



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 06:04 PM BST

PDB ID : 3MDJ
Title : ER Aminopeptidase, ERAP1, Bound to the Zinc Aminopeptidase Inhibitor, Bestatin
Authors : Nguyen, T.T.; Stern, L.J.
Deposited on : 2010-03-30
Resolution : 2.95 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

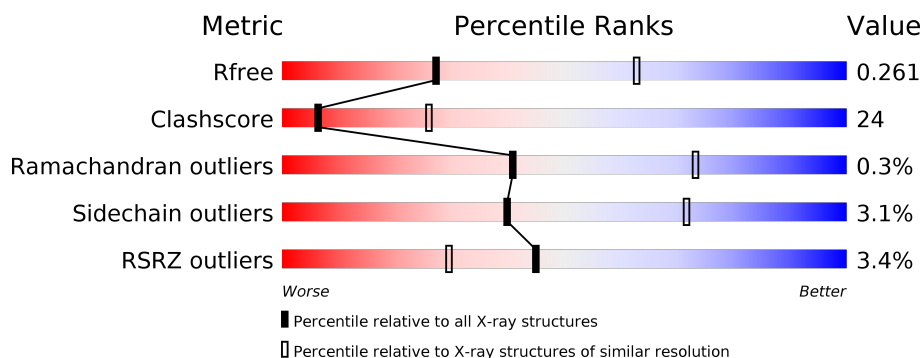
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 $\leq 5\%$. 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	921	<div> <div>2%</div> <div> <div>51%</div> <div>36%</div> <div>11%</div> </div> </div>
1	B	921	<div> <div>4%</div> <div> <div>54%</div> <div>33%</div> <div>11%</div> </div> </div>
1	C	921	<div> <div>3%</div> <div> <div>50%</div> <div>38%</div> <div>11%</div> </div> </div>
2	D	5	<div> <div>20%</div> <div>60%</div> <div>20%</div> </div>
2	F	5	<div> <div>20%</div> <div>40%</div> <div>40%</div> </div>
3	E	2	<div> <div>50%</div> <div>50%</div> </div>

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
2	NAG	F	1	X	-	-	-
5	BES	A	1001	-	-	-	X
5	BES	B	1001	-	-	X	-
6	NAG	A	6001	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20163 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 Endoplasmic reticulum aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	818	Total	C	N	O	S	55	0	0
			6625	4271	1096	1227	31			
1	B	821	Total	C	N	O	S	50	0	0
			6643	4281	1099	1232	31			
1	C	819	Total	C	N	O	S	68	0	0
			6634	4276	1097	1230	31			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	ASP	GLY	SEE REMARK 999	UNP Q9NZ08
A	514	ARG	GLY	SEE REMARK 999	UNP Q9NZ08
A	528	ARG	LYS	SEE REMARK 999	UNP Q9NZ08
A	730	GLU	GLN	SEE REMARK 999	UNP Q9NZ08
A	940	HIS	-	expression tag	UNP Q9NZ08
A	941	ASP	-	expression tag	UNP Q9NZ08
A	942	PRO	-	expression tag	UNP Q9NZ08
A	943	GLU	-	expression tag	UNP Q9NZ08
A	944	ALA	-	expression tag	UNP Q9NZ08
A	945	ASP	-	expression tag	UNP Q9NZ08
A	946	ALA	-	expression tag	UNP Q9NZ08
A	947	THR	-	expression tag	UNP Q9NZ08
A	948	GLY	-	expression tag	UNP Q9NZ08
A	949	LEU	-	expression tag	UNP Q9NZ08
A	950	GLU	-	expression tag	UNP Q9NZ08
A	951	ARG	-	expression tag	UNP Q9NZ08
A	952	MET	-	expression tag	UNP Q9NZ08
A	953	LEU	-	expression tag	UNP Q9NZ08
A	954	GLU	-	expression tag	UNP Q9NZ08
A	955	SER	-	expression tag	UNP Q9NZ08
A	956	ARG	-	expression tag	UNP Q9NZ08
A	957	GLY	-	expression tag	UNP Q9NZ08
B	346	ASP	GLY	SEE REMARK 999	UNP Q9NZ08

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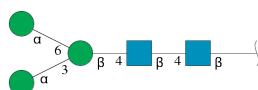
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	ARG	GLY	SEE REMARK 999	UNP Q9NZ08
B	528	ARG	LYS	SEE REMARK 999	UNP Q9NZ08
B	730	GLU	GLN	SEE REMARK 999	UNP Q9NZ08
B	940	HIS	-	expression tag	UNP Q9NZ08
B	941	ASP	-	expression tag	UNP Q9NZ08
B	942	PRO	-	expression tag	UNP Q9NZ08
B	943	GLU	-	expression tag	UNP Q9NZ08
B	944	ALA	-	expression tag	UNP Q9NZ08
B	945	ASP	-	expression tag	UNP Q9NZ08
B	946	ALA	-	expression tag	UNP Q9NZ08
B	947	THR	-	expression tag	UNP Q9NZ08
B	948	GLY	-	expression tag	UNP Q9NZ08
B	949	LEU	-	expression tag	UNP Q9NZ08
B	950	GLU	-	expression tag	UNP Q9NZ08
B	951	ARG	-	expression tag	UNP Q9NZ08
B	952	MET	-	expression tag	UNP Q9NZ08
B	953	LEU	-	expression tag	UNP Q9NZ08
B	954	GLU	-	expression tag	UNP Q9NZ08
B	955	SER	-	expression tag	UNP Q9NZ08
B	956	ARG	-	expression tag	UNP Q9NZ08
B	957	GLY	-	expression tag	UNP Q9NZ08
C	346	ASP	GLY	SEE REMARK 999	UNP Q9NZ08
C	514	ARG	GLY	SEE REMARK 999	UNP Q9NZ08
C	528	ARG	LYS	SEE REMARK 999	UNP Q9NZ08
C	730	GLU	GLN	SEE REMARK 999	UNP Q9NZ08
C	940	HIS	-	expression tag	UNP Q9NZ08
C	941	ASP	-	expression tag	UNP Q9NZ08
C	942	PRO	-	expression tag	UNP Q9NZ08
C	943	GLU	-	expression tag	UNP Q9NZ08
C	944	ALA	-	expression tag	UNP Q9NZ08
C	945	ASP	-	expression tag	UNP Q9NZ08
C	946	ALA	-	expression tag	UNP Q9NZ08
C	947	THR	-	expression tag	UNP Q9NZ08
C	948	GLY	-	expression tag	UNP Q9NZ08
C	949	LEU	-	expression tag	UNP Q9NZ08
C	950	GLU	-	expression tag	UNP Q9NZ08
C	951	ARG	-	expression tag	UNP Q9NZ08
C	952	MET	-	expression tag	UNP Q9NZ08
C	953	LEU	-	expression tag	UNP Q9NZ08
C	954	GLU	-	expression tag	UNP Q9NZ08
C	955	SER	-	expression tag	UNP Q9NZ08
C	956	ARG	-	expression tag	UNP Q9NZ08

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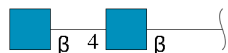
Chain	Residue	Modelled	Actual	Comment	Reference
C	957	GLY	-	expression tag	UNP Q9NZ08

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

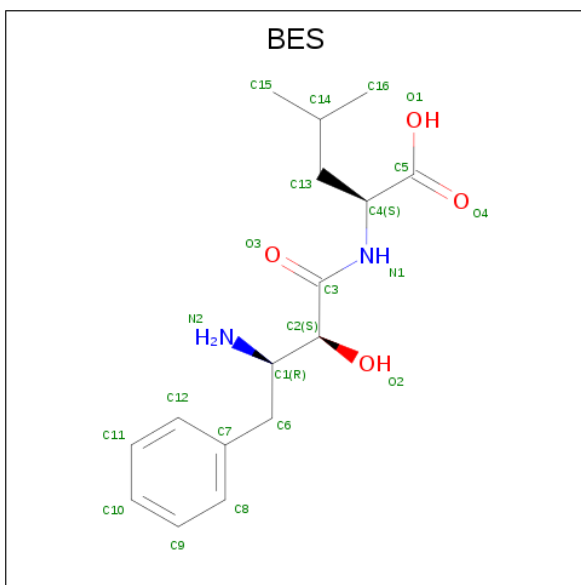


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

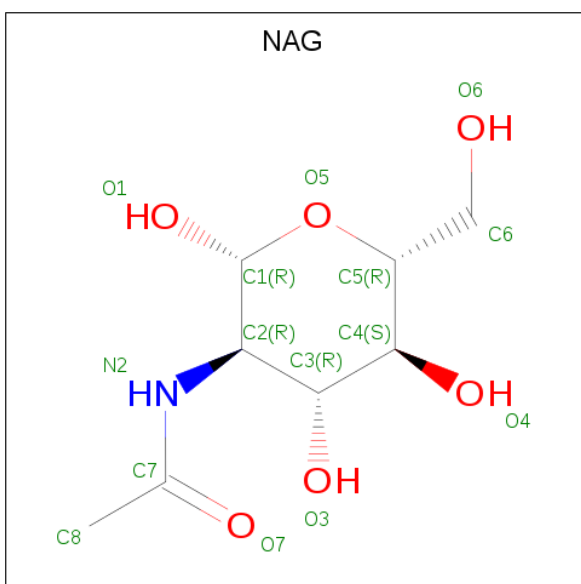
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (three-letter code: BES) (formula: C₁₆H₂₄N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			22	16	2	4		
5	B	1	Total	C	N	O	0	0
			22	16	2	4		
5	C	1	Total	C	N	O	0	0
			22	16	2	4		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

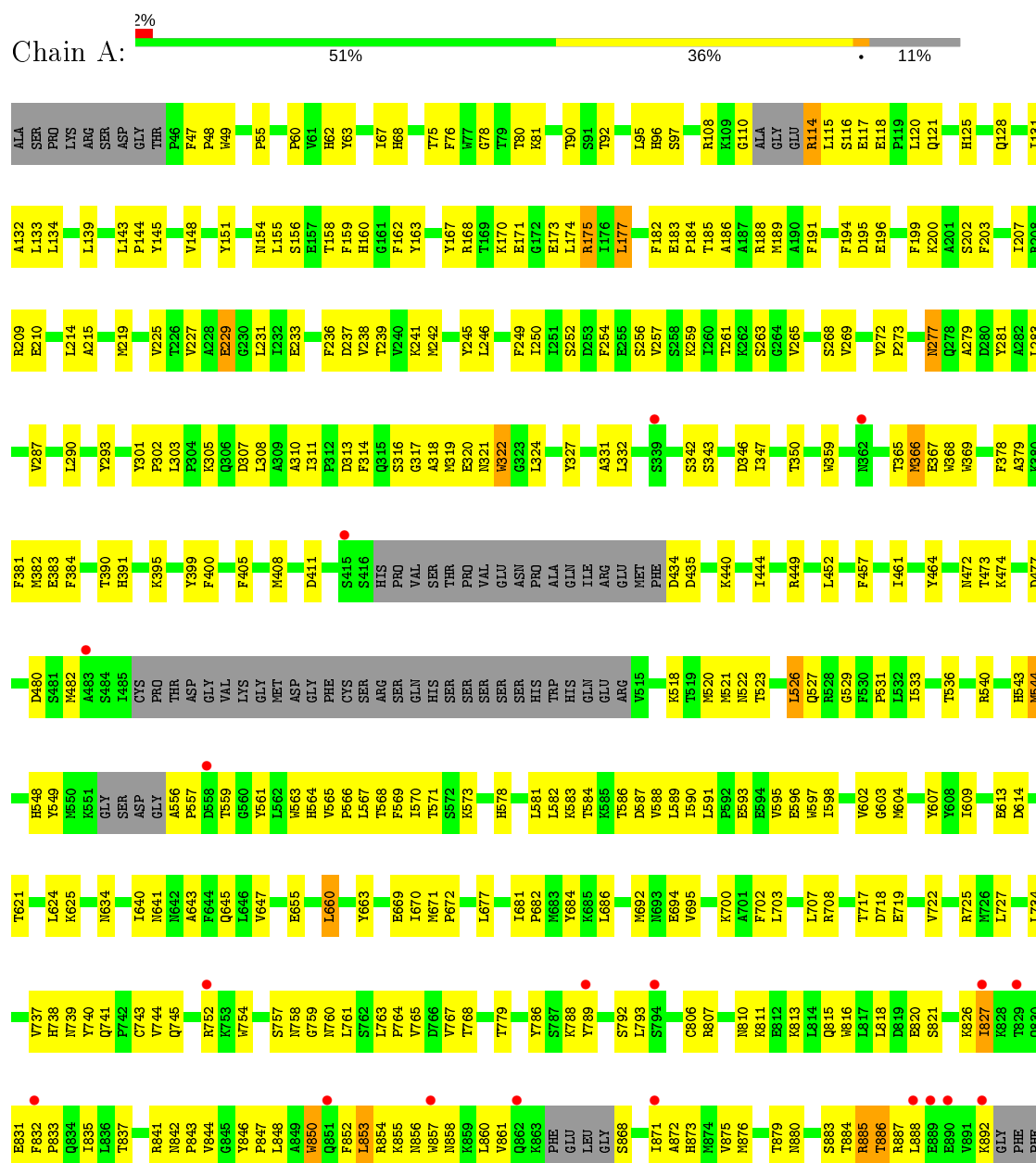


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

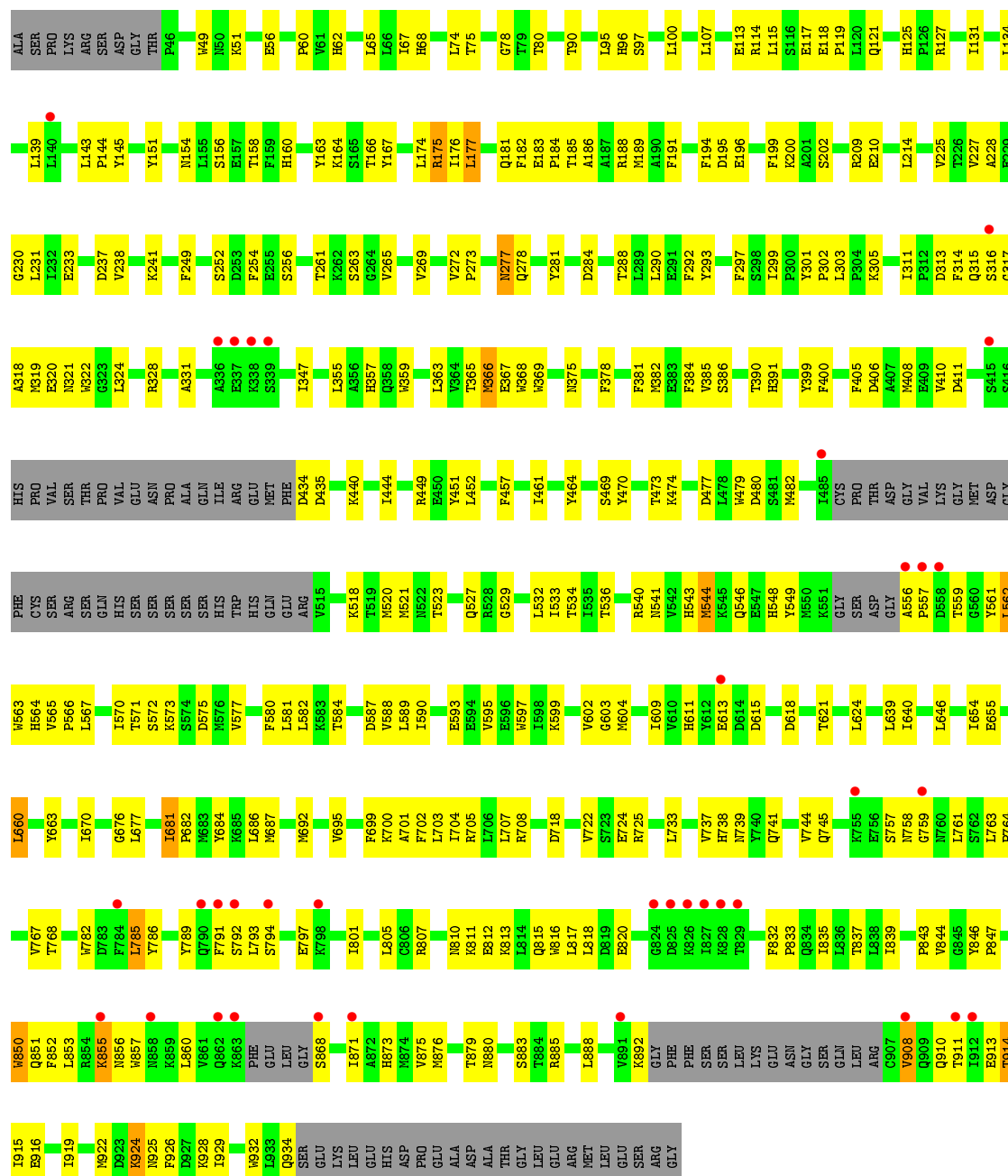
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Endoplasmic reticulum aminopeptidase 1



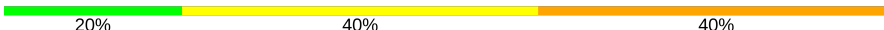


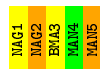
• Molecule 1: Endoplasmic reticulum aminopeptidase 1



WORLDWIDE
PDB
PROTEIN DATA BANK

nose

Chain F: 



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

Chain E: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.03 Å 234.63 Å 95.86 Å 90.00° 103.59° 90.00°	Depositor
Resolution (Å)	38.11 – 2.95 38.11 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.11-2.95) 99.8 (38.11-2.95)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.95 Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.199 , 0.264 0.195 , 0.261	Depositor DCC
R_{free} test set	3208 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20163	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BES, ZN, BMA, NAG, MAN

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	0.27	0/6785	0.45	0/9195
1	B	0.28	0/6804	0.46	0/9222
1	C	0.27	0/6794	0.45	0/9207
All	All	0.27	0/20383	0.45	0/27624

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6625	0	6567	327	0
1	B	6643	0	6582	315	0
1	C	6634	0	6574	322	0
2	D	61	0	52	4	0
2	F	61	0	52	1	0
3	E	28	0	25	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	22	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	22	0	22	10	0
5	C	22	0	23	6	0
6	A	28	0	26	1	0
6	B	14	0	13	0	0
All	All	20163	0	19958	955	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 24.

All (955) 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:640:ILE:HD11	1:C:663:TYR:HE2	1.13	1.12
1:B:113:GLU:O	1:B:117:GLU:HG3	1.49	1.12
1:A:210:GLU:HG3	2:D:1:NAG:H83	1.37	1.07
1:A:875:VAL:HG11	1:A:908:VAL:CG2	1.86	1.04
1:C:319:MET:HE1	5:C:1001:BES:HN21	1.23	1.03
1:C:640:ILE:HD11	1:C:663:TYR:CE2	1.95	1.02
1:B:320:GLU:OE1	5:B:1001:BES:N2	1.93	1.01
1:A:571:THR:HG22	1:A:573:LYS:H	1.21	1.01
1:A:588:VAL:HG11	1:B:241:LYS:HD2	1.42	1.00
1:A:737:VAL:HG13	1:A:807:ARG:HH21	1.24	1.00
1:B:621:THR:HG22	1:B:660:LEU:HG	1.41	0.99
1:C:314:PHE:CE2	1:C:316:SER:HB2	1.97	0.99
1:C:143:LEU:HD12	1:C:144:PRO:HD2	1.43	0.99
1:A:875:VAL:HG11	1:A:908:VAL:HG21	1.41	0.99
1:B:318:ALA:O	5:B:1001:BES:H61	1.63	0.99
1:A:210:GLU:HG3	2:D:1:NAG:C8	1.92	0.99
1:C:621:THR:HG22	1:C:660:LEU:HD13	1.43	0.99
1:C:68:HIS:HE1	1:C:231:LEU:HD21	1.28	0.98
1:C:113:GLU:HG2	1:C:114:ARG:H	1.22	0.98
1:A:143:LEU:HD12	1:A:144:PRO:HD2	1.45	0.97
1:B:143:LEU:HD12	1:B:144:PRO:HD2	1.46	0.96
1:B:314:PHE:CE2	1:B:316:SER:HB2	2.01	0.94
1:B:544:MET:HG3	1:B:582:LEU:HD23	1.50	0.93
1:C:227:VAL:HG21	1:C:233:GLU:HB2	1.50	0.93
1:B:261:THR:HG22	1:B:265:VAL:H	1.32	0.92
1:A:533:ILE:HD13	1:A:567:LEU:HD21	1.51	0.92
1:B:737:VAL:HG13	1:B:807:ARG:HH21	1.31	0.91
1:B:549:TYR:CE1	1:B:609:ILE:HD11	2.06	0.91
1:C:108:ARG:HG2	1:C:117:GLU:HG2	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLN:HB3	1:B:134:LEU:HB2	1.57	0.87
1:B:856:ASN:O	1:B:860:LEU:HB2	1.74	0.87
1:A:60:PRO:HG3	1:A:194:PHE:CD2	2.11	0.86
1:A:737:VAL:HG13	1:A:807:ARG:NH2	1.90	0.86
1:B:763:LEU:HG	1:B:768:THR:HG22	1.59	0.84
1:A:621:THR:HG22	1:A:660:LEU:HG	1.60	0.84
1:B:185:THR:HG23	1:B:188:ARG:CZ	2.07	0.83
1:C:810:ASN:HD22	1:C:813:LYS:HD3	1.44	0.83
1:A:227:VAL:HG21	1:A:233:GLU:HB2	1.59	0.83
1:B:316:SER:HB3	5:B:1001:BES:H8	1.62	0.82
1:A:314:PHE:CE2	1:A:316:SER:HB2	2.14	0.82
1:B:182:PHE:HA	1:B:186:ALA:HB3	1.58	0.82
1:C:544:MET:SD	1:C:582:LEU:HD23	2.19	0.82
1:C:182:PHE:HA	1:C:186:ALA:HB3	1.62	0.81
1:A:96:HIS:HD2	1:A:195:ASP:H	1.27	0.81
1:C:314:PHE:HE2	1:C:316:SER:HB2	1.44	0.81
1:A:121:GLN:HB3	1:A:134:LEU:HB2	1.62	0.80
1:A:381:PHE:HZ	1:A:449:ARG:HD2	1.46	0.80
1:A:763:LEU:HG	1:A:768:THR:HG22	1.63	0.80
1:A:872:ALA:O	1:A:875:VAL:HG12	1.81	0.80
1:C:621:THR:HG22	1:C:660:LEU:CD1	2.10	0.80
1:A:182:PHE:HA	1:A:186:ALA:HB3	1.64	0.80
1:C:570:ILE:HG23	1:C:602:VAL:HG21	1.64	0.80
1:C:60:PRO:HG3	1:C:194:PHE:CD2	2.16	0.79
1:B:473:THR:HG23	1:B:477:ASP:HB2	1.64	0.79
1:B:875:VAL:CG1	1:B:908:VAL:HG11	2.12	0.79
1:A:473:THR:HG23	1:A:477:ASP:HB2	1.64	0.79
1:A:681:ILE:HA	1:A:684:TYR:CE2	2.17	0.78
1:C:875:VAL:CG1	1:C:908:VAL:HG11	2.12	0.78
1:C:113:GLU:HG2	1:C:114:ARG:N	1.97	0.78
1:B:621:THR:HG22	1:B:660:LEU:CG	2.13	0.78
1:A:80:THR:HG23	1:A:151:TYR:HE1	1.47	0.78
1:B:536:THR:OG1	1:B:613:GLU:HG3	1.84	0.77
1:C:261:THR:HG23	1:C:263:SER:H	1.48	0.77
1:C:473:THR:HG23	1:C:477:ASP:HB2	1.65	0.77
1:A:350:THR:HA	5:A:1001:BES:H162	1.66	0.77
1:B:883:SER:HB2	1:B:922:MET:HG3	1.67	0.77
1:A:90:THR:HG22	1:A:92:THR:H	1.50	0.77
1:C:571:THR:HG22	1:C:573:LYS:H	1.50	0.77
1:A:75:THR:HG22	1:A:154:ASN:OD1	1.85	0.76
1:B:261:THR:HG23	1:B:263:SER:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:SER:H	1:C:317:GLY:HA2	1.49	0.76
1:B:227:VAL:HG21	1:B:233:GLU:HB2	1.66	0.76
1:B:319:MET:SD	1:B:320:GLU:OE1	2.44	0.76
1:A:156:SER:OG	1:A:158:THR:HG22	1.85	0.76
1:A:549:TYR:CE1	1:A:609:ILE:HD11	2.21	0.76
1:C:856:ASN:O	1:C:860:LEU:HB2	1.86	0.76
1:A:875:VAL:HG11	1:A:908:VAL:HG22	1.67	0.75
1:B:588:VAL:HG11	1:C:241:LYS:HD2	1.67	0.75
1:A:888:LEU:HD21	1:A:915:ILE:HG21	1.68	0.75
1:A:816:TRP:O	1:A:820:GLU:HG2	1.86	0.75
1:B:185:THR:O	1:B:185:THR:HG22	1.86	0.75
1:C:319:MET:CE	5:C:1001:BES:HN21	1.98	0.75
1:C:261:THR:HG22	1:C:265:VAL:H	1.50	0.75
1:A:571:THR:HG22	1:A:573:LYS:N	1.98	0.75
1:A:559:THR:HG22	1:A:561:TYR:H	1.50	0.75
1:C:185:THR:O	1:C:185:THR:HG22	1.86	0.74
1:A:185:THR:HG23	1:A:188:ARG:CZ	2.17	0.74
1:B:670:ILE:HD11	1:B:724:GLU:HG3	1.68	0.74
1:C:581:LEU:CD1	1:C:583:LYS:HG3	2.18	0.74
1:B:786:TYR:O	1:B:789:TYR:HB3	1.88	0.73
1:B:908:VAL:O	1:B:908:VAL:HG12	1.87	0.73
1:A:202:SER:OG	1:A:238:VAL:HG12	1.89	0.73
1:C:811:LYS:HE2	1:C:844:VAL:CG1	2.19	0.73
1:B:96:HIS:HD2	1:B:195:ASP:H	1.34	0.73
1:A:183:GLU:HB2	1:A:319:MET:HE1	1.71	0.73
1:C:322:TRP:CE2	1:C:362:ASN:HB3	2.23	0.72
1:A:856:ASN:O	1:A:860:LEU:HB2	1.88	0.72
1:B:571:THR:HG22	1:B:573:LYS:H	1.54	0.72
1:B:113:GLU:O	1:B:117:GLU:CG	2.35	0.72
1:C:68:HIS:CE1	1:C:231:LEU:HD21	2.20	0.72
1:C:908:VAL:O	1:C:908:VAL:HG12	1.88	0.72
1:A:810:ASN:ND2	1:A:813:LYS:HE2	2.04	0.72
1:B:60:PRO:HG3	1:B:194:PHE:CD2	2.25	0.72
1:C:166:THR:HG22	1:C:176:ILE:HD13	1.72	0.72
1:A:581:LEU:CD1	1:A:583:LYS:HG3	2.20	0.71
1:C:640:ILE:CD1	1:C:663:TYR:HE2	1.98	0.71
1:A:319:MET:SD	1:A:320:GLU:OE1	2.48	0.71
1:A:588:VAL:HG12	1:A:589:LEU:N	2.04	0.71
1:C:875:VAL:HG11	1:C:908:VAL:HG11	1.72	0.71
1:A:367:GLU:OE1	1:A:474:LYS:HE3	1.90	0.70
1:B:580:PHE:HZ	1:B:587:ASP:OD2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:VAL:HG13	1:B:807:ARG:NH2	2.06	0.70
1:B:156:SER:OG	1:B:158:THR:HG22	1.91	0.70
1:C:681:ILE:HB	1:C:682:PRO:HD3	1.73	0.70
1:A:261:THR:HG22	1:A:265:VAL:H	1.56	0.70
1:A:759:GLY:HA3	1:A:788:LYS:HE3	1.74	0.70
1:A:185:THR:HG22	1:A:185:THR:O	1.91	0.70
1:A:67:ILE:HD11	1:A:207:ILE:HD12	1.74	0.70
1:A:571:THR:CG2	1:A:573:LYS:H	2.01	0.69
1:A:888:LEU:HD21	1:A:915:ILE:CG2	2.22	0.69
1:C:185:THR:HG23	1:C:188:ARG:CZ	2.21	0.69
1:A:588:VAL:HG11	1:B:241:LYS:CD	2.21	0.69
1:C:540:ARG:HD2	1:C:591:LEU:O	1.92	0.69
1:B:549:TYR:CD1	1:B:609:ILE:HD11	2.27	0.68
1:C:228:ALA:HB3	1:C:231:LEU:HB2	1.75	0.68
1:A:681:ILE:HB	1:A:682:PRO:HD3	1.74	0.68
1:B:390:THR:HG22	1:B:391:HIS:CD2	2.28	0.68
1:B:399:TYR:OH	1:B:722:VAL:HB	1.92	0.68
1:B:595:VAL:HG12	1:B:597:TRP:H	1.58	0.68
1:C:96:HIS:HD2	1:C:195:ASP:H	1.41	0.68
1:A:570:ILE:HG23	1:A:602:VAL:HG21	1.75	0.68
1:C:533:ILE:HD13	1:C:567:LEU:HD21	1.74	0.68
1:C:319:MET:HE1	5:C:1001:BES:N2	2.05	0.68
1:C:316:SER:N	1:C:317:GLY:HA2	2.08	0.68
1:A:200:LYS:HB2	1:A:241:LYS:HE2	1.75	0.67
1:B:381:PHE:HZ	1:B:449:ARG:HD2	1.58	0.67
1:C:852:PHE:CZ	1:C:856:ASN:ND2	2.61	0.67
1:B:49:TRP:CH2	1:B:51:LYS:HD2	2.29	0.67
1:C:571:THR:HG22	1:C:573:LYS:N	2.10	0.67
1:B:533:ILE:CD1	1:B:567:LEU:HD21	2.25	0.67
1:C:759:GLY:HA3	1:C:788:LYS:HE3	1.76	0.66
1:C:692:MET:SD	1:C:926:PHE:HZ	2.18	0.66
1:B:321:ASN:HB2	1:B:324:LEU:O	1.96	0.66
1:B:763:LEU:CG	1:B:768:THR:HG22	2.24	0.66
1:A:318:ALA:O	5:A:1001:BES:H61	1.95	0.66
1:A:760:ASN:OD1	6:A:6001:NAG:O5	2.13	0.66
1:A:321:ASN:HB2	1:A:324:LEU:O	1.96	0.66
1:A:908:VAL:O	1:A:908:VAL:HG12	1.94	0.66
1:C:546:GLN:HE21	1:C:582:LEU:HD12	1.61	0.66
1:B:464:TYR:OH	1:B:473:THR:HG21	1.96	0.65
1:B:588:VAL:HG12	1:B:589:LEU:N	2.10	0.65
1:B:677:LEU:HD21	1:B:707:LEU:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:763:LEU:HD12	1:B:764:PRO:HD2	1.78	0.65
1:B:875:VAL:HG12	1:B:908:VAL:HG11	1.77	0.65
1:A:200:LYS:CE	1:A:365:THR:HG22	2.26	0.65
1:B:559:THR:HG22	1:B:561:TYR:H	1.62	0.65
1:C:671:MET:HB3	1:C:672:PRO:HD3	1.77	0.65
1:A:571:THR:HG23	1:A:595:VAL:HG11	1.78	0.65
1:C:113:GLU:CG	1:C:114:ARG:H	2.05	0.65
1:A:621:THR:HG22	1:A:660:LEU:CG	2.26	0.65
1:A:540:ARG:HD2	1:A:591:LEU:O	1.96	0.65
1:A:763:LEU:CG	1:A:768:THR:HG22	2.27	0.65
1:A:832:PHE:N	1:A:833:PRO:HD2	2.12	0.65
1:B:261:THR:HG22	1:B:265:VAL:N	2.07	0.65
1:B:183:GLU:HB3	1:B:319:MET:HE3	1.78	0.65
1:B:80:THR:HG21	1:B:191:PHE:HB2	1.79	0.64
1:A:390:THR:HG22	1:A:391:HIS:CD2	2.33	0.64
1:A:80:THR:HG21	1:A:191:PHE:HB2	1.80	0.64
1:A:916:GLU:HA	1:A:919:ILE:HD12	1.80	0.64
1:C:121:GLN:HB3	1:C:134:LEU:HB2	1.78	0.64
1:C:156:SER:OG	1:C:158:THR:HG22	1.97	0.64
1:A:139:LEU:HD22	1:A:145:TYR:CE1	2.33	0.64
1:A:81:LYS:HG2	1:A:148:VAL:HG13	1.79	0.64
1:A:883:SER:HB2	1:A:922:MET:HG3	1.80	0.64
1:A:533:ILE:CD1	1:A:567:LEU:HD21	2.27	0.64
1:B:316:SER:N	1:B:317:GLY:HA2	2.11	0.64
1:B:700:LYS:HD3	1:B:738:HIS:HD2	1.62	0.64
1:B:737:VAL:CG1	1:B:807:ARG:HH21	2.06	0.64
1:C:384:PHE:CE2	1:C:400:PHE:HD1	2.15	0.64
1:A:259:LYS:HD3	1:A:287:VAL:HG21	1.80	0.64
1:A:316:SER:N	1:A:317:GLY:HA2	2.11	0.64
1:B:181:GLN:HE22	1:B:319:MET:CE	2.11	0.64
1:B:677:LEU:O	1:B:681:ILE:HG13	1.98	0.64
1:A:700:LYS:HD3	1:A:738:HIS:HD2	1.63	0.64
1:C:764:PRO:O	1:C:768:THR:HG23	1.98	0.63
1:A:108:ARG:HG2	1:A:117:GLU:HG3	1.79	0.63
1:B:167:TYR:CE1	1:B:175:ARG:HB2	2.34	0.63
1:C:581:LEU:HD12	1:C:583:LYS:HG3	1.80	0.63
1:B:832:PHE:N	1:B:833:PRO:HD2	2.13	0.63
1:C:737:VAL:HG11	1:C:807:ARG:NH2	2.13	0.63
1:A:544:MET:HG3	1:A:582:LEU:HD23	1.81	0.63
1:B:114:ARG:HA	1:B:117:GLU:HG3	1.81	0.63
1:C:319:MET:SD	1:C:320:GLU:OE1	2.56	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:837:THR:HG21	1:C:873:HIS:NE2	2.14	0.63
1:B:114:ARG:HA	1:B:117:GLU:CD	2.19	0.63
1:C:700:LYS:HD3	1:C:738:HIS:CD2	2.34	0.63
1:C:97:SER:CB	1:C:131:ILE:HD11	2.28	0.63
1:A:200:LYS:HB3	1:A:241:LYS:HG2	1.81	0.63
1:C:875:VAL:HG12	1:C:908:VAL:HG11	1.81	0.63
1:B:875:VAL:HG11	1:B:908:VAL:HG11	1.78	0.63
1:A:671:MET:HB3	1:A:672:PRO:HD3	1.80	0.62
1:B:261:THR:CG2	1:B:265:VAL:H	2.10	0.62
1:A:96:HIS:CD2	1:A:195:ASP:H	2.15	0.62
1:A:677:LEU:HD21	1:A:707:LEU:HD11	1.81	0.62
1:B:640:ILE:HD11	1:B:676:GLY:HA2	1.81	0.62
1:C:700:LYS:HD3	1:C:738:HIS:HD2	1.64	0.62
1:C:57:TYR:CE1	1:C:90:THR:HG21	2.34	0.62
1:C:75:THR:HG22	1:C:154:ASN:OD1	1.99	0.62
1:B:764:PRO:O	1:B:768:THR:HG23	1.98	0.62
1:B:541:ASN:OD1	1:C:241:LYS:HG3	1.99	0.62
1:C:67:ILE:HD13	1:C:249:PHE:CZ	2.34	0.62
1:A:316:SER:H	1:A:317:GLY:HA2	1.65	0.62
1:C:810:ASN:ND2	1:C:813:LYS:HD3	2.13	0.62
1:A:911:THR:O	1:A:915:ILE:HG13	1.99	0.62
1:A:700:LYS:HD3	1:A:738:HIS:CD2	2.35	0.61
1:B:540:ARG:HD3	1:B:593:GLU:HA	1.82	0.61
1:B:314:PHE:HE2	1:B:316:SER:HB2	1.62	0.61
1:C:68:HIS:HE1	1:C:231:LEU:CD2	2.10	0.61
1:A:117:GLU:O	1:A:118:GLU:HG2	1.99	0.61
1:A:522:ASN:HB3	1:A:526:LEU:HD22	1.82	0.61
1:C:692:MET:SD	1:C:926:PHE:CZ	2.93	0.61
1:A:764:PRO:O	1:A:768:THR:HG23	1.99	0.61
1:B:534:THR:HG21	1:B:613:GLU:OE2	2.00	0.61
1:A:670:ILE:HD13	1:A:727:LEU:HD22	1.82	0.61
1:B:565:VAL:CG1	1:B:582:LEU:HB3	2.30	0.61
1:A:97:SER:CB	1:A:131:ILE:HD11	2.30	0.61
1:A:549:TYR:CD1	1:A:609:ILE:HD11	2.36	0.61
1:B:139:LEU:HD22	1:B:145:TYR:CE1	2.35	0.61
1:B:888:LEU:HD11	1:B:919:ILE:CD1	2.31	0.61
1:A:96:HIS:HD2	1:A:195:ASP:N	1.96	0.61
1:B:543:HIS:CD2	1:B:588:VAL:HG22	2.36	0.61
1:C:318:ALA:O	5:C:1001:BES:H2	2.00	0.61
1:A:185:THR:HG23	1:A:188:ARG:NH2	2.16	0.60
1:A:464:TYR:OH	1:A:473:THR:HG21	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:THR:HG23	1:B:263:SER:N	2.16	0.60
1:A:581:LEU:HD12	1:A:583:LYS:HG3	1.81	0.60
1:A:115:LEU:HD12	1:A:116:SER:H	1.67	0.60
1:C:564:HIS:CD2	1:C:583:LYS:HG2	2.37	0.60
1:C:684:TYR:CD1	1:C:700:LYS:HE2	2.36	0.60
1:C:711:ILE:HD13	1:C:735:ALA:HB2	1.83	0.60
1:B:480:ASP:OD1	1:B:518:LYS:HE2	2.01	0.60
1:C:754:TRP:NE1	1:C:759:GLY:HA2	2.16	0.60
1:A:810:ASN:HD22	1:A:813:LYS:HE2	1.67	0.60
1:B:700:LYS:HD3	1:B:738:HIS:CD2	2.35	0.60
1:C:200:LYS:CE	1:C:365:THR:HG22	2.32	0.60
1:B:757:SER:N	1:B:758:ASN:HA	2.17	0.60
1:A:595:VAL:HG12	1:A:597:TRP:H	1.66	0.60
1:B:114:ARG:HA	1:B:117:GLU:CG	2.32	0.60
1:C:334:PHE:CE1	1:C:338:LYS:HB3	2.37	0.60
1:A:875:VAL:CG2	1:A:908:VAL:HG11	2.31	0.60
1:B:527:GLN:OE1	1:B:563:TRP:NE1	2.34	0.60
1:B:67:ILE:HD13	1:B:249:PHE:CZ	2.36	0.60
1:B:367:GLU:OE1	1:B:474:LYS:HE3	2.01	0.60
1:B:571:THR:HG23	1:B:595:VAL:HG11	1.84	0.60
1:B:757:SER:HB3	1:B:759:GLY:N	2.16	0.59
1:C:183:GLU:HB3	1:C:319:MET:HE3	1.82	0.59
1:A:703:LEU:HD21	1:A:734:LEU:HD21	1.84	0.59
1:B:544:MET:HG3	1:B:582:LEU:CD2	2.27	0.59
1:C:559:THR:CG2	1:C:561:TYR:H	2.15	0.59
1:A:757:SER:N	1:A:758:ASN:HA	2.17	0.59
1:B:316:SER:HB3	5:B:1001:BES:C8	2.31	0.59
1:B:546:GLN:HE21	1:B:582:LEU:HD12	1.67	0.59
1:A:531:PRO:HB3	1:A:563:TRP:CE3	2.38	0.59
1:A:588:VAL:HG12	1:A:589:LEU:H	1.67	0.59
1:C:883:SER:HB2	1:C:922:MET:HG3	1.84	0.59
1:B:363:LEU:HD11	1:B:469:SER:HB2	1.85	0.59
1:B:384:PHE:CE1	1:B:400:PHE:HB2	2.37	0.59
1:B:660:LEU:O	1:B:663:TYR:HD2	1.86	0.59
1:C:832:PHE:N	1:C:833:PRO:HD2	2.18	0.59
1:A:293:TYR:HE2	1:A:382:MET:HG3	1.67	0.59
1:A:660:LEU:O	1:A:663:TYR:HD2	1.85	0.59
1:B:807:ARG:HH12	1:B:843:PRO:HD2	1.68	0.59
1:B:166:THR:HG22	1:B:176:ILE:HD13	1.84	0.59
1:B:565:VAL:HG12	1:B:582:LEU:HB3	1.85	0.59
1:A:155:LEU:HG	1:A:162:PHE:CE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:GLN:HE21	1:A:745:GLN:NE2	2.00	0.58
1:C:754:TRP:CG	1:C:763:LEU:HD11	2.38	0.58
1:A:225:VAL:O	1:A:227:VAL:HG23	2.04	0.58
1:B:741:GLN:HE21	1:B:745:GLN:NE2	2.00	0.58
1:B:115:LEU:HD22	1:B:115:LEU:N	2.18	0.58
1:B:319:MET:SD	1:B:320:GLU:CD	2.81	0.58
1:B:692:MET:SD	1:B:926:PHE:CZ	2.96	0.58
1:A:571:THR:HG23	1:A:595:VAL:CG1	2.34	0.58
1:B:80:THR:HG23	1:B:151:TYR:HE1	1.68	0.58
1:B:313:ASP:O	1:B:315:GLN:HG2	2.04	0.58
1:B:807:ARG:NH1	1:B:843:PRO:HD2	2.19	0.58
1:A:523:THR:O	1:A:527:GLN:HB2	2.03	0.58
1:B:78:GLY:HA3	1:B:151:TYR:CZ	2.38	0.58
1:C:795:SER:OG	1:C:797:GLU:HB3	2.03	0.58
1:A:655:GLU:HB2	1:A:932:TRP:HD1	1.69	0.58
1:B:816:TRP:O	1:B:820:GLU:HG2	2.03	0.58
1:A:261:THR:HG22	1:A:265:VAL:N	2.19	0.58
1:B:237:ASP:OD1	1:B:238:VAL:N	2.37	0.58
1:C:520:MET:SD	1:C:566:PRO:HG3	2.44	0.58
1:B:741:GLN:HE21	1:B:745:GLN:HE21	1.50	0.58
1:C:321:ASN:HB2	1:C:324:LEU:O	2.03	0.58
1:C:588:VAL:HG12	1:C:589:LEU:N	2.19	0.58
1:B:559:THR:CG2	1:B:561:TYR:H	2.17	0.57
1:C:381:PHE:HZ	1:C:449:ARG:HD2	1.69	0.57
1:C:384:PHE:CE1	1:C:400:PHE:HB2	2.39	0.57
1:C:457:PHE:CE2	1:C:461:ILE:HD11	2.39	0.57
1:C:846:TYR:CG	1:C:847:PRO:HD3	2.39	0.57
1:A:643:ALA:O	1:A:647:VAL:HG23	2.05	0.57
1:B:284:ASP:O	1:B:288:THR:HG23	2.04	0.57
1:A:559:THR:CG2	1:A:561:TYR:H	2.16	0.57
1:A:588:VAL:CG1	1:A:589:LEU:N	2.66	0.57
1:B:846:TYR:N	1:B:847:PRO:CD	2.67	0.57
1:C:816:TRP:O	1:C:820:GLU:HG2	2.04	0.57
1:C:89:PRO:O	1:C:90:THR:HG23	2.04	0.57
1:B:451:TYR:HD2	1:B:452:LEU:HD12	1.69	0.57
1:C:850:TRP:O	1:C:854:ARG:HG3	2.05	0.57
1:B:852:PHE:CZ	1:B:856:ASN:ND2	2.72	0.57
1:C:660:LEU:O	1:C:663:TYR:HD2	1.87	0.57
1:C:464:TYR:OH	1:C:473:THR:HG21	2.05	0.57
1:A:68:HIS:HE1	1:A:231:LEU:HD21	1.70	0.57
1:A:717:THR:OG1	1:A:719:GLU:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:TYR:O	1:A:789:TYR:HB3	2.05	0.57
1:B:615:ASP:HB2	1:B:618:ASP:HB2	1.85	0.57
1:B:681:ILE:HB	1:B:682:PRO:HD3	1.86	0.57
1:A:261:THR:HG23	1:A:263:SER:H	1.70	0.56
1:A:237:ASP:OD1	1:A:238:VAL:N	2.37	0.56
1:A:588:VAL:CG1	1:A:589:LEU:H	2.17	0.56
1:A:739:ASN:HA	1:A:744:VAL:HG21	1.87	0.56
1:B:523:THR:O	1:B:563:TRP:CD1	2.58	0.56
1:C:733:LEU:O	1:C:737:VAL:HG23	2.05	0.56
1:B:139:LEU:HD22	1:B:145:TYR:HE1	1.70	0.56
1:C:261:THR:HG22	1:C:265:VAL:N	2.19	0.56
1:C:408:MET:HG2	1:C:530:PHE:CE2	2.40	0.56
1:A:327:TYR:HE1	1:A:350:THR:HG22	1.70	0.56
1:B:572:SER:OG	1:B:595:VAL:HG13	2.06	0.56
1:A:200:LYS:HB2	1:A:241:LYS:CE	2.35	0.56
1:A:708:ARG:HG2	1:A:708:ARG:HH11	1.70	0.56
1:B:319:MET:CE	5:B:1001:BES:HN21	2.19	0.56
1:B:810:ASN:CB	1:B:813:LYS:HD2	2.35	0.56
1:A:741:GLN:HE21	1:A:745:GLN:HE21	1.52	0.56
1:A:754:TRP:NE1	1:A:759:GLY:HA2	2.20	0.56
1:B:621:THR:CG2	1:B:660:LEU:HG	2.25	0.56
1:C:156:SER:HB3	1:C:163:TYR:HB3	1.88	0.56
1:C:80:THR:HG21	1:C:191:PHE:HB2	1.86	0.56
1:C:559:THR:HG22	1:C:561:TYR:H	1.71	0.56
1:C:699:PHE:O	1:C:703:LEU:HD13	2.05	0.56
1:B:293:TYR:HE2	1:B:382:MET:HG3	1.70	0.56
1:C:757:SER:N	1:C:758:ASN:HA	2.21	0.56
1:C:757:SER:HB3	1:C:759:GLY:N	2.20	0.56
1:A:272:VAL:HG13	1:A:273:PRO:HD2	1.86	0.56
1:B:281:TYR:CD2	1:B:347:ILE:HD11	2.40	0.56
1:B:876:MET:O	1:B:880:ASN:HB2	2.05	0.56
1:C:281:TYR:CD2	1:C:347:ILE:HD11	2.41	0.56
1:B:913:GLU:O	1:B:916:GLU:HB3	2.06	0.56
1:A:540:ARG:HD3	1:A:593:GLU:HA	1.87	0.55
1:B:791:PHE:H	1:B:791:PHE:HD2	1.54	0.55
1:A:183:GLU:HB2	1:A:319:MET:CE	2.36	0.55
1:A:564:HIS:CD2	1:A:583:LYS:HG2	2.40	0.55
1:A:621:THR:O	1:A:625:LYS:HG3	2.06	0.55
1:B:49:TRP:CZ2	1:B:51:LYS:HD2	2.40	0.55
1:B:785:LEU:HD22	1:B:801:ILE:HG23	1.88	0.55
1:C:542:VAL:HB	1:C:589:LEU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:ILE:HG23	1:A:684:TYR:CZ	2.41	0.55
1:B:281:TYR:HD2	1:B:347:ILE:HD11	1.72	0.55
1:C:230:GLY:C	1:C:231:LEU:HD12	2.26	0.55
1:C:293:TYR:HE2	1:C:382:MET:HG3	1.70	0.55
1:C:383:GLU:O	1:C:387:VAL:HG23	2.06	0.55
1:C:544:MET:HG3	1:C:582:LEU:CD2	2.36	0.55
1:A:853:LEU:O	1:A:857:TRP:HB2	2.06	0.55
1:B:692:MET:SD	1:B:926:PHE:HZ	2.28	0.55
1:C:535:ILE:HG13	1:C:600:PHE:CD1	2.41	0.55
1:A:621:THR:CG2	1:A:660:LEU:HG	2.35	0.55
1:A:837:THR:HG21	1:A:873:HIS:NE2	2.21	0.55
1:B:62:HIS:HE1	1:B:238:VAL:HG13	1.71	0.55
1:C:811:LYS:HE2	1:C:844:VAL:HG13	1.88	0.55
1:C:549:TYR:HE1	1:C:649:ILE:HD13	1.70	0.55
1:B:457:PHE:CD1	1:B:482:MET:HE3	2.42	0.55
1:B:807:ARG:HH12	1:B:843:PRO:CD	2.19	0.55
1:C:97:SER:HB3	1:C:131:ILE:HD11	1.87	0.55
1:C:533:ILE:CD1	1:C:567:LEU:HD21	2.36	0.55
1:B:797:GLU:O	1:B:801:ILE:HG13	2.07	0.55
1:C:699:PHE:CE2	1:C:703:LEU:HD11	2.42	0.55
1:A:757:SER:HB3	1:A:759:GLY:N	2.22	0.55
1:A:927:ASP:O	1:A:931:VAL:HG23	2.07	0.55
1:C:741:GLN:HB3	1:C:742:PRO:HD3	1.89	0.55
1:A:327:TYR:CE1	1:A:350:THR:HG22	2.40	0.54
1:B:185:THR:O	1:B:185:THR:CG2	2.54	0.54
1:C:524:TRP:CZ2	1:C:565:VAL:HG22	2.43	0.54
1:C:846:TYR:CD2	1:C:847:PRO:HD3	2.42	0.54
1:B:911:THR:O	1:B:915:ILE:HG13	2.08	0.54
1:C:803:PHE:O	1:C:807:ARG:HG2	2.07	0.54
1:B:520:MET:SD	1:B:566:PRO:HG3	2.48	0.54
1:B:97:SER:CB	1:B:131:ILE:HD11	2.36	0.54
1:C:219:MET:HE2	1:C:239:THR:HA	1.90	0.54
1:C:546:GLN:HE21	1:C:582:LEU:CD1	2.20	0.54
1:B:812:GLU:O	1:B:816:TRP:HB2	2.08	0.54
1:B:533:ILE:HD12	1:B:567:LEU:HD21	1.89	0.54
1:B:811:LYS:HE2	1:B:844:VAL:CG1	2.38	0.54
1:C:707:LEU:O	1:C:711:ILE:HG13	2.07	0.54
1:A:876:MET:O	1:A:880:ASN:HB2	2.07	0.54
1:B:793:LEU:HG	1:B:794:SER:OG	2.07	0.54
1:C:310:ALA:HB2	1:C:332:LEU:HD23	1.90	0.54
1:A:449:ARG:O	1:A:452:LEU:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:THR:HG22	1:C:391:HIS:CD2	2.42	0.54
1:A:590:ILE:HG13	1:B:470:TYR:CG	2.42	0.53
1:B:640:ILE:HD11	1:B:676:GLY:CA	2.38	0.53
1:C:803:PHE:CE2	1:C:807:ARG:HG3	2.43	0.53
1:A:167:TYR:CE1	1:A:175:ARG:HB2	2.42	0.53
1:A:806:CYS:SG	1:A:835:ILE:HG23	2.49	0.53
1:A:868:SER:HA	1:A:871:ILE:HG12	1.90	0.53
1:B:588:VAL:CG1	1:B:589:LEU:N	2.71	0.53
1:A:67:ILE:HD11	1:A:207:ILE:CD1	2.37	0.53
1:A:399:TYR:OH	1:A:722:VAL:HB	2.07	0.53
1:B:183:GLU:OE1	1:B:320:GLU:OE2	2.26	0.53
1:B:96:HIS:HD2	1:B:195:ASP:N	2.03	0.53
1:A:185:THR:CG2	1:A:188:ARG:CZ	2.85	0.53
1:A:76:PHE:HD1	1:A:155:LEU:HD12	1.73	0.53
1:C:322:TRP:CE2	1:C:362:ASN:CB	2.91	0.53
1:C:399:TYR:OH	1:C:722:VAL:HB	2.07	0.53
1:A:888:LEU:CD2	1:A:915:ILE:HG21	2.38	0.53
1:B:853:LEU:O	1:B:857:TRP:HB2	2.08	0.53
1:C:444:ILE:HG22	1:C:521:MET:HE1	1.89	0.53
1:B:115:LEU:H	1:B:115:LEU:CD2	2.22	0.53
1:B:115:LEU:CD2	1:B:115:LEU:N	2.71	0.53
1:B:156:SER:HB3	1:B:163:TYR:HB3	1.90	0.53
1:C:611:HIS:CE1	1:C:617:TRP:HE1	2.27	0.53
1:B:580:PHE:CZ	1:B:587:ASP:OD2	2.59	0.53
1:C:185:THR:O	1:C:185:THR:CG2	2.56	0.53
1:C:225:VAL:O	1:C:227:VAL:HG23	2.08	0.53
1:C:571:THR:CG2	1:C:573:LYS:H	2.19	0.53
1:B:181:GLN:HE22	1:B:319:MET:HE3	1.73	0.53
1:B:916:GLU:HA	1:B:919:ILE:HD12	1.90	0.53
1:C:786:TYR:O	1:C:789:TYR:HB3	2.09	0.53
1:A:281:TYR:CD2	1:A:347:ILE:HD11	2.44	0.53
1:A:540:ARG:NH2	1:B:302:PRO:O	2.42	0.53
1:C:139:LEU:HD22	1:C:145:TYR:CE1	2.44	0.53
1:A:763:LEU:HD12	1:A:764:PRO:HD2	1.90	0.52
1:B:96:HIS:CD2	1:B:195:ASP:H	2.20	0.52
1:C:81:LYS:HG2	1:C:148:VAL:HG13	1.91	0.52
1:B:571:THR:HG22	1:B:573:LYS:N	2.22	0.52
1:B:910:GLN:O	1:B:914:THR:HG22	2.09	0.52
1:C:343:SER:O	1:C:347:ILE:HG23	2.09	0.52
1:A:365:THR:O	1:A:472:ASN:HA	2.08	0.52
1:A:63:TYR:CD1	1:A:203:PHE:CE1	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:TYR:CE2	1:B:272:VAL:HG13	2.45	0.52
1:B:582:LEU:CD1	1:B:584:THR:O	2.57	0.52
1:C:888:LEU:HD21	1:C:915:ILE:CG2	2.40	0.52
1:B:230:GLY:C	1:B:231:LEU:HD12	2.30	0.52
1:C:261:THR:HG23	1:C:263:SER:N	2.21	0.52
1:C:621:THR:CG2	1:C:660:LEU:HD13	2.29	0.52
1:C:810:ASN:HD22	1:C:813:LYS:CD	2.20	0.52
1:C:836:LEU:HD22	1:C:874:MET:HE3	1.91	0.52
1:C:449:ARG:O	1:C:452:LEU:O	2.27	0.52
1:C:440:LYS:O	1:C:444:ILE:HG12	2.09	0.52
1:B:185:THR:HG23	1:B:188:ARG:NH2	2.24	0.52
1:C:313:ASP:O	1:C:315:GLN:HG2	2.08	0.52
1:C:717:THR:OG1	1:C:719:GLU:HG2	2.10	0.52
1:A:120:LEU:HD13	1:A:133:LEU:HB3	1.92	0.52
1:B:75:THR:HG22	1:B:154:ASN:OD1	2.10	0.52
1:C:60:PRO:HG3	1:C:194:PHE:CG	2.44	0.52
1:C:327:TYR:CD2	1:C:332:LEU:HD22	2.45	0.52
1:C:117:GLU:O	1:C:118:GLU:HG3	2.08	0.51
1:C:200:LYS:HE3	1:C:365:THR:HG22	1.92	0.51
1:C:214:LEU:HD23	1:C:252:SER:O	2.10	0.51
1:C:684:TYR:HB3	1:C:699:PHE:CD2	2.45	0.51
1:C:286:ALA:O	1:C:290:LEU:HG	2.10	0.51
1:C:259:LYS:HD3	1:C:287:VAL:HG21	1.92	0.51
1:A:405:PHE:CZ	1:A:604:MET:SD	3.03	0.51
1:A:582:LEU:CD1	1:A:584:THR:O	2.58	0.51
1:B:183:GLU:HB3	1:B:319:MET:CE	2.40	0.51
1:B:615:ASP:HB2	1:B:618:ASP:CG	2.31	0.51
1:B:68:HIS:HE1	1:B:231:LEU:HD21	1.75	0.51
1:A:110:GLY:HA3	1:A:114:ARG:O	2.11	0.51
1:A:655:GLU:HB2	1:A:932:TRP:CD1	2.45	0.51
1:B:532:LEU:HD11	1:B:646:LEU:HD21	1.92	0.51
1:C:237:ASP:OD1	1:C:238:VAL:N	2.43	0.51
1:B:888:LEU:HD11	1:B:919:ILE:HD11	1.93	0.51
1:C:571:THR:HG22	1:C:574:SER:H	1.75	0.51
1:C:621:THR:O	1:C:625:LYS:HG3	2.10	0.51
1:A:97:SER:HB2	1:A:131:ILE:HD11	1.91	0.51
1:A:308:LEU:N	1:A:308:LEU:HD12	2.26	0.51
1:C:670:ILE:HD13	1:C:727:LEU:HD22	1.92	0.51
1:A:170:LYS:HG3	1:A:171:GLU:OE2	2.10	0.51
1:A:565:VAL:HG12	1:A:582:LEU:HB3	1.93	0.51
1:C:322:TRP:CD2	1:C:362:ASN:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:595:VAL:HG12	1:C:597:TRP:H	1.76	0.51
1:C:367:GLU:OE1	1:C:474:LYS:HE3	2.10	0.51
1:A:408:MET:HE1	1:A:609:ILE:HG23	1.92	0.50
1:A:533:ILE:HD11	1:A:565:VAL:HG11	1.93	0.50
1:A:761:LEU:HD12	1:A:761:LEU:O	2.10	0.50
1:C:694:GLU:O	1:C:698:GLN:HG3	2.11	0.50
1:A:473:THR:CG2	1:A:474:LYS:N	2.74	0.50
1:A:844:VAL:HG12	1:A:844:VAL:O	2.10	0.50
1:B:536:THR:HB	1:B:543:HIS:HB2	1.93	0.50
1:C:677:LEU:HD21	1:C:707:LEU:HD11	1.92	0.50
1:C:851:GLN:O	1:C:855:LYS:HG3	2.12	0.50
1:B:357:HIS:CE1	1:B:375:ASN:ND2	2.80	0.50
1:B:655:GLU:OE2	1:B:928:LYS:HD3	2.11	0.50
1:C:586:THR:O	1:C:587:ASP:OD1	2.29	0.50
1:A:277:ASN:HD22	1:A:277:ASN:N	2.10	0.50
1:B:181:GLN:HE22	1:B:319:MET:HE2	1.76	0.50
1:B:737:VAL:CG1	1:B:807:ARG:NH2	2.72	0.50
1:C:812:GLU:O	1:C:816:TRP:HB2	2.11	0.50
1:C:782:TRP:CD2	1:C:813:LYS:HE3	2.47	0.50
1:C:876:MET:O	1:C:880:ASN:HB2	2.11	0.50
1:A:573:LYS:HG3	1:A:595:VAL:HG22	1.92	0.50
1:A:757:SER:H	1:A:758:ASN:HA	1.76	0.50
1:A:842:ASN:OD1	1:A:843:PRO:HD2	2.11	0.50
1:C:368:TRP:CG	1:C:369:TRP:N	2.79	0.50
1:C:682:PRO:O	1:C:686:LEU:HD13	2.11	0.50
1:B:185:THR:CG2	1:B:188:ARG:CZ	2.86	0.50
1:B:449:ARG:O	1:B:452:LEU:O	2.30	0.50
1:C:100:LEU:HD22	1:C:151:TYR:HD2	1.77	0.50
1:C:549:TYR:CE1	1:C:609:ILE:HD11	2.46	0.50
1:A:718:ASP:HB3	1:A:725:ARG:NH1	2.26	0.50
1:B:186:ALA:O	1:B:189:MET:HB2	2.11	0.50
1:B:908:VAL:HG12	1:B:911:THR:HB	1.93	0.50
1:C:571:THR:HG23	1:C:595:VAL:CG1	2.41	0.50
1:A:290:LEU:HD12	1:A:359:TRP:HH2	1.77	0.50
1:B:311:ILE:HB	1:B:314:PHE:HB2	1.92	0.50
1:B:523:THR:O	1:B:563:TRP:NE1	2.45	0.50
1:C:737:VAL:CG1	1:C:807:ARG:NH2	2.75	0.50
1:C:907:CYS:C	1:C:909:GLN:H	2.15	0.50
1:A:256:SER:HA	1:A:269:VAL:O	2.12	0.50
1:A:408:MET:CE	1:A:609:ILE:HG23	2.42	0.50
1:C:125:HIS:CD2	1:C:128:GLN:H	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:884:THR:HG22	1:C:886:THR:H	1.77	0.50
1:C:925:ASN:O	1:C:929:ILE:HG13	2.11	0.50
1:A:588:VAL:CG1	1:B:241:LYS:HD2	2.29	0.49
1:C:571:THR:HG23	1:C:595:VAL:HG11	1.94	0.49
1:A:440:LYS:HE3	1:A:607:TYR:CE2	2.48	0.49
1:A:80:THR:HG23	1:A:151:TYR:CE1	2.36	0.49
1:B:479:TRP:CH2	1:B:521:MET:HE2	2.48	0.49
1:C:314:PHE:CE2	1:C:316:SER:CB	2.84	0.49
1:A:281:TYR:HD2	1:A:347:ILE:HD11	1.76	0.49
1:A:846:TYR:CG	1:A:847:PRO:HD3	2.47	0.49
1:B:875:VAL:HB	1:B:908:VAL:HG21	1.94	0.49
1:C:346:ASP:O	1:C:350:THR:HG23	2.12	0.49
1:A:586:THR:O	1:A:587:ASP:OD1	2.31	0.49
1:B:125:HIS:CD2	1:B:127:ARG:HB3	2.47	0.49
1:C:262:LYS:HG3	1:C:291:GLU:OE2	2.12	0.49
1:C:764:PRO:HB2	1:C:767:VAL:HG22	1.93	0.49
1:C:643:ALA:O	1:C:647:VAL:HG23	2.12	0.49
1:B:366:MET:HG3	1:B:368:TRP:O	2.12	0.49
1:C:183:GLU:HB3	1:C:319:MET:CE	2.42	0.49
1:A:139:LEU:HD22	1:A:145:TYR:HE1	1.75	0.49
1:A:440:LYS:O	1:A:444:ILE:HG12	2.12	0.49
1:A:624:LEU:HD12	1:A:660:LEU:HD21	1.93	0.49
1:A:718:ASP:OD2	1:A:765:VAL:HG22	2.13	0.49
1:A:850:TRP:CE2	1:A:854:ARG:NH1	2.81	0.49
1:A:875:VAL:HG21	1:A:908:VAL:HG11	1.95	0.49
1:B:290:LEU:HD12	1:B:359:TRP:HH2	1.77	0.49
1:B:761:LEU:HD12	1:B:761:LEU:O	2.13	0.49
1:A:177:LEU:HD13	1:A:254:PHE:CZ	2.48	0.49
1:B:107:LEU:HD11	1:B:145:TYR:HB3	1.94	0.49
1:B:210:GLU:HG3	3:E:1:NAG:H82	1.95	0.49
1:B:785:LEU:CD2	1:B:801:ILE:HG23	2.43	0.49
1:C:348:THR:HG21	1:C:391:HIS:CD2	2.48	0.49
1:C:737:VAL:CG1	1:C:807:ARG:HH21	2.25	0.49
1:A:480:ASP:OD1	1:A:518:LYS:HE2	2.12	0.49
1:A:760:ASN:C	1:A:760:ASN:OD1	2.51	0.49
1:B:844:VAL:O	1:B:844:VAL:HG12	2.13	0.49
1:A:200:LYS:HE2	1:A:365:THR:CG2	2.43	0.48
1:A:908:VAL:HG12	1:A:911:THR:HB	1.95	0.48
1:B:316:SER:CB	5:B:1001:BES:H8	2.37	0.48
1:B:534:THR:HG22	1:B:613:GLU:HG2	1.95	0.48
1:C:908:VAL:CG1	1:C:908:VAL:O	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:PHE:CE2	1:B:400:PHE:HD1	2.32	0.48
1:C:588:VAL:CG1	1:C:589:LEU:N	2.76	0.48
1:A:47:PHE:HA	1:A:48:PRO:HD3	1.61	0.48
1:A:604:MET:HE1	1:A:634:ASN:HB3	1.95	0.48
1:B:225:VAL:O	1:B:227:VAL:HG23	2.13	0.48
1:B:888:LEU:O	1:B:892:LYS:HG3	2.13	0.48
1:C:78:GLY:HA3	1:C:151:TYR:CZ	2.48	0.48
1:B:214:LEU:HD23	1:B:252:SER:O	2.14	0.48
1:B:319:MET:HE2	5:B:1001:BES:C8	2.43	0.48
1:B:533:ILE:HD13	1:B:567:LEU:HD21	1.95	0.48
1:A:536:THR:HB	1:A:543:HIS:HB2	1.95	0.48
1:A:811:LYS:HE2	1:A:844:VAL:CG1	2.43	0.48
1:A:831:GLU:HG2	1:A:835:ILE:HD11	1.95	0.48
1:C:350:THR:HA	5:C:1001:BES:H162	1.95	0.48
1:B:924:LYS:NZ	1:B:924:LYS:HB2	2.29	0.48
1:C:125:HIS:NE2	1:C:128:GLN:HG3	2.29	0.48
1:C:165:SER:O	1:C:177:LEU:HD23	2.14	0.48
1:B:571:THR:HG23	1:B:595:VAL:CG1	2.43	0.48
1:B:815:GLN:HA	1:B:818:LEU:HD12	1.96	0.48
1:B:908:VAL:HG13	1:B:911:THR:OG1	2.14	0.48
1:C:139:LEU:HD22	1:C:145:TYR:HE1	1.78	0.48
1:A:669:GLU:O	1:A:672:PRO:HD2	2.14	0.48
1:B:292:PHE:CZ	1:B:386:SER:HA	2.49	0.48
1:B:319:MET:HE1	5:B:1001:BES:HN21	1.78	0.48
1:B:378:PHE:CE1	1:B:461:ILE:HD13	2.48	0.48
1:C:325:THR:HG23	1:C:327:TYR:CE2	2.48	0.48
1:C:544:MET:CG	1:C:582:LEU:HD23	2.43	0.48
1:C:846:TYR:N	1:C:847:PRO:CD	2.76	0.48
1:A:210:GLU:HG3	2:D:1:NAG:H82	1.86	0.48
1:A:67:ILE:O	1:A:67:ILE:HG13	2.13	0.48
1:C:444:ILE:CG2	1:C:521:MET:HE1	2.43	0.48
1:C:754:TRP:CE2	1:C:759:GLY:HA2	2.49	0.48
1:A:444:ILE:HG22	1:A:521:MET:HE1	1.96	0.48
1:A:821:SER:HA	1:A:827:ILE:HG23	1.96	0.48
1:B:367:GLU:OE1	1:B:474:LYS:CE	2.62	0.48
1:B:62:HIS:ND1	1:B:202:SER:HB2	2.29	0.48
1:B:457:PHE:CD1	1:B:482:MET:CE	2.97	0.47
1:B:615:ASP:HB2	1:B:618:ASP:CB	2.44	0.47
1:B:682:PRO:O	1:B:686:LEU:HD13	2.14	0.47
1:C:290:LEU:CD2	1:C:355:LEU:HD13	2.44	0.47
1:A:565:VAL:CG1	1:A:582:LEU:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:TYR:CD2	1:B:847:PRO:HD3	2.49	0.47
1:B:316:SER:H	1:B:317:GLY:HA2	1.77	0.47
1:B:49:TRP:CZ2	1:B:51:LYS:HB2	2.49	0.47
1:B:782:TRP:HZ2	1:B:817:LEU:HD11	1.79	0.47
1:B:701:ALA:O	1:B:705:ARG:HG3	2.14	0.47
1:B:704:ILE:O	1:B:708:ARG:HB2	2.15	0.47
1:B:588:VAL:CG1	1:C:241:LYS:HD2	2.39	0.47
1:A:740:TYR:O	1:A:744:VAL:HG23	2.14	0.47
1:B:837:THR:HG21	1:B:873:HIS:NE2	2.29	0.47
1:C:916:GLU:HA	1:C:919:ILE:HD12	1.96	0.47
1:A:202:SER:OG	1:A:238:VAL:CG1	2.61	0.47
1:B:582:LEU:HD11	1:B:584:THR:O	2.13	0.47
1:C:544:MET:SD	1:C:580:PHE:CE2	3.07	0.47
1:A:569:PHE:CZ	1:A:589:LEU:HD21	2.50	0.47
1:A:826:LYS:O	1:A:827:ILE:HB	2.15	0.47
1:A:846:TYR:N	1:A:847:PRO:CD	2.77	0.47
1:B:588:VAL:CG1	1:B:589:LEU:H	2.28	0.47
1:C:371:ASP:OD1	1:C:475:ASN:ND2	2.48	0.47
1:A:115:LEU:HD12	1:A:116:SER:N	2.29	0.47
1:A:229:GLU:HA	1:A:229:GLU:OE1	2.15	0.47
1:A:257:VAL:HG23	1:A:283:LEU:HD22	1.96	0.47
1:C:405:PHE:CZ	1:C:604:MET:SD	3.08	0.47
1:C:613:GLU:HG3	1:C:614:ASP:N	2.29	0.47
1:C:853:LEU:O	1:C:857:TRP:HB2	2.15	0.47
1:B:532:LEU:HD12	1:B:609:ILE:O	2.15	0.47
1:A:246:LEU:CD2	1:A:320:GLU:HG2	2.45	0.47
1:A:159:PHE:CE1	1:A:313:ASP:HB3	2.49	0.47
1:B:200:LYS:CE	1:B:365:THR:HG22	2.45	0.47
1:C:53:ARG:HD3	1:C:368:TRP:CH2	2.50	0.47
1:C:624:LEU:O	1:C:628:HIS:HB3	2.15	0.47
1:B:272:VAL:HG13	1:B:273:PRO:HD2	1.97	0.47
1:B:570:ILE:HG23	1:B:602:VAL:HG21	1.95	0.47
1:A:160:HIS:CD2	1:A:186:ALA:HB2	2.50	0.46
1:C:100:LEU:HD22	1:C:151:TYR:CD2	2.50	0.46
1:C:710:LEU:CD2	1:C:731:LEU:HD11	2.45	0.46
1:A:692:MET:SD	1:A:926:PHE:CZ	3.08	0.46
1:C:334:PHE:HE1	1:C:338:LYS:HB3	1.79	0.46
1:A:582:LEU:HD11	1:A:584:THR:O	2.14	0.46
1:A:63:TYR:HB2	1:A:203:PHE:CD1	2.50	0.46
1:C:227:VAL:HG21	1:C:233:GLU:CB	2.33	0.46
1:C:733:LEU:HA	1:C:770:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:LEU:HD11	1:C:919:ILE:CD1	2.44	0.46
1:A:384:PHE:CE2	1:A:400:PHE:HD1	2.34	0.46
1:B:314:PHE:HE2	1:B:317:GLY:C	2.19	0.46
1:C:133:LEU:HD13	1:C:147:VAL:HG11	1.97	0.46
1:C:181:GLN:OE1	1:C:319:MET:HE3	2.15	0.46
1:C:757:SER:H	1:C:758:ASN:HA	1.81	0.46
1:A:200:LYS:HE2	1:A:365:THR:HG22	1.98	0.46
1:A:565:VAL:HA	1:A:566:PRO:HD3	1.68	0.46
1:B:297:PHE:O	1:B:299:ILE:HG13	2.15	0.46
1:A:156:SER:HG	1:A:158:THR:HG22	1.81	0.46
1:A:852:PHE:CZ	1:A:856:ASN:ND2	2.79	0.46
1:B:763:LEU:CD2	1:B:768:THR:HG22	2.45	0.46
1:C:281:TYR:HD2	1:C:347:ILE:HD11	1.80	0.46
1:C:544:MET:HG3	1:C:582:LEU:HD21	1.98	0.46
1:C:806:CYS:SG	1:C:835:ILE:HG23	2.55	0.46
1:A:858:ASN:O	1:A:861:VAL:HG22	2.16	0.46
1:C:615:ASP:HB3	1:C:618:ASP:HB2	1.98	0.46
1:C:761:LEU:O	1:C:761:LEU:HD12	2.16	0.46
1:C:844:VAL:O	1:C:844:VAL:HG12	2.16	0.46
1:C:89:PRO:O	1:C:90:THR:CG2	2.64	0.46
1:B:925:ASN:O	1:B:929:ILE:HG13	2.15	0.46
1:B:702:PHE:CZ	1:B:932:TRP:CH2	3.04	0.46
1:A:268:SER:HB2	1:A:307:ASP:OD1	2.16	0.46
1:A:641:ASN:O	1:A:645:GLN:HG3	2.15	0.46
1:B:654:ILE:HB	1:B:925:ASN:ND2	2.30	0.46
1:B:846:TYR:CG	1:B:847:PRO:HD3	2.51	0.46
1:C:196:GLU:HB2	1:C:199:PHE:HD2	1.80	0.46
1:C:384:PHE:HE1	1:C:396:VAL:O	1.99	0.46
1:C:580:PHE:CD1	1:C:589:LEU:HD13	2.51	0.46
1:C:913:GLU:O	1:C:916:GLU:HB3	2.16	0.46
1:A:269:VAL:HG11	1:A:279:ALA:HB1	1.98	0.45
1:A:875:VAL:HG22	1:A:908:VAL:HG11	1.97	0.45
1:B:590:ILE:HG13	1:C:470:TYR:CG	2.52	0.45
1:B:868:SER:HA	1:B:871:ILE:HG12	1.97	0.45
1:A:156:SER:HB3	1:A:163:TYR:HB3	1.97	0.45
1:C:411:ASP:OD1	1:C:529:GLY:HA2	2.15	0.45
1:C:879:THR:OG1	1:C:911:THR:HG21	2.16	0.45
1:C:827:ILE:HD11	1:C:830:GLN:HE21	1.81	0.45
1:A:261:THR:HG23	1:A:263:SER:N	2.31	0.45
1:A:681:ILE:HG23	1:A:684:TYR:OH	2.17	0.45
1:C:319:MET:SD	1:C:320:GLU:CD	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:LEU:O	1:A:892:LYS:HG3	2.16	0.45
1:B:227:VAL:HG21	1:B:233:GLU:CB	2.42	0.45
1:B:876:MET:HG2	1:B:911:THR:OG1	2.17	0.45
1:A:331:ALA:HA	1:A:347:ILE:HG22	1.99	0.45
1:A:613:GLU:HG3	1:A:614:ASP:N	2.31	0.45
1:A:640:ILE:HD11	1:A:663:TYR:CE2	2.52	0.45
1:A:694:GLU:HG2	1:A:695:VAL:N	2.30	0.45
1:B:181:GLN:NE2	5:B:1001:BES:C9	2.80	0.45
1:B:875:VAL:CB	1:B:908:VAL:HG21	2.47	0.45
1:C:684:TYR:HA	1:C:687:MET:SD	2.57	0.45
1:A:434:ASP:OD1	1:A:435:ASP:N	2.48	0.45
1:A:548:HIS:HB2	1:A:561:TYR:HB2	1.98	0.45
1:A:848:LEU:O	1:A:852:PHE:HB2	2.17	0.45
1:B:355:LEU:HD23	1:B:355:LEU:HA	1.79	0.45
1:B:65:LEU:HD23	1:B:80:THR:HB	1.99	0.45
1:B:757:SER:H	1:B:758:ASN:HA	1.82	0.45
1:C:177:LEU:HD13	1:C:254:PHE:CZ	2.52	0.45
1:C:655:GLU:HB3	1:C:932:TRP:CD1	2.52	0.45
1:C:667:GLU:HG2	1:C:672:PRO:HB2	1.99	0.45
1:A:62:HIS:ND1	1:A:202:SER:HB3	2.31	0.45
1:B:548:HIS:ND1	1:B:559:THR:HG21	2.32	0.45
1:C:378:PHE:CZ	1:C:382:MET:HE2	2.52	0.45
1:C:582:LEU:HD11	1:C:584:THR:O	2.17	0.45
1:B:687:MET:SD	1:B:695:VAL:HG12	2.57	0.45
1:C:227:VAL:CG2	1:C:233:GLU:HB2	2.34	0.45
1:B:156:SER:HB3	1:B:163:TYR:CB	2.47	0.44
1:A:846:TYR:CD2	1:A:847:PRO:HD3	2.53	0.44
1:A:868:SER:HA	1:A:871:ILE:CD1	2.48	0.44
1:B:718:ASP:HB3	1:B:725:ARG:NH1	2.32	0.44
1:C:384:PHE:O	1:C:385:VAL:C	2.54	0.44
1:C:604:MET:HG2	1:C:604:MET:O	2.17	0.44
1:A:131:ILE:HG22	1:A:132:ALA:N	2.32	0.44
1:C:405:PHE:HZ	1:C:604:MET:SD	2.40	0.44
1:C:647:VAL:HA	1:C:652:LEU:O	2.17	0.44
1:C:852:PHE:CE1	1:C:856:ASN:ND2	2.85	0.44
1:A:215:ALA:HA	1:A:250:ILE:O	2.18	0.44
1:A:763:LEU:CD2	1:A:768:THR:HG22	2.46	0.44
1:B:301:TYR:HA	1:B:302:PRO:HD3	1.80	0.44
1:C:457:PHE:CD1	1:C:482:MET:HE3	2.52	0.44
1:C:47:PHE:HA	1:C:48:PRO:HD3	1.62	0.44
1:C:65:LEU:HD22	1:C:80:THR:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:THR:CG2	1:A:185:THR:O	2.63	0.44
1:A:49:TRP:CZ3	1:A:55:PRO:HG3	2.52	0.44
1:B:185:THR:HG23	1:B:188:ARG:NE	2.33	0.44
1:B:411:ASP:OD1	1:B:529:GLY:N	2.51	0.44
1:C:876:MET:HG2	1:C:911:THR:OG1	2.18	0.44
1:C:183:GLU:OE1	1:C:320:GLU:OE2	2.35	0.44
1:B:256:SER:HA	1:B:269:VAL:O	2.17	0.44
1:B:56:GLU:H	1:B:56:GLU:HG2	1.63	0.44
1:B:595:VAL:HG12	1:B:597:TRP:N	2.29	0.44
1:A:324:LEU:HG	1:A:324:LEU:O	2.18	0.44
1:A:879:THR:OG1	1:A:911:THR:HG21	2.17	0.44
1:B:74:LEU:HD13	1:B:164:LYS:HD3	2.00	0.44
1:A:613:GLU:HG3	1:A:614:ASP:H	1.83	0.44
1:A:682:PRO:O	1:A:686:LEU:HD13	2.17	0.44
1:B:791:PHE:N	1:B:791:PHE:CD2	2.86	0.44
1:C:436:VAL:O	1:C:439:ASP:HB2	2.17	0.44
1:A:97:SER:HB3	1:A:131:ILE:CG1	2.48	0.43
1:A:139:LEU:HB3	1:A:145:TYR:CE1	2.53	0.43
1:A:227:VAL:CG2	1:A:233:GLU:HB2	2.38	0.43
1:B:534:THR:CG2	1:B:613:GLU:HG2	2.49	0.43
1:B:670:ILE:HD11	1:B:724:GLU:HA	2.00	0.43
1:C:277:ASN:HD22	1:C:277:ASN:N	2.16	0.43
1:C:537:VAL:HG22	1:C:542:VAL:HG22	1.99	0.43
1:C:797:GLU:O	1:C:801:ILE:HG13	2.18	0.43
1:A:556:ALA:HB3	1:A:557:PRO:HD3	1.99	0.43
1:B:160:HIS:CD2	1:B:186:ALA:HB2	2.54	0.43
1:B:196:GLU:HB2	1:B:199:PHE:HD2	1.84	0.43
1:C:384:PHE:CE2	1:C:400:PHE:CD1	3.03	0.43
1:C:367:GLU:OE1	1:C:474:LYS:CE	2.66	0.43
1:C:565:VAL:HA	1:C:566:PRO:HD3	1.71	0.43
1:C:754:TRP:HA	1:C:757:SER:HB2	2.00	0.43
1:A:708:ARG:HG2	1:A:708:ARG:NH1	2.34	0.43
1:C:125:HIS:CE1	1:C:128:GLN:NE2	2.87	0.43
1:C:457:PHE:CE2	1:C:461:ILE:CD1	3.01	0.43
1:C:68:HIS:CE1	1:C:231:LEU:CD2	2.94	0.43
1:A:314:PHE:HE2	1:A:316:SER:HB2	1.77	0.43
1:A:604:MET:HG2	1:A:604:MET:O	2.17	0.43
1:A:907:CYS:C	1:A:909:GLN:H	2.22	0.43
1:B:444:ILE:HG22	1:B:521:MET:HE1	2.01	0.43
1:B:739:ASN:HA	1:B:744:VAL:HG21	2.00	0.43
1:C:345:LEU:HD11	1:C:396:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:PHE:CD1	1:C:482:MET:CE	3.01	0.43
1:C:544:MET:SD	1:C:567:LEU:HD12	2.59	0.43
1:C:94:ILE:HD12	1:C:94:ILE:N	2.33	0.43
1:B:434:ASP:HB3	1:B:435:ASP:H	1.70	0.43
1:C:858:ASN:O	1:C:861:VAL:HG22	2.19	0.43
1:A:214:LEU:HD23	1:A:252:SER:O	2.18	0.43
1:A:219:MET:HG2	1:A:239:THR:HG22	2.01	0.43
1:A:368:TRP:CG	1:A:369:TRP:N	2.87	0.43
1:B:405:PHE:CZ	1:B:604:MET:SD	3.12	0.43
1:B:611:HIS:ND1	1:B:646:LEU:HD13	2.32	0.43
1:B:879:THR:OG1	1:B:911:THR:HG21	2.18	0.43
1:C:160:HIS:CD2	1:C:186:ALA:HB2	2.54	0.43
1:C:373:TRP:HA	1:C:438:TYR:CE2	2.53	0.43
1:C:544:MET:SD	1:C:580:PHE:CD2	3.12	0.43
1:B:378:PHE:HE1	1:B:461:ILE:HD13	1.82	0.43
1:B:684:TYR:C	1:B:684:TYR:CD1	2.92	0.43
1:B:793:LEU:O	1:B:794:SER:HB2	2.19	0.43
1:C:185:THR:CG2	1:C:188:ARG:CZ	2.95	0.43
1:C:159:PHE:CE1	1:C:313:ASP:HB3	2.54	0.43
1:C:380:LYS:HE3	1:C:435:ASP:OD1	2.18	0.43
1:C:572:SER:OG	1:C:595:VAL:HG13	2.18	0.43
1:C:701:ALA:O	1:C:705:ARG:HG3	2.18	0.43
1:C:868:SER:HA	1:C:871:ILE:HG12	1.99	0.43
1:A:568:THR:HA	1:A:578:HIS:O	2.19	0.43
1:B:118:GLU:HA	1:B:119:PRO:HD3	1.92	0.43
1:B:449:ARG:O	1:B:449:ARG:HG2	2.19	0.43
1:B:888:LEU:HD21	1:B:915:ILE:CG2	2.49	0.43
1:C:810:ASN:CB	1:C:813:LYS:HD3	2.49	0.43
1:A:457:PHE:CD1	1:A:482:MET:HE3	2.54	0.43
1:B:115:LEU:HD13	1:B:115:LEU:HA	1.79	0.43
1:A:78:GLY:HA3	1:A:151:TYR:CZ	2.54	0.42
1:A:590:ILE:HG13	1:B:470:TYR:CD1	2.53	0.42
1:B:792:SER:OG	1:B:793:LEU:N	2.51	0.42
1:C:620:LEU:HD13	1:C:639:LEU:HD21	2.01	0.42
1:C:741:GLN:HE21	1:C:745:GLN:NE2	2.17	0.42
1:C:782:TRP:CE2	1:C:805:LEU:HD22	2.54	0.42
1:A:293:TYR:CE2	1:A:382:MET:HG3	2.52	0.42
1:A:810:ASN:ND2	1:A:813:LYS:HG3	2.34	0.42
1:A:815:GLN:HA	1:A:818:LEU:HD12	2.02	0.42
1:B:177:LEU:HD13	1:B:254:PHE:CZ	2.54	0.42
1:B:328:ARG:CZ	1:B:331:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:782:TRP:CE2	1:B:805:LEU:HD22	2.54	0.42
1:B:888:LEU:HD21	1:B:915:ILE:HG22	2.01	0.42
1:C:373:TRP:HA	1:C:438:TYR:CD2	2.54	0.42
1:C:850:TRP:CE3	1:C:850:TRP:HA	2.54	0.42
1:A:261:THR:CG2	1:A:265:VAL:H	2.29	0.42
1:A:411:ASP:CG	1:A:529:GLY:HA2	2.39	0.42
1:B:408:MET:CE	1:B:609:ILE:HG23	2.49	0.42
1:C:269:VAL:HG11	1:C:279:ALA:HB1	2.01	0.42
1:C:480:ASP:OD1	1:C:518:LYS:HE2	2.19	0.42
1:C:543:HIS:NE2	1:C:586:THR:OG1	2.42	0.42
1:A:569:PHE:CD1	1:A:598:ILE:HD11	2.55	0.42
1:A:681:ILE:HD13	1:A:684:TYR:OH	2.20	0.42
1:A:885:ARG:O	1:A:888:LEU:HB2	2.20	0.42
1:B:702:PHE:CE1	1:B:932:TRP:CZ3	3.08	0.42
1:C:107:LEU:HB2	1:C:120:LEU:HD21	2.01	0.42
1:A:311:ILE:HB	1:A:314:PHE:HB2	2.00	0.42
1:A:343:SER:O	1:A:347:ILE:HG23	2.19	0.42
1:A:473:THR:HG22	1:A:474:LYS:N	2.33	0.42
1:A:595:VAL:HG12	1:A:596:GLU:N	2.34	0.42
1:B:702:PHE:CE1	1:B:932:TRP:HZ3	2.38	0.42
1:C:128:GLN:O	1:C:130:GLN:HG3	2.20	0.42
2:F:2:NAG:O7	2:F:5:MAN:H62	2.20	0.42
1:A:183:GLU:HA	1:A:184:PRO:HA	1.82	0.42
1:A:621:THR:HG22	1:A:660:LEU:CD2	2.49	0.42
1:B:314:PHE:CE2	1:B:317:GLY:C	2.93	0.42
1:C:556:ALA:N	1:C:557:PRO:CD	2.82	0.42
1:C:732:LEU:CD1	1:C:767:VAL:HG12	2.49	0.42
1:C:888:LEU:O	1:C:892:LYS:HG3	2.20	0.42
1:A:125:HIS:CE1	1:A:128:GLN:NE2	2.88	0.42
1:A:207:ILE:HG12	1:A:236:PHE:HE1	1.85	0.42
1:A:457:PHE:CD1	1:A:482:MET:CE	3.03	0.42
1:A:520:MET:HA	1:A:564:HIS:HB2	2.01	0.42
1:B:384:PHE:O	1:B:385:VAL:C	2.57	0.42
1:B:556:ALA:N	1:B:557:PRO:CD	2.82	0.42
1:C:125:HIS:HD2	1:C:128:GLN:H	1.66	0.42
1:C:473:THR:CG2	1:C:474:LYS:N	2.82	0.42
1:C:613:GLU:HG3	1:C:614:ASP:H	1.85	0.42
1:A:366:MET:HG3	1:A:368:TRP:O	2.19	0.42
1:A:367:GLU:OE1	1:A:474:LYS:CE	2.63	0.42
1:A:872:ALA:O	1:A:875:VAL:CG1	2.61	0.42
1:B:599:LYS:HE2	1:B:639:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:THR:O	1:B:139:LEU:HG	2.20	0.42
1:C:464:TYR:CE1	1:C:473:THR:HG21	2.55	0.42
1:C:850:TRP:HE3	1:C:850:TRP:HA	1.84	0.42
1:A:379:ALA:O	1:A:383:GLU:HG3	2.20	0.42
1:A:702:PHE:CZ	1:A:932:TRP:CH2	3.08	0.42
1:B:181:GLN:NE2	5:B:1001:BES:H9	2.35	0.42
1:B:835:ILE:O	1:B:839:ILE:HG13	2.20	0.42
1:C:924:LYS:HD3	1:C:924:LYS:O	2.20	0.42
1:A:168:ARG:HA	1:A:173:GLU:O	2.20	0.42
1:A:850:TRP:HE3	1:A:850:TRP:HA	1.85	0.42
1:C:378:PHE:CZ	1:C:382:MET:CE	3.03	0.42
1:A:245:TYR:HE2	1:A:320:GLU:OE2	2.03	0.41
1:A:67:ILE:HD13	1:A:249:PHE:CE1	2.55	0.41
1:A:314:PHE:HE2	1:A:317:GLY:C	2.24	0.41
1:A:544:MET:HE2	1:A:567:LEU:CD1	2.50	0.41
1:A:792:SER:O	1:A:793:LEU:HB2	2.20	0.41
1:B:562:LEU:HD22	1:B:562:LEU:HA	1.92	0.41
1:C:366:MET:HG3	1:C:368:TRP:O	2.20	0.41
1:C:478:LEU:HD13	1:C:479:TRP:CZ3	2.55	0.41
1:C:698:GLN:HE21	1:C:698:GLN:HB3	1.70	0.41
1:A:186:ALA:O	1:A:189:MET:HB2	2.19	0.41
1:A:411:ASP:OD1	1:A:529:GLY:N	2.51	0.41
1:A:603:GLY:O	1:A:604:MET:HB3	2.20	0.41
1:A:752:ARG:HB2	1:A:752:ARG:HE	1.60	0.41
1:B:440:LYS:O	1:B:444:ILE:HG12	2.20	0.41
1:B:520:MET:HG3	1:B:564:HIS:HB2	2.03	0.41
1:C:411:ASP:OD1	1:C:529:GLY:N	2.53	0.41
1:C:754:TRP:CD1	1:C:763:LEU:HD11	2.55	0.41
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.90	0.41
1:A:842:ASN:HA	1:A:843:PRO:HD2	1.92	0.41
1:B:100:LEU:HD22	1:B:151:TYR:CD2	2.56	0.41
1:B:390:THR:CG2	1:B:391:HIS:CD2	3.02	0.41
1:B:733:LEU:O	1:B:737:VAL:HG23	2.19	0.41
1:C:322:TRP:CZ2	1:C:363:LEU:HA	2.56	0.41
1:A:67:ILE:CD1	1:A:249:PHE:CE1	3.03	0.41
1:A:807:ARG:NH1	1:A:843:PRO:HD2	2.35	0.41
1:B:97:SER:HB3	1:B:131:ILE:HD11	2.01	0.41
1:B:183:GLU:HA	1:B:184:PRO:HA	1.78	0.41
1:B:850:TRP:CE3	1:B:850:TRP:HA	2.56	0.41
1:C:185:THR:HG23	1:C:188:ARG:NH2	2.35	0.41
1:A:229:GLU:OE1	2:D:4:MAN:O2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:ARG:HH12	1:A:843:PRO:HD2	1.84	0.41
1:A:884:THR:HG22	1:A:886:THR:H	1.86	0.41
1:B:97:SER:HB3	1:B:131:ILE:CG1	2.51	0.41
1:C:544:MET:HG3	1:C:582:LEU:HD23	2.01	0.41
1:C:755:LYS:C	1:C:757:SER:H	2.24	0.41
1:A:242:MET:HB3	1:A:322:TRP:CZ3	2.55	0.41
1:A:764:PRO:O	1:A:767:VAL:HG22	2.20	0.41
1:A:884:THR:HB	1:A:887:ARG:HB2	2.02	0.41
1:B:228:ALA:HB3	1:B:231:LEU:HB2	2.02	0.41
1:B:451:TYR:CD2	1:B:452:LEU:HD12	2.51	0.41
1:B:850:TRP:HE3	1:B:850:TRP:HA	1.85	0.41
1:A:155:LEU:HG	1:A:162:PHE:CD2	2.56	0.41
1:A:200:LYS:CB	1:A:241:LYS:HG2	2.49	0.41
1:A:342:SER:O	1:A:346:ASP:N	2.44	0.41
1:A:378:PHE:CE1	1:A:461:ILE:HD13	2.55	0.41
1:B:277:ASN:ND2	1:B:278:GLN:HG3	2.36	0.41
1:B:368:TRP:CG	1:B:369:TRP:N	2.89	0.41
1:B:520:MET:HG3	1:B:564:HIS:CB	2.51	0.41
1:B:624:LEU:HD12	1:B:660:LEU:HD21	2.03	0.41
1:B:699:PHE:HE2	1:B:703:LEU:HD11	1.86	0.41
1:B:810:ASN:HB2	1:B:813:LYS:HD2	2.03	0.41
1:C:183:GLU:HA	1:C:184:PRO:HA	1.85	0.41
1:C:328:ARG:CZ	1:C:331:ALA:HB2	2.51	0.41
1:C:731:LEU:HD23	1:C:731:LEU:HA	1.75	0.41
1:A:320:GLU:OE1	1:A:320:GLU:N	2.46	0.41
1:B:851:GLN:O	1:B:855:LYS:HG3	2.20	0.41
1:A:162:PHE:CD1	1:A:249:PHE:HE1	2.39	0.41
1:A:319:MET:HE1	1:A:320:GLU:OE2	2.21	0.41
1:A:850:TRP:CE3	1:A:850:TRP:HA	2.55	0.41
1:B:406:ASP:O	1:B:410:VAL:HG23	2.21	0.41
1:C:739:ASN:HA	1:C:744:VAL:HG21	2.02	0.41
1:A:62:HIS:HE1	1:A:238:VAL:HG13	1.86	0.41
1:A:301:TYR:HA	1:A:302:PRO:HD3	1.86	0.41
1:B:681:ILE:N	1:B:682:PRO:CD	2.84	0.41
1:B:764:PRO:HB2	1:B:767:VAL:HG22	2.02	0.41
1:C:548:HIS:ND1	1:C:559:THR:HG21	2.36	0.41
1:A:556:ALA:N	1:A:557:PRO:CD	2.84	0.40
1:B:331:ALA:HA	1:B:347:ILE:HG22	2.03	0.40
1:B:533:ILE:HD11	1:B:565:VAL:HG11	2.03	0.40
1:B:810:ASN:CG	1:B:813:LYS:HD2	2.42	0.40
1:B:815:GLN:O	1:B:818:LEU:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:908:VAL:HG13	1:C:911:THR:OG1	2.21	0.40
1:A:177:LEU:HD13	1:A:254:PHE:HZ	1.86	0.40
1:A:310:ALA:HB2	1:A:332:LEU:HD23	2.03	0.40
1:A:758:ASN:C	1:A:760:ASN:N	2.73	0.40
1:B:556:ALA:HB3	1:B:557:PRO:HD3	2.02	0.40
1:C:125:HIS:CD2	1:C:128:GLN:HG3	2.57	0.40
1:C:337:GLU:HG3	1:C:337:GLU:O	2.21	0.40
1:C:710:LEU:HG	1:C:731:LEU:CD1	2.51	0.40
1:C:827:ILE:CD1	1:C:830:GLN:HE21	2.34	0.40
1:B:114:ARG:CA	1:B:117:GLU:HG3	2.49	0.40
1:B:603:GLY:O	1:B:604:MET:HB3	2.20	0.40
1:C:96:HIS:CD2	1:C:195:ASP:HB3	2.56	0.40
1:C:357:HIS:CE1	1:C:375:ASN:ND2	2.89	0.40
1:A:139:LEU:HB3	1:A:145:TYR:HE1	1.87	0.40
1:A:196:GLU:HB2	1:A:199:PHE:HD2	1.86	0.40
1:A:449:ARG:HG3	1:A:457:PHE:CG	2.56	0.40
1:A:595:VAL:HG12	1:A:597:TRP:N	2.36	0.40
1:B:277:ASN:HD22	1:B:277:ASN:N	2.19	0.40
1:C:183:GLU:OE1	5:C:1001:BES:N2	2.55	0.40
1:C:167:TYR:CE1	1:C:175:ARG:HB2	2.57	0.40
1:C:261:THR:CG2	1:C:265:VAL:HB	2.51	0.40
1:C:911:THR:O	1:C:915:ILE:HG13	2.21	0.40
1:A:707:LEU:O	1:A:708:ARG:C	2.59	0.40
1:A:837:THR:O	1:A:841:ARG:HG3	2.21	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	804/921 (87%)	750 (93%)	50 (6%)	4 (0%)	29 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	809/921 (88%)	755 (93%)	52 (6%)	2 (0%)	47	79
1	C	805/921 (87%)	753 (94%)	51 (6%)	1 (0%)	51	83
All	All	2418/2763 (88%)	2258 (93%)	153 (6%)	7 (0%)	41	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	908	VAL
1	A	229	GLU
1	A	908	VAL
1	B	908	VAL
1	A	855	LYS
1	B	855	LYS
1	A	827	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	733/819 (90%)	710 (97%)	23 (3%)	40	71
1	B	734/819 (90%)	711 (97%)	23 (3%)	40	71
1	C	734/819 (90%)	711 (97%)	23 (3%)	40	71
All	All	2201/2457 (90%)	2132 (97%)	69 (3%)	40	71

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	A	114	ARG
1	A	174	LEU
1	A	175	ARG
1	A	177	LEU
1	A	209	ARG
1	A	277	ASN

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Mol	Chain	Res	Type
1	A	303	LEU
1	A	305	LYS
1	A	322	TRP
1	A	366	MET
1	A	395	LYS
1	A	526	LEU
1	A	544	MET
1	A	660	LEU
1	A	743	CYS
1	A	779	THR
1	A	850	TRP
1	A	853	LEU
1	A	885	ARG
1	A	886	THR
1	A	924	LYS
1	A	934	GLN
1	B	95	LEU
1	B	174	LEU
1	B	175	ARG
1	B	177	LEU
1	B	209	ARG
1	B	277	ASN
1	B	303	LEU
1	B	305	LYS
1	B	322	TRP
1	B	366	MET
1	B	544	MET
1	B	562	LEU
1	B	575	ASP
1	B	577	VAL
1	B	581	LEU
1	B	660	LEU
1	B	681	ILE
1	B	785	LEU
1	B	850	TRP
1	B	885	ARG
1	B	914	THR
1	B	924	LYS
1	B	934	GLN
1	C	95	LEU
1	C	175	ARG
1	C	209	ARG

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Mol	Chain	Res	Type
1	C	261	THR
1	C	277	ASN
1	C	303	LEU
1	C	305	LYS
1	C	322	TRP
1	C	366	MET
1	C	395	LYS
1	C	413	LEU
1	C	478	LEU
1	C	526	LEU
1	C	559	THR
1	C	575	ASP
1	C	577	VAL
1	C	694	GLU
1	C	743	CYS
1	C	752	ARG
1	C	783	ASP
1	C	790	GLN
1	C	850	TRP
1	C	924	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	96	HIS
1	A	98	HIS
1	A	125	HIS
1	A	128	GLN
1	A	160	HIS
1	A	181	GLN
1	A	277	ASN
1	A	306	GLN
1	A	391	HIS
1	A	527	GLN
1	A	634	ASN
1	A	641	ASN
1	A	645	GLN
1	A	698	GLN
1	A	745	GLN
1	A	830	GLN
1	A	934	GLN

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Mol	Chain	Res	Type
1	B	96	HIS
1	B	125	HIS
1	B	160	HIS
1	B	181	GLN
1	B	277	ASN
1	B	357	HIS
1	B	391	HIS
1	B	446	ASN
1	B	634	ASN
1	B	698	GLN
1	B	745	GLN
1	B	925	ASN
1	B	934	GLN
1	C	68	HIS
1	C	96	HIS
1	C	125	HIS
1	C	128	GLN
1	C	160	HIS
1	C	277	ASN
1	C	357	HIS
1	C	391	HIS
1	C	446	ASN
1	C	546	GLN
1	C	564	HIS
1	C	628	HIS
1	C	634	ASN
1	C	698	GLN
1	C	745	GLN
1	C	810	ASN
1	C	830	GLN

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 ⓘ

12 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
2	NAG	D	1	1,2	14,14,15	0.87	0	17,19,21	2.00	6 (35%)
2	NAG	D	2	2	14,14,15	0.63	0	17,19,21	2.45	3 (17%)
2	BMA	D	3	2	11,11,12	0.42	0	15,15,17	0.81	0
2	MAN	D	4	2	11,11,12	0.60	0	15,15,17	0.92	0
2	MAN	D	5	2	11,11,12	0.93	1 (9%)	15,15,17	1.88	3 (20%)
3	NAG	E	1	1,3	14,14,15	0.77	0	17,19,21	1.22	2 (11%)
3	NAG	E	2	3	14,14,15	0.64	0	17,19,21	2.49	3 (17%)
2	NAG	F	1	1,2	14,14,15	1.06	3 (21%)	17,19,21	1.88	6 (35%)
2	NAG	F	2	2	14,14,15	0.71	0	17,19,21	2.86	4 (23%)
2	BMA	F	3	2	11,11,12	0.39	0	15,15,17	0.83	1 (6%)
2	MAN	F	4	2	11,11,12	0.46	0	15,15,17	0.78	0
2	MAN	F	5	2	11,11,12	0.79	0	15,15,17	1.38	2 (13%)

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
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	F	4	2	-	0/2/19/22	0/1/1/1
2	MAN	F	5	2	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C4-C3	-2.11	1.47	1.52
2	F	1	NAG	O5-C1	2.07	1.47	1.43
2	D	5	MAN	O5-C5	2.06	1.47	1.43
2	F	1	NAG	O4-C4	-2.06	1.38	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	O5-C5-C6	-9.25	92.71	107.20
2	D	2	NAG	O5-C5-C6	-8.17	94.40	107.20
3	E	2	NAG	O5-C5-C6	-8.07	94.55	107.20
2	D	5	MAN	O5-C5-C6	4.78	114.70	107.20
2	F	2	NAG	C6-C5-C4	4.24	122.93	113.00
2	F	1	NAG	O4-C4-C3	-4.15	100.75	110.35
3	E	2	NAG	C6-C5-C4	4.14	122.70	113.00
2	D	2	NAG	C6-C5-C4	4.04	122.48	113.00
2	F	5	MAN	O5-C5-C6	3.97	113.42	107.20
3	E	2	NAG	C4-C3-C2	-3.54	105.84	111.02
2	F	2	NAG	C4-C3-C2	-3.51	105.88	111.02
2	D	5	MAN	C6-C5-C4	-3.39	105.05	113.00
2	F	2	NAG	C1-O5-C5	-3.39	107.60	112.19
2	D	1	NAG	O3-C3-C4	-3.36	102.59	110.35
2	D	1	NAG	C3-C4-C5	-3.27	104.41	110.24
2	D	1	NAG	O4-C4-C3	-3.20	102.96	110.35
2	D	1	NAG	O3-C3-C2	-3.18	102.88	109.47
2	D	2	NAG	C4-C3-C2	-2.90	106.77	111.02
3	E	1	NAG	C1-O5-C5	2.81	115.99	112.19
2	F	1	NAG	C3-C4-C5	-2.54	105.72	110.24
2	F	3	BMA	O5-C5-C6	2.44	111.02	107.20
2	F	1	NAG	C1-C2-N2	2.40	114.59	110.49
2	D	1	NAG	O5-C5-C6	2.39	110.96	107.20
2	F	5	MAN	C6-C5-C4	-2.28	107.66	113.00
2	F	1	NAG	O3-C3-C2	-2.22	104.87	109.47
3	E	1	NAG	O5-C5-C6	2.17	110.60	107.20
2	D	1	NAG	C1-C2-N2	2.15	114.16	110.49
2	F	1	NAG	O3-C3-C4	-2.14	105.39	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	MAN	O3-C3-C4	-2.10	105.49	110.35
2	F	1	NAG	O4-C4-C5	-2.04	104.24	109.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1	NAG	C1

All (1) torsion outliers are listed below:

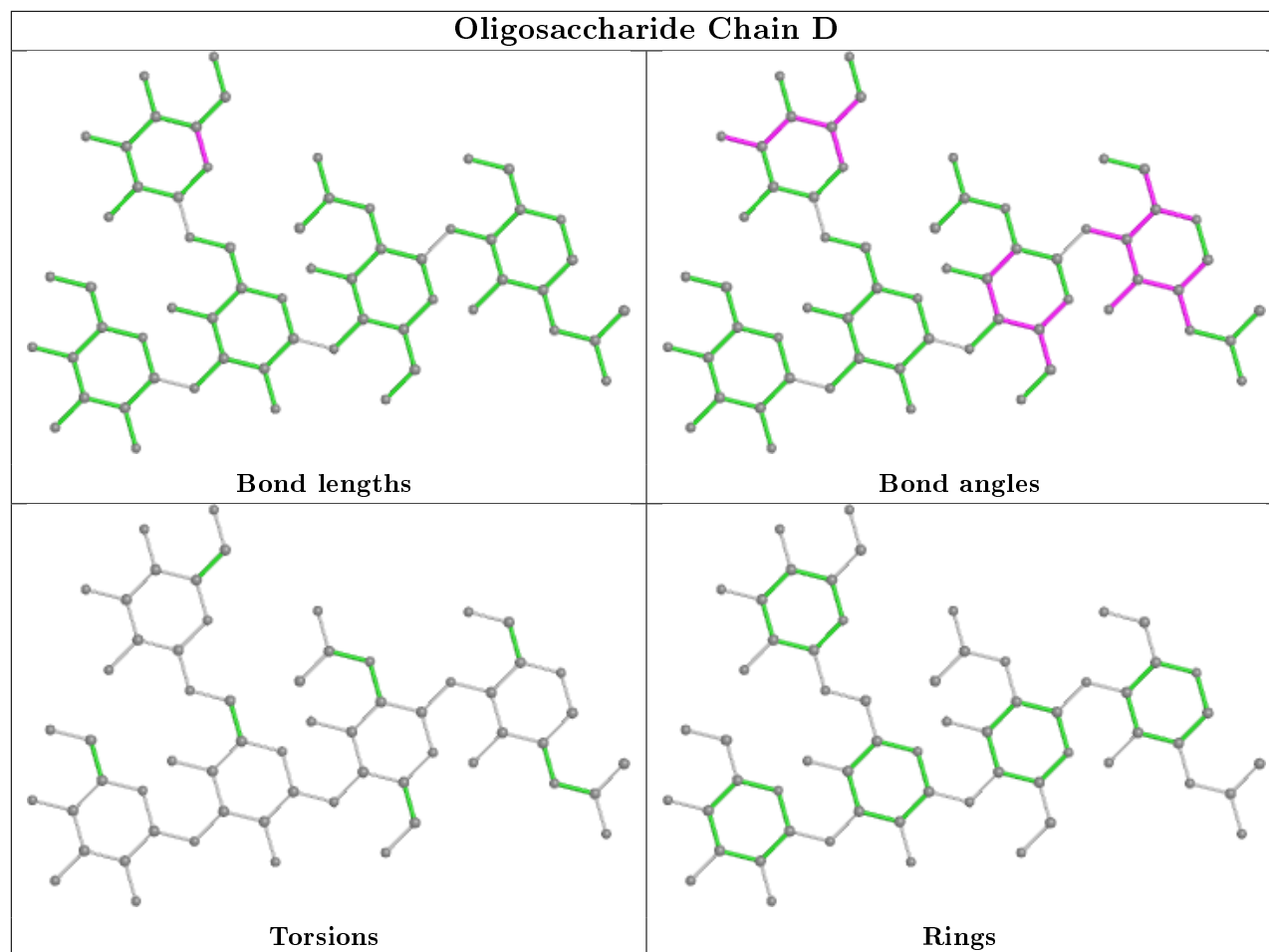
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C3-C2-N2-C7

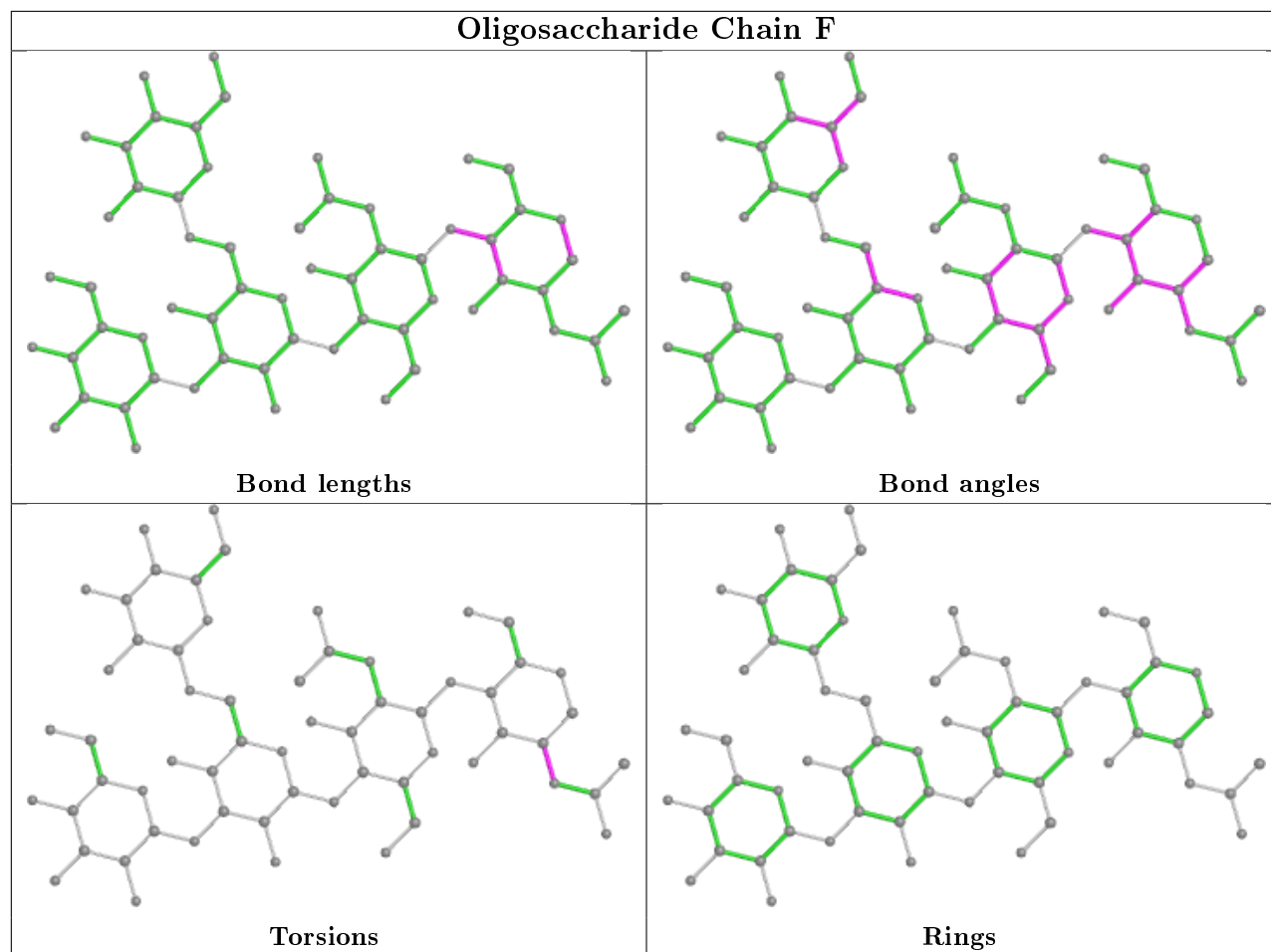
There are no ring outliers.

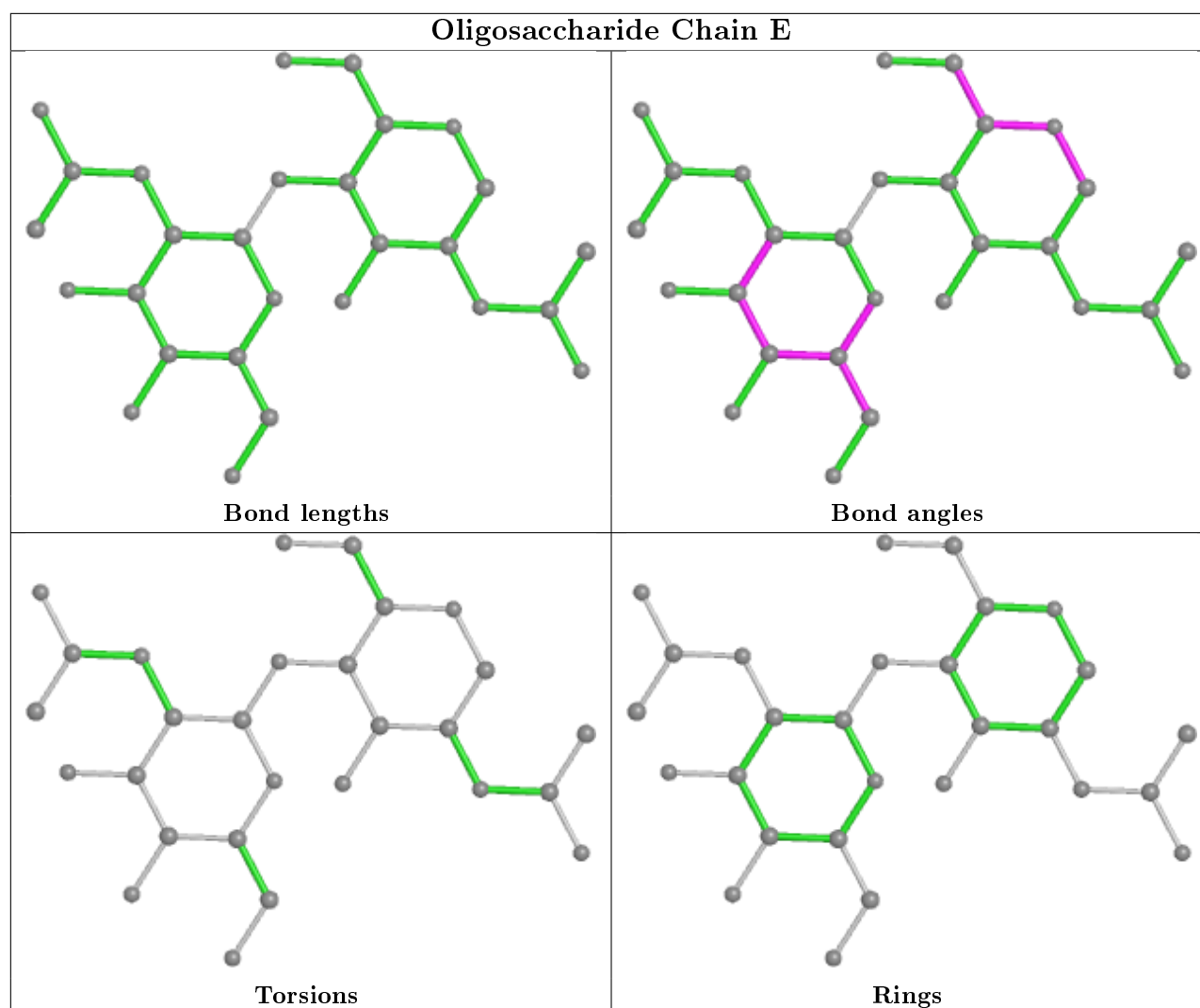
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	5	MAN	1	0
3	E	1	NAG	1	0
2	D	1	NAG	3	0
2	F	2	NAG	1	0
2	D	4	MAN	1	0

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







5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	A	6001	1	14,14,15	1.25	2 (14%)	17,19,21	1.53	5 (29%)
5	BES	B	1001	4	19,22,22	0.49	0	23,29,29	0.93	1 (4%)
5	BES	A	1001	4	19,22,22	0.46	0	23,29,29	0.82	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BES	C	1001	4	19,22,22	0.42	0	23,29,29	0.98	2 (8%)
6	NAG	B	6000	1	14,14,15	0.65	0	17,19,21	0.98	1 (5%)
6	NAG	A	6000	1	14,14,15	0.93	1 (7%)	17,19,21	1.46	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
6	NAG	A	6001	1	1/1/5/7	2/6/23/26	0/1/1/1
5	BES	B	1001	4	-	3/20/24/24	0/1/1/1
5	BES	A	1001	4	-	3/20/24/24	0/1/1/1
5	BES	C	1001	4	-	3/20/24/24	0/1/1/1
6	NAG	B	6000	1	-	2/6/23/26	0/1/1/1
6	NAG	A	6000	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	6001	NAG	C1-C2	3.05	1.56	1.52
6	A	6001	NAG	O5-C1	2.74	1.48	1.43
6	A	6000	NAG	O5-C1	2.33	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	6000	NAG	C1-O5-C5	3.44	116.85	112.19
6	A	6001	NAG	O5-C1-C2	-3.06	106.46	111.29
6	A	6001	NAG	C6-C5-C4	-2.88	106.26	113.00
5	C	1001	BES	C4-N1-C3	-2.87	118.88	123.19
6	A	6000	NAG	O5-C5-C6	2.76	111.53	107.20
6	A	6001	NAG	C1-O5-C5	2.73	115.90	112.19
6	A	6001	NAG	O5-C5-C6	2.43	111.01	107.20
5	B	1001	BES	C4-N1-C3	-2.35	119.67	123.19
6	A	6000	NAG	O5-C1-C2	-2.23	107.77	111.29
5	C	1001	BES	C13-C4-N1	-2.16	105.95	109.80
6	B	6000	NAG	C1-O5-C5	2.06	114.99	112.19
5	A	1001	BES	C7-C6-C1	-2.02	109.17	113.46
6	A	6001	NAG	C4-C3-C2	-2.00	108.08	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	6001	NAG	C1

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	6001	NAG	C8-C7-N2-C2
6	A	6001	NAG	O7-C7-N2-C2
6	B	6000	NAG	C8-C7-N2-C2
6	B	6000	NAG	O7-C7-N2-C2
6	A	6000	NAG	C8-C7-N2-C2
6	A	6000	NAG	O7-C7-N2-C2
5	B	1001	BES	O2-C2-C3-N1
5	A	1001	BES	O2-C2-C3-N1
5	B	1001	BES	C5-C4-N1-C3
5	B	1001	BES	O2-C2-C3-O3
5	C	1001	BES	O2-C2-C3-N1
5	A	1001	BES	O2-C2-C3-O3
5	C	1001	BES	O2-C2-C3-O3
5	C	1001	BES	C5-C4-N1-C3
5	A	1001	BES	C5-C4-N1-C3

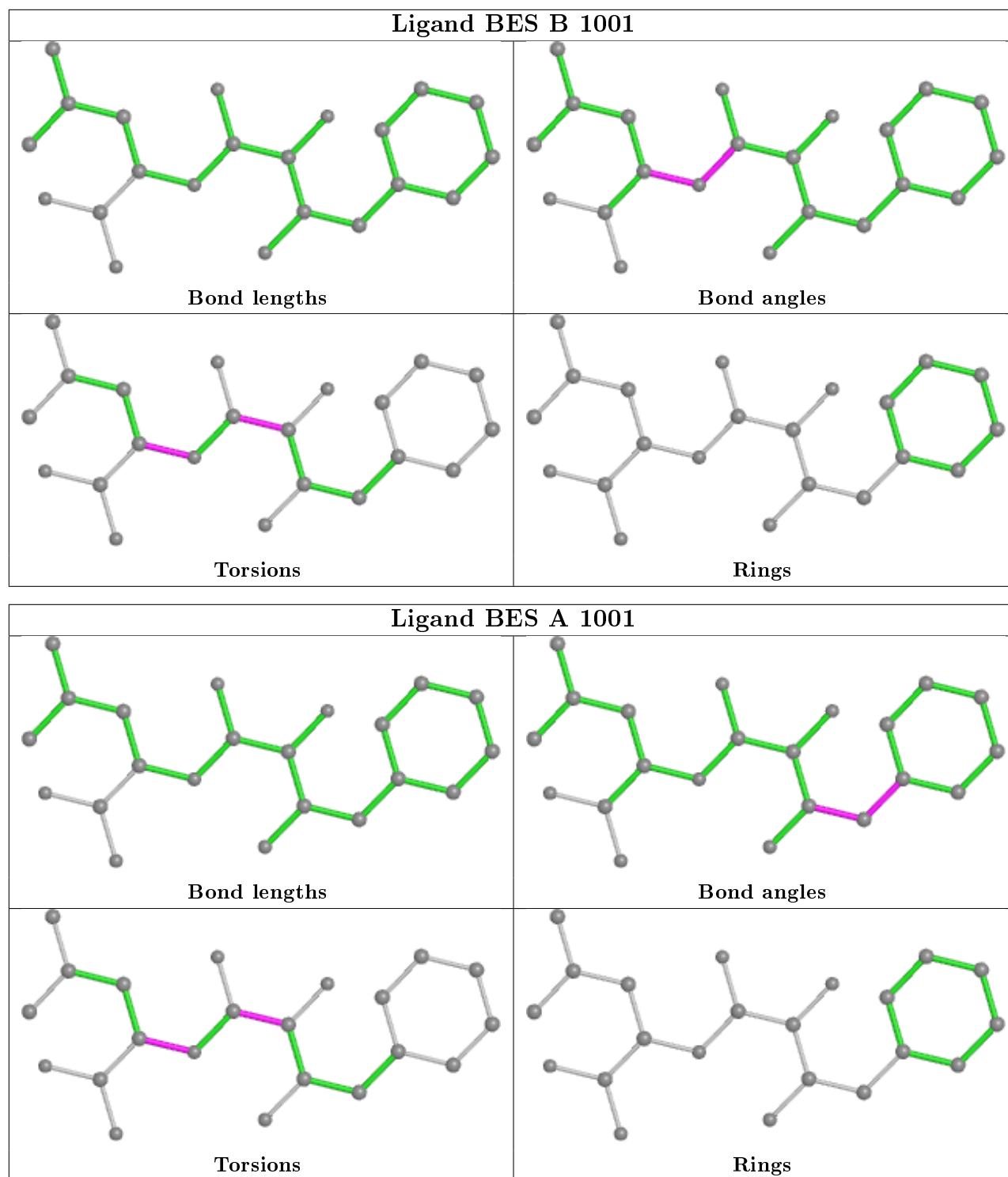
There are no ring outliers.

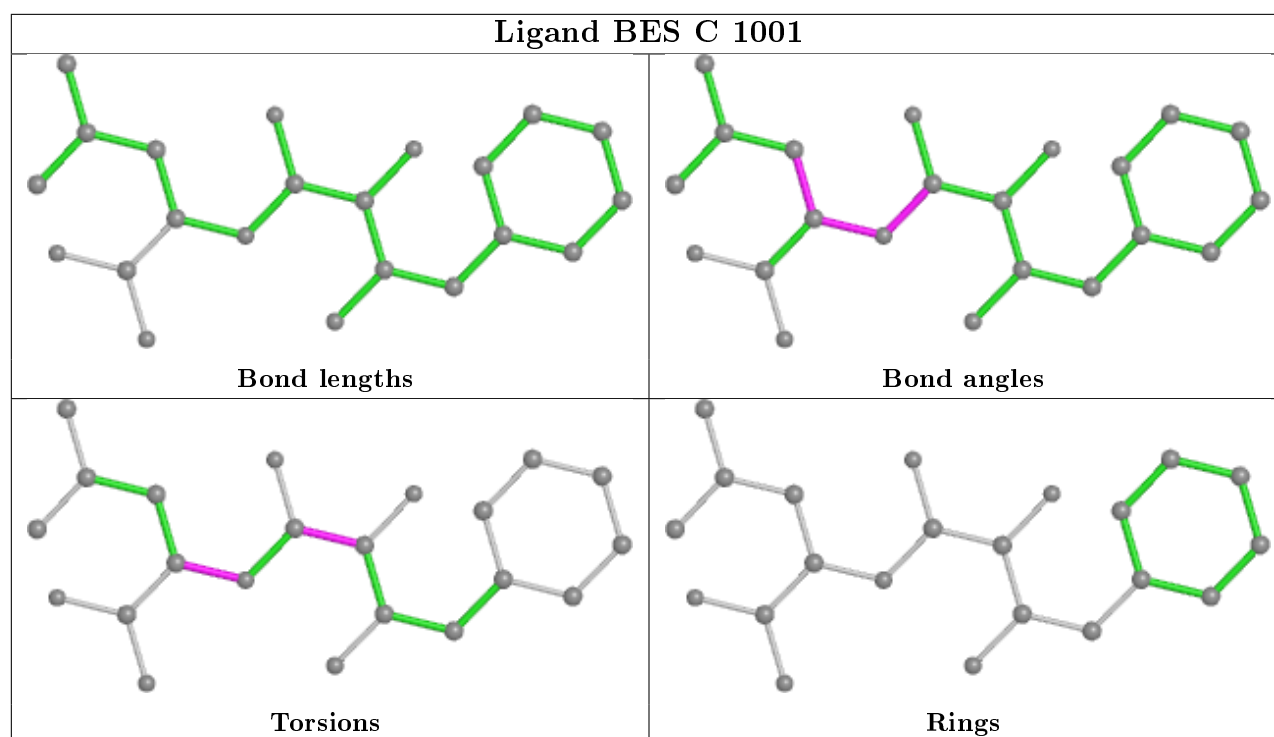
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	6001	NAG	1	0
5	B	1001	BES	10	0
5	A	1001	BES	2	0
5	C	1001	BES	6	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 than 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, 95th 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	818/921 (88%)	-0.23	20 (2%)	59 42	26, 57, 133, 238	11 (1%)
1	B	821/921 (89%)	-0.15	36 (4%)	34 21	24, 57, 130, 223	11 (1%)
1	C	818/921 (88%)	-0.25	27 (3%)	46 30	28, 57, 130, 223	12 (1%)
All	All	2457/2763 (88%)	-0.21	83 (3%)	45 29	24, 57, 131, 238	34 (1%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	339	SER	9.6
1	B	558	ASP	8.8
1	B	794	SER	8.5
1	B	557	PRO	8.4
1	B	339	SER	7.4
1	B	827	ILE	7.4
1	B	825	ASP	7.3
1	B	826	LYS	7.1
1	A	829	THR	6.0
1	C	794	SER	5.6
1	B	829	THR	5.5
1	B	792	SER	4.7
1	C	907	CYS	4.6
1	C	791	PHE	4.6
1	C	793	LEU	4.5
1	B	911	THR	4.5
1	B	556	ALA	4.5
1	A	889	GLU	4.3
1	C	762	SER	4.3
1	C	792	SER	4.2
1	B	824	GLY	4.2
1	A	857	TRP	4.1
1	C	757	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	339	SER	4.0
1	C	558	ASP	3.9
1	C	908	VAL	3.8
1	B	790	GLN	3.7
1	B	338	LYS	3.7
1	B	791	PHE	3.7
1	B	908	VAL	3.7
1	C	789	TYR	3.6
1	C	824	GLY	3.5
1	B	862	GLN	3.5
1	B	828	LYS	3.4
1	A	907	CYS	3.4
1	A	794	SER	3.2
1	A	832	PHE	3.2
1	B	912	ILE	3.2
1	C	829	THR	3.2
1	C	869	SER	3.2
1	B	759	GLY	3.1
1	A	871	ILE	3.0
1	B	337	GLU	3.0
1	A	851	GLN	2.8
1	A	415	SER	2.8
1	C	110	GLY	2.7
1	B	855	LYS	2.7
1	C	825	ASP	2.6
1	A	862	GLN	2.5
1	B	858	ASN	2.5
1	A	827	ILE	2.4
1	B	891	VAL	2.4
1	B	784	PHE	2.4
1	A	892	LYS	2.4
1	C	860	LEU	2.4
1	B	336	ALA	2.3
1	B	613	GLU	2.3
1	A	888	LEU	2.3
1	C	760	ASN	2.3
1	B	863	LYS	2.3
1	C	857	TRP	2.3
1	B	798	LYS	2.3
1	C	858	ASN	2.3
1	C	485	ILE	2.3
1	C	909	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	892	LYS	2.3
1	B	485	ILE	2.2
1	B	755	LYS	2.2
1	B	140	LEU	2.2
1	A	890	GLU	2.2
1	C	830	GLN	2.2
1	B	871	ILE	2.2
1	A	752	ARG	2.2
1	A	558	ASP	2.2
1	B	415	SER	2.2
1	B	868	SER	2.1
1	C	415	SER	2.1
1	C	850	TRP	2.1
1	A	789	TYR	2.1
1	C	911	THR	2.1
1	A	362	ASN	2.0
1	A	483	ALA	2.0
1	B	316	SER	2.0

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

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

6.3 Carbohydrates ⓘ

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, 95th 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
2	MAN	D	4	11/12	0.56	0.34	111,168,187,189	0
3	NAG	E	2	14/15	0.75	0.25	118,161,189,212	0
2	MAN	F	5	11/12	0.81	0.35	86,142,212,223	0
2	MAN	D	5	11/12	0.83	0.30	33,95,172,209	0
2	MAN	F	4	11/12	0.84	0.24	75,95,103,110	0
2	BMA	F	3	11/12	0.85	0.26	43,135,191,223	0
2	NAG	F	2	14/15	0.86	0.34	47,135,257,284	0
2	NAG	D	2	14/15	0.88	0.18	60,85,108,108	0
2	BMA	D	3	11/12	0.89	0.17	51,86,129,131	0
2	NAG	D	1	14/15	0.89	0.21	49,90,110,161	0

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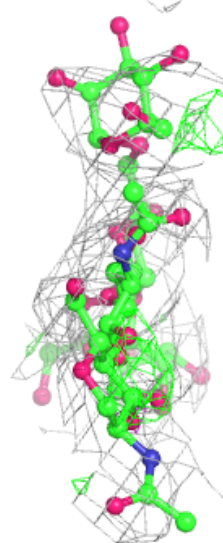
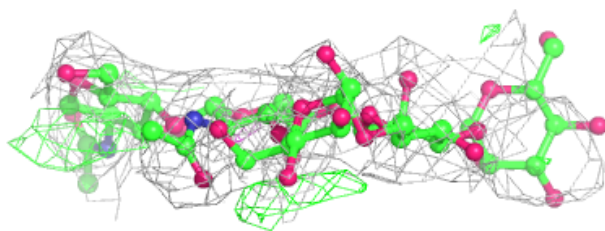
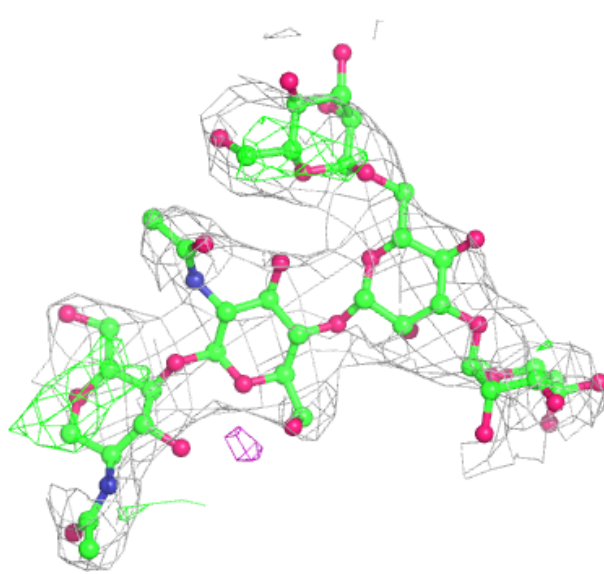
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	F	1	14/15	0.90	0.19	20,79,110,127	0
3	NAG	E	1	14/15	0.91	0.21	50,93,110,139	0

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.

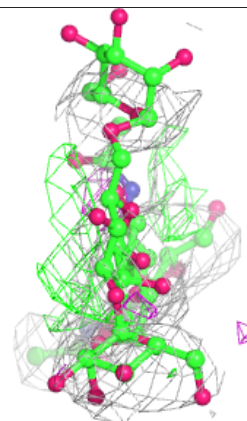
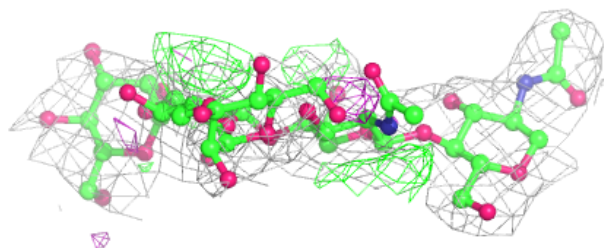
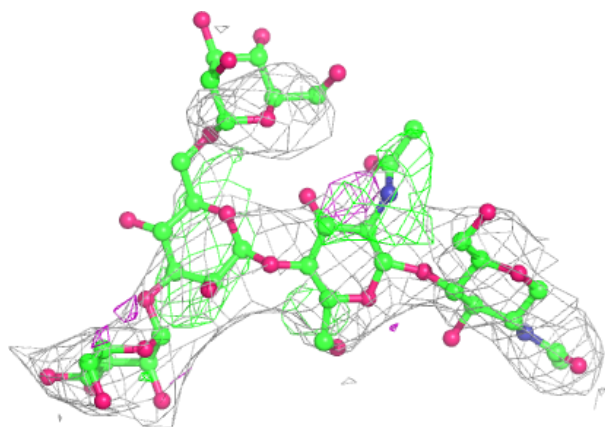
Electron density around Chain D:

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

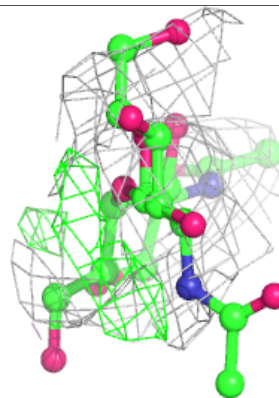
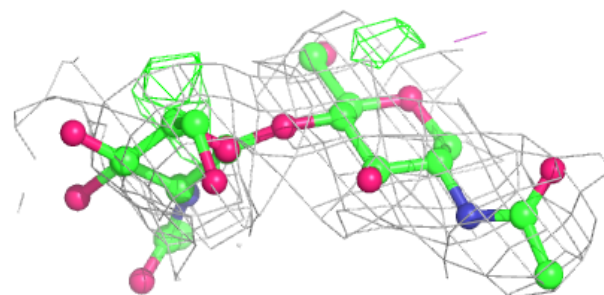
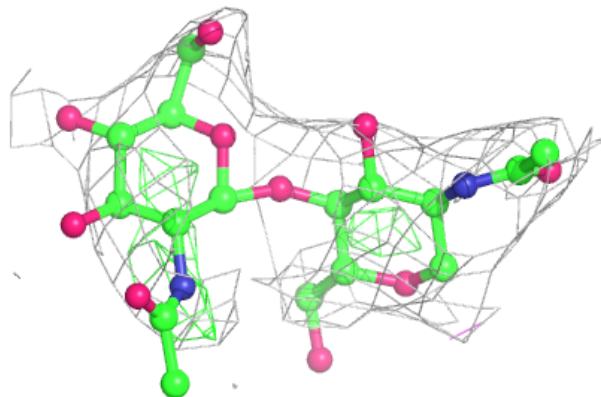


Electron density around Chain F:

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

**Electron density around Chain E:**

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

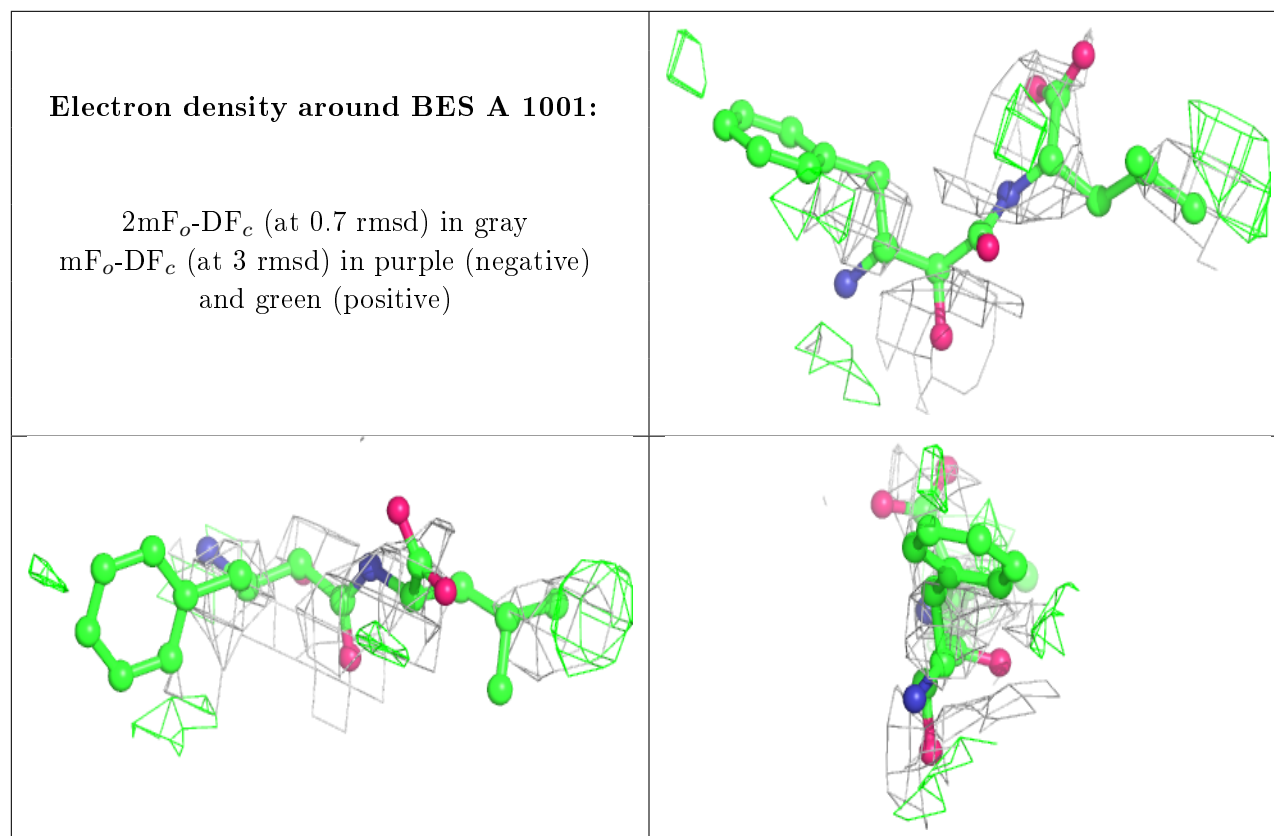


6.4 Ligands ⓘ

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, 95th 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.

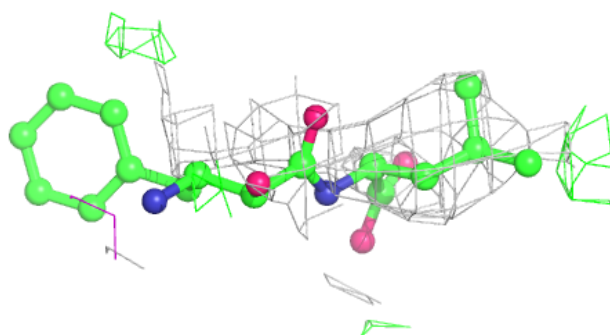
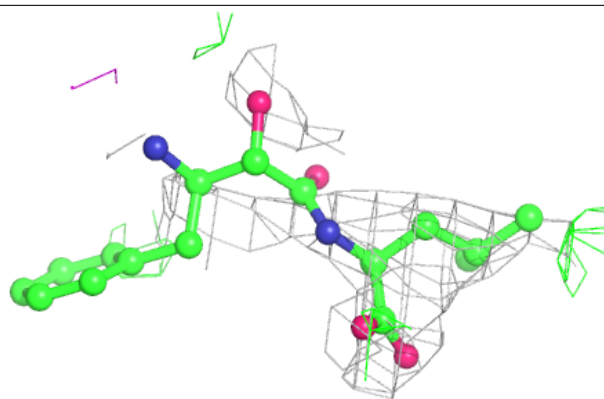
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	A	6001	14/15	0.74	0.17	72,140,150,153	0
6	NAG	B	6000	14/15	0.74	0.28	59,128,146,153	0
5	BES	A	1001	22/22	0.78	0.45	86,184,208,217	0
5	BES	C	1001	22/22	0.82	0.37	79,178,213,218	0
6	NAG	A	6000	14/15	0.82	0.19	76,119,141,145	0
5	BES	B	1001	22/22	0.88	0.38	121,167,185,218	0
4	ZN	B	1000	1/1	0.99	0.11	38,38,38,38	0
4	ZN	C	1000	1/1	0.99	0.12	38,38,38,38	0
4	ZN	A	1000	1/1	0.99	0.13	40,40,40,40	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.

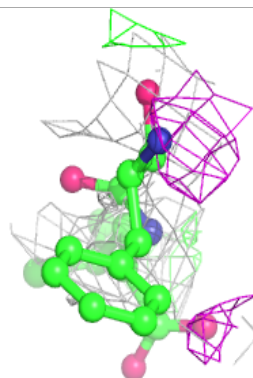
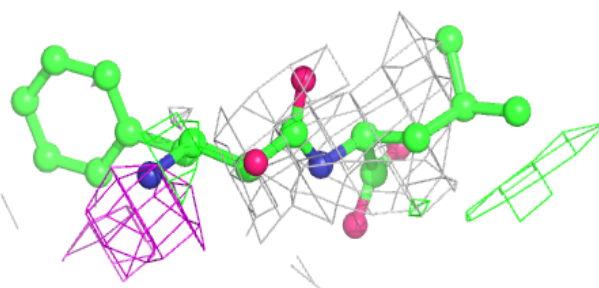
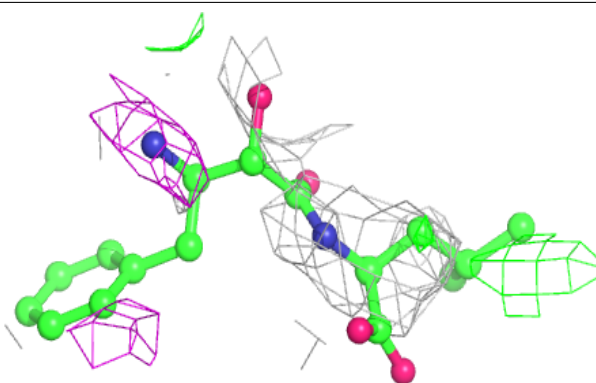


Electron density around BES C 1001:

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

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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6.5 Other polymers

There are no such residues in this entry.