 (5%)	46,59,59	1.99	11 (23%)
5	SO4	A	807	-	4,4,4	0.21	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	805	1	14,14,15	0.66	0	17,19,21	2.27	5 (29%)
5	SO4	B	806	-	4,4,4	0.15	0	6,6,6	0.41	0
6	BLD	B	807	-	36,37,37	1.64	2 (5%)	46,59,59	2.03	14 (30%)
4	NAG	B	805	1	14,14,15	0.45	0	17,19,21	2.49	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	805	1	-	2/6/23/26	0/1/1/1
4	NAG	A	806	-	-	5/6/23/26	0/1/1/1
6	BLD	A	808	-	-	7/20/85/85	0/4/4/4
6	BLD	B	807	-	-	5/20/85/85	0/4/4/4
4	NAG	B	805	1	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	807	BLD	O07-C06	8.65	1.45	1.34
6	A	808	BLD	O07-C06	8.32	1.44	1.34
4	A	806	NAG	O5-C1	-2.37	1.39	1.43
6	A	808	BLD	O07-C07	-2.13	1.42	1.45
6	B	807	BLD	O07-C07	-2.05	1.42	1.45

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	805	NAG	C1-O5-C5	6.70	121.27	112.19
4	B	805	NAG	C3-C4-C5	-5.91	99.70	110.24
6	A	808	BLD	C05-C04-C03	5.87	120.13	111.90
4	A	805	NAG	C2-N2-C7	-5.77	114.68	122.90
6	A	808	BLD	C14-C08-C09	-4.88	102.56	109.09
6	A	808	BLD	C11-C09-C08	-4.88	104.72	111.75
6	B	807	BLD	C01-C02-C03	4.74	116.81	111.36
6	B	807	BLD	C10-C01-C02	4.57	121.59	114.09
6	B	807	BLD	C05-C04-C03	4.45	118.13	111.90
4	A	805	NAG	C1-O5-C5	4.17	117.84	112.19
6	B	807	BLD	C01-C10-C05	4.05	113.51	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	805	NAG	C4-C3-C2	-3.98	105.19	111.02
6	A	808	BLD	C07-O07-C06	-3.98	115.39	121.01
6	B	807	BLD	C11-C09-C08	-3.80	106.28	111.75
4	A	806	NAG	O3-C3-C4	-3.64	101.93	110.35
6	B	807	BLD	C04-C03-C02	3.57	114.69	110.27
6	B	807	BLD	C12-C13-C17	3.24	121.42	116.57
4	A	806	NAG	O4-C4-C5	3.19	117.21	109.30
6	A	808	BLD	C04-C05-C10	3.11	117.08	112.80
6	A	808	BLD	O23-C23-C24	2.78	115.67	109.49
6	B	807	BLD	C04-C05-C10	2.67	116.47	112.80
6	A	808	BLD	O22-C22-C20	2.66	115.40	109.49
6	B	807	BLD	C16-C17-C13	-2.62	100.69	103.84
6	B	807	BLD	C19-C10-C01	-2.59	105.03	108.97
4	A	805	NAG	O5-C1-C2	2.55	115.31	111.29
6	A	808	BLD	C13-C17-C20	-2.52	115.98	118.89
6	A	808	BLD	C01-C10-C05	2.46	110.98	107.06
4	B	805	NAG	O4-C4-C3	2.41	115.91	110.35
4	A	806	NAG	O5-C1-C2	-2.38	107.54	111.29
4	A	805	NAG	C6-C5-C4	-2.34	107.52	113.00
6	B	807	BLD	O22-C22-C20	2.33	114.68	109.49
4	B	805	NAG	O4-C4-C5	2.33	115.09	109.30
6	B	807	BLD	C28-C24-C23	2.26	115.95	111.39
6	A	808	BLD	C16-C15-C14	-2.21	100.76	105.13
6	B	807	BLD	C13-C17-C20	2.11	121.33	118.89
4	B	805	NAG	O5-C5-C6	2.08	110.47	107.20
6	B	807	BLD	O23-C23-C24	2.07	114.09	109.49
6	A	808	BLD	C19-C10-C05	2.06	113.43	109.88

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	808	BLD	C23-C24-C25-C27
6	B	807	BLD	C20-C22-C23-C24
6	B	807	BLD	C23-C24-C25-C27
4	A	805	NAG	C4-C5-C6-O6
4	A	806	NAG	O5-C5-C6-O6
4	A	805	NAG	O5-C5-C6-O6
6	A	808	BLD	O22-C22-C23-O23
6	B	807	BLD	O22-C22-C23-O23
4	A	806	NAG	C4-C5-C6-O6
4	B	805	NAG	C8-C7-N2-C2

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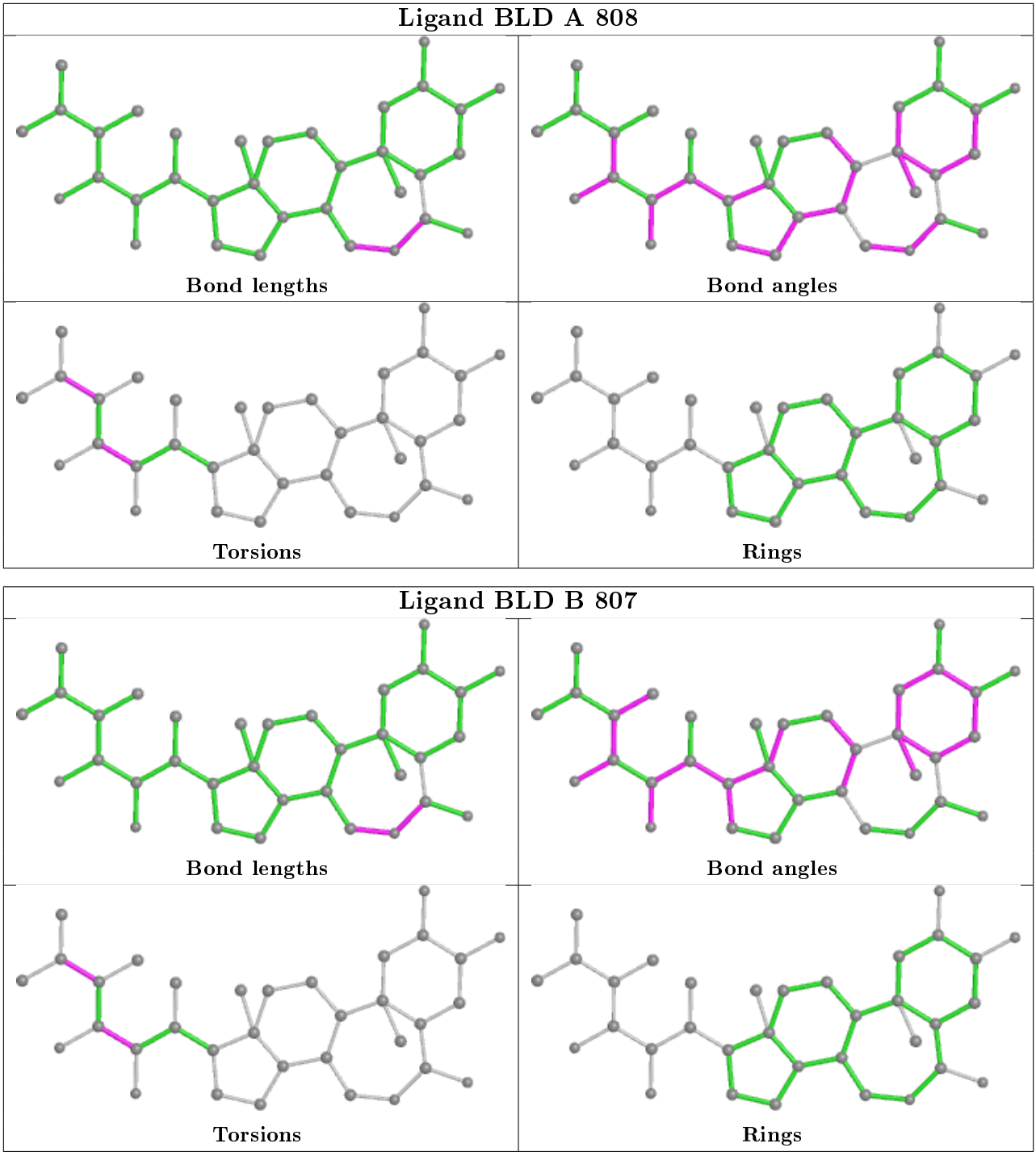
Mol	Chain	Res	Type	Atoms
4	B	805	NAG	O7-C7-N2-C2
4	B	805	NAG	C4-C5-C6-O6
6	B	807	BLD	O22-C22-C23-C24
4	B	805	NAG	O5-C5-C6-O6
6	A	808	BLD	C23-C24-C25-C26
6	A	808	BLD	C20-C22-C23-C24
6	A	808	BLD	C20-C22-C23-O23
6	A	808	BLD	O22-C22-C23-C24
6	B	807	BLD	C20-C22-C23-O23
6	A	808	BLD	C28-C24-C25-C27
4	A	806	NAG	C8-C7-N2-C2
4	A	806	NAG	O7-C7-N2-C2
4	A	806	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	806	NAG	1	0
6	A	808	BLD	8	0
4	A	805	NAG	3	0
6	B	807	BLD	4	0
4	B	805	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	733/767 (95%)	0.35	28 (3%)	40	26	0, 21, 83, 178	0
1	B	734/767 (95%)	0.35	34 (4%)	32	20	0, 28, 94, 199	0
2	C	175/201 (87%)	0.38	11 (6%)	20	11	0, 27, 76, 152	0
2	D	175/201 (87%)	0.37	15 (8%)	10	6	0, 27, 83, 133	0
All	All	1817/1936 (93%)	0.35	88 (4%)	30	19	0, 25, 89, 199	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	75	LEU	4.0
1	A	670	ILE	3.7
2	D	194	PHE	3.7
1	A	694	ILE	3.4
2	C	147	LEU	3.3
1	B	415	LYS	3.3
1	B	30	GLN	3.2
1	B	241	LEU	3.0
1	A	589	ALA	3.0
2	D	136	LEU	3.0
1	A	269	THR	3.0
2	D	147	LEU	3.0
1	B	493	LEU	2.9
1	A	74	VAL	2.9
1	B	74	VAL	2.8
1	B	295	TYR	2.7
1	A	296	LEU	2.7
1	B	756	PHE	2.7
2	D	145	LEU	2.7
1	B	685	LEU	2.6
2	D	88	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	180	LEU	2.6
1	A	274	LEU	2.6
2	D	99	LEU	2.6
1	B	452	LEU	2.5
1	B	743	PRO	2.5
2	D	140	LYS	2.5
2	D	171	LEU	2.5
2	D	75	LEU	2.5
1	B	288	LEU	2.5
2	C	73	VAL	2.5
1	B	755	LYS	2.5
1	A	528	ILE	2.5
2	D	112	LEU	2.4
1	A	276	ILE	2.4
2	D	157	PRO	2.4
1	A	699	GLY	2.4
2	D	73	VAL	2.4
2	C	180	ILE	2.4
1	B	614	ASN	2.4
1	A	313	GLY	2.4
1	B	471	LEU	2.4
1	A	742	ILE	2.4
1	B	55	TRP	2.4
1	A	153	LEU	2.4
1	B	733	LEU	2.3
1	A	674	ILE	2.3
1	A	698	VAL	2.3
2	D	169	LEU	2.3
1	B	528	ILE	2.3
1	B	615	LEU	2.3
2	C	171	LEU	2.3
1	B	469	LEU	2.3
1	A	515	ASN	2.3
1	B	274	LEU	2.3
1	B	731	ILE	2.3
1	A	722	MET	2.2
1	A	563	ILE	2.2
1	B	699	GLY	2.2
2	C	164	LEU	2.2
2	C	194	PHE	2.2
1	B	694	ILE	2.2
1	A	99	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	508	LEU	2.2
1	B	180	LEU	2.1
1	A	649	THR	2.1
1	A	415	LYS	2.1
1	A	616	LEU	2.1
1	B	703	GLY	2.1
1	B	595	LYS	2.1
2	C	88	LEU	2.1
2	C	179	ASP	2.1
1	A	540	ILE	2.1
2	D	160	LEU	2.1
1	B	428	PHE	2.1
2	C	121	LEU	2.1
2	C	132	ILE	2.1
1	B	150	LEU	2.1
1	A	576	ILE	2.0
1	B	670	ILE	2.0
1	A	598	VAL	2.0
1	A	592	ILE	2.0
1	B	563	ILE	2.0
2	D	186	PHE	2.0
1	B	576	ILE	2.0
1	A	355	GLU	2.0
1	B	406	ILE	2.0
1	B	356	LEU	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. 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	B-factors(Å^2)	Q<0.9
3	NAG	E	2	14/15	0.81	0.29	32,44,52,63	0
3	NAG	G	2	14/15	0.88	0.26	53,53,53,53	0
3	NAG	F	2	14/15	0.88	0.27	10,29,35,35	0

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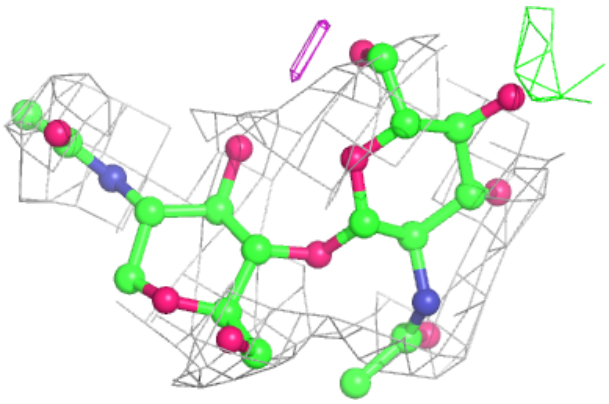
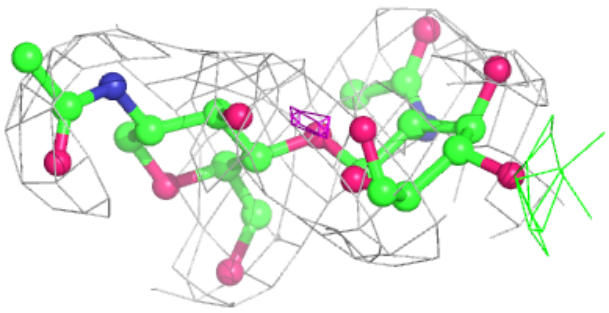
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	F	1	14/15	0.89	0.25	33,33,33,33	0
3	NAG	H	2	14/15	0.90	0.17	39,39,39,39	0
3	NAG	H	1	14/15	0.92	0.21	40,40,40,40	0
3	NAG	G	1	14/15	0.93	0.22	15,17,21,22	0
3	NAG	E	1	14/15	0.94	0.23	8,12,17,22	0

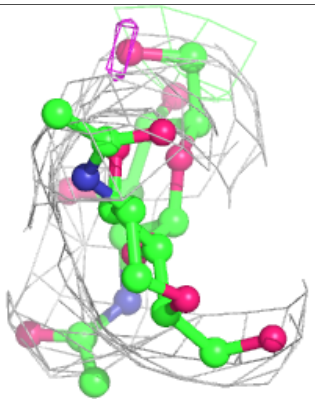
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

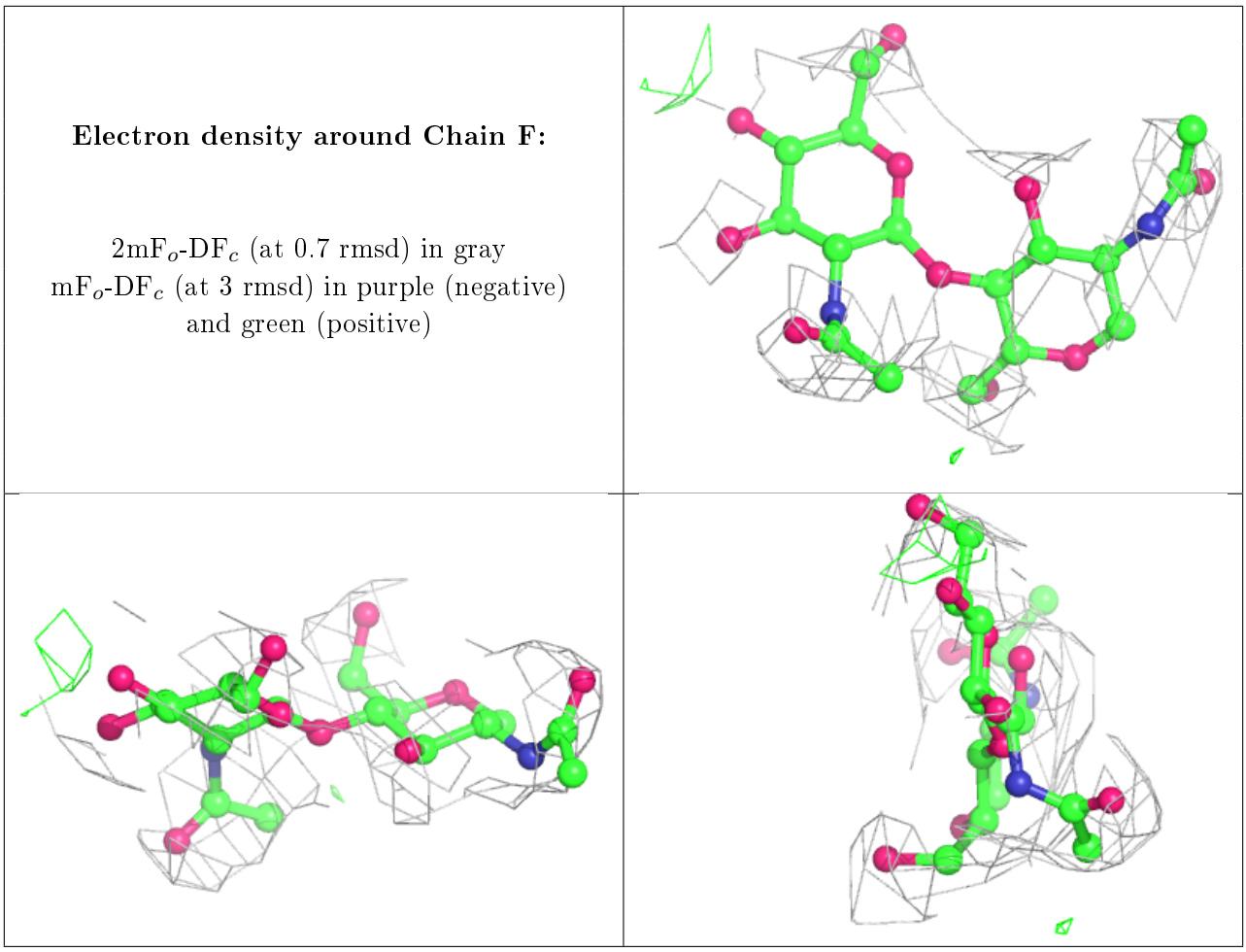






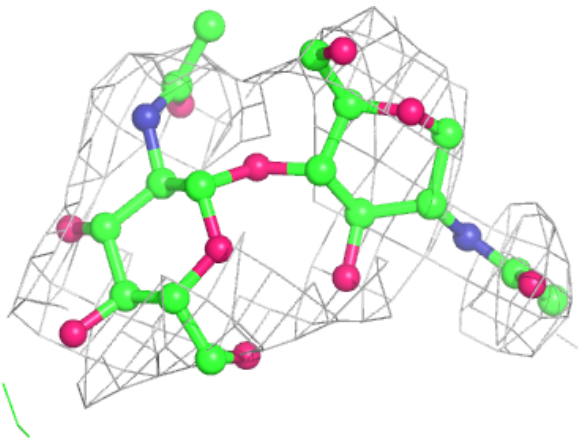
Electron density around Chain F:

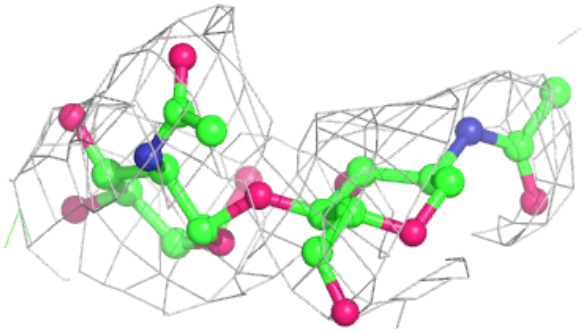
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

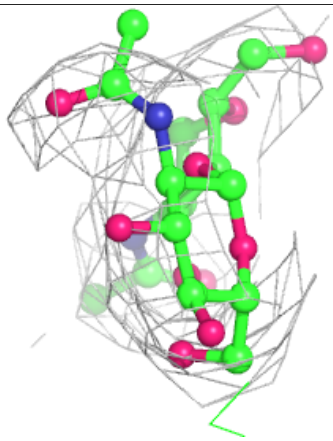


Electron density around Chain G:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

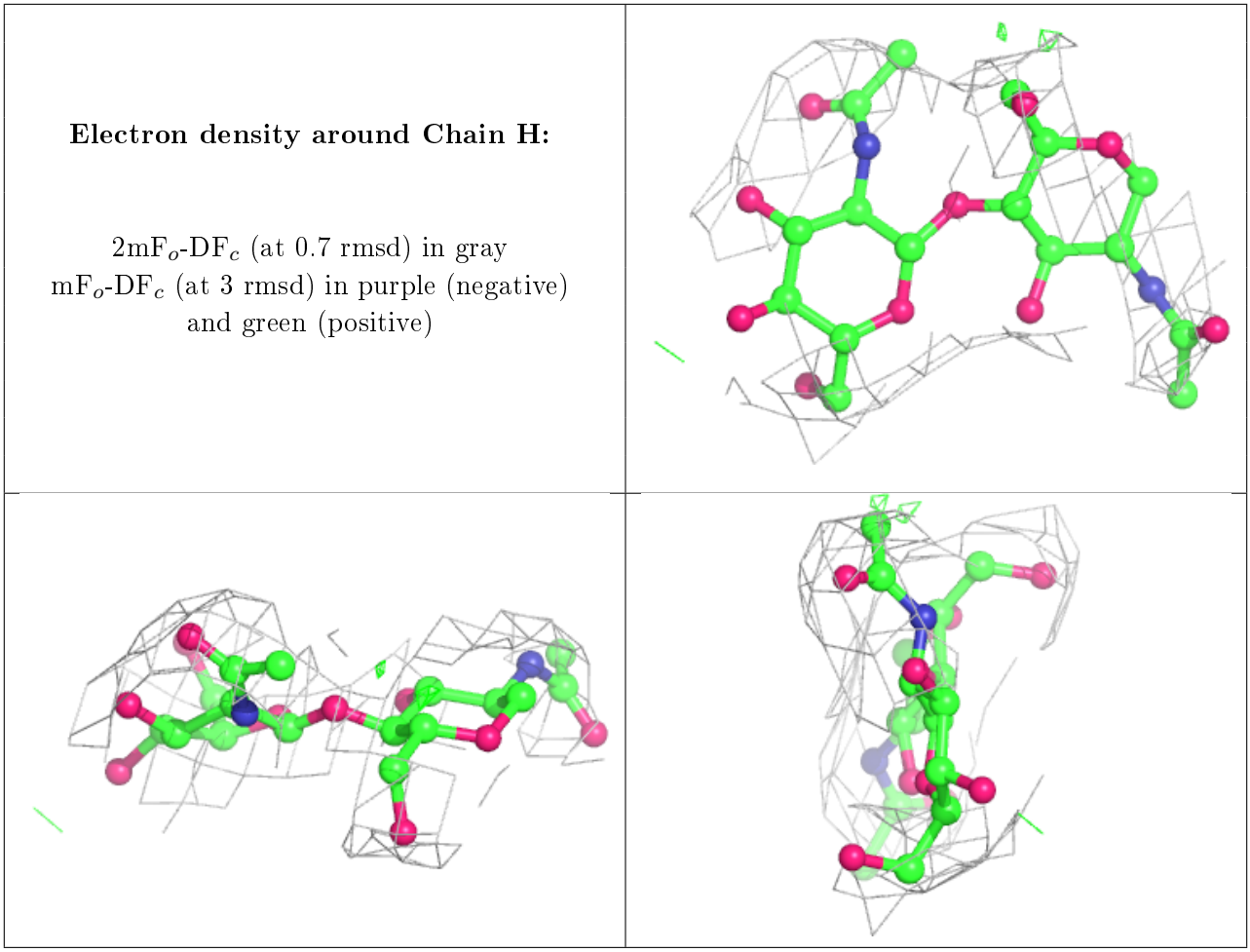






Electron density around Chain H:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



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. 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.

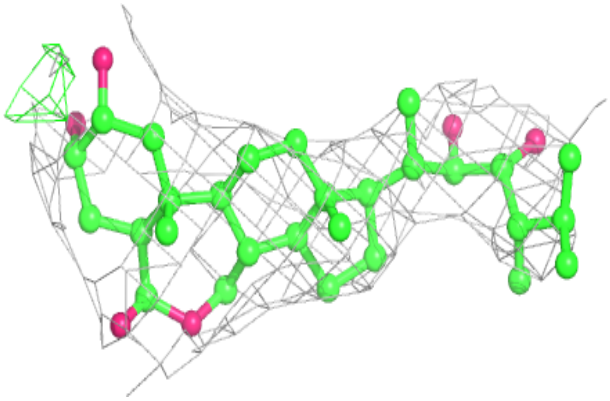
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	B	805	14/15	0.77	0.33	29,29,29,29	0
5	SO4	A	807	5/5	0.83	0.22	64,64,64,64	0
5	SO4	B	806	5/5	0.86	0.21	72,72,72,72	0
4	NAG	A	806	14/15	0.86	0.24	35,35,35,35	0
4	NAG	A	805	14/15	0.90	0.26	46,46,46,46	0
6	BLD	B	807	34/34	0.94	0.47	5,13,22,23	0
6	BLD	A	808	34/34	0.95	0.50	1,7,15,17	0

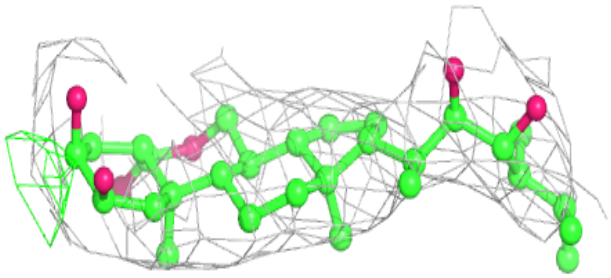
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

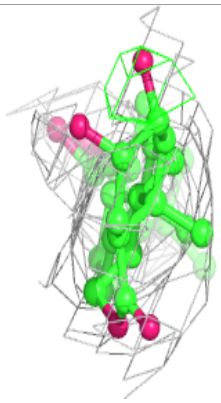
orientation to approximate a three-dimensional view.

Electron density around BLD B 807:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

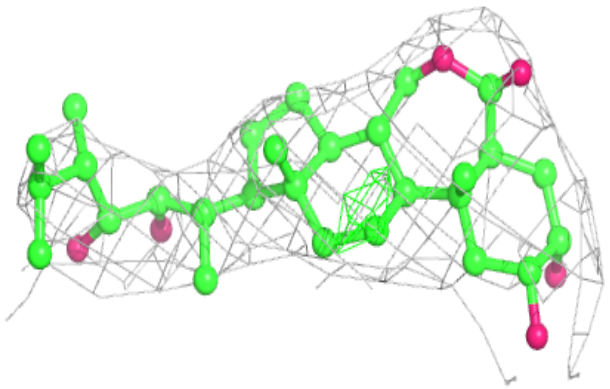


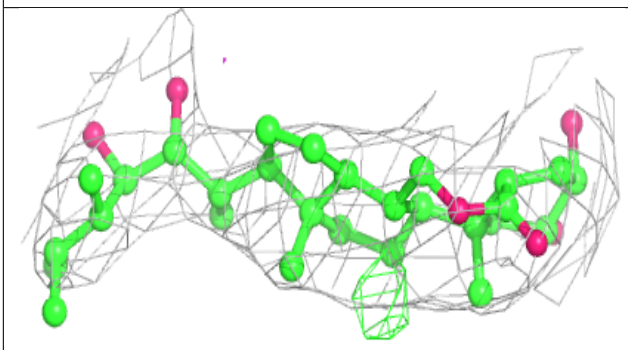


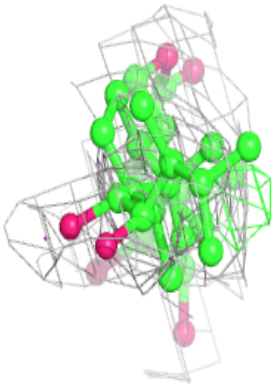


Electron density around BLD A 808:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.