



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:35 AM UTC

PDB ID : 3OBV / pdb_00003obv
Title : Autoinhibited Formin mDia1 Structure
Authors : Tomchick, D.R.; Rosen, M.K.; Otomo, T.
Deposited on : 2010-08-09
Resolution : 2.75 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

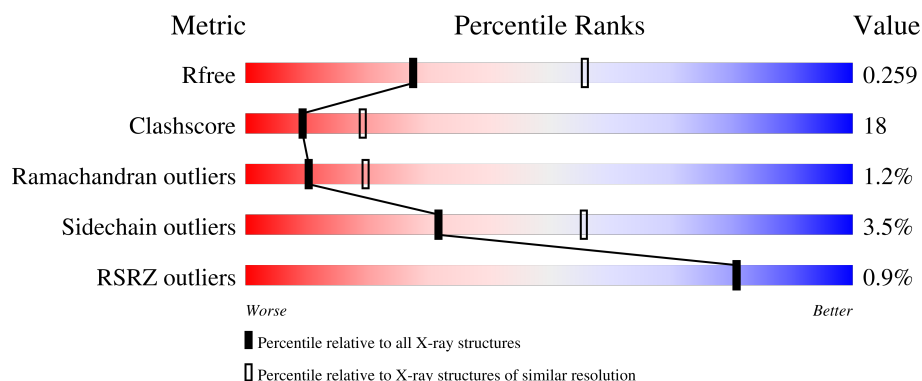
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

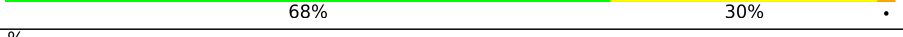
The reported resolution of this entry is 2.75 Å.

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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 of 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	327	
1	B	327	
1	C	327	
1	D	327	
2	E	457	

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Mol	Chain	Length	Quality of chain
2	F	457	
2	G	457	
2	H	457	
3	I	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLC	I	1	X	-	-	-
3	FRU	I	2	X	-	-	-
3	GLC	J	1	X	-	-	-
3	FRU	J	2	X	-	-	-
3	GLC	K	1	X	-	-	-
3	FRU	K	2	X	-	-	-
3	GLC	L	1	X	-	-	-
3	FRU	L	2	X	-	-	-
3	GLC	M	1	X	-	-	-
3	FRU	M	2	X	-	-	-
3	GLC	N	1	X	-	-	-
3	FRU	N	2	X	-	-	-
3	GLC	O	1	X	-	-	-
3	FRU	O	2	X	-	-	-
3	GLC	P	1	X	-	-	-
3	FRU	P	2	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 24400 atoms, of which 176 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.

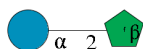
- Molecule 1 is a protein called Protein diaphanous homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2589	1625	445	497	22			
1	B	319	Total	C	N	O	S	0	0	0
			2571	1617	443	489	22			
1	C	322	Total	C	N	O	S	0	0	0
			2589	1625	445	497	22			
1	D	327	Total	C	N	O	S	0	0	0
			2632	1651	453	506	22			

- Molecule 2 is a protein called Protein diaphanous homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	419	Total	C	N	O	S	0	0	0
			3410	2154	579	656	21			
2	F	419	Total	C	N	O	S	0	0	0
			3414	2155	582	656	21			
2	G	420	Total	C	N	O	S	0	0	0
			3421	2160	583	657	21			
2	H	419	Total	C	N	O	S	0	0	0
			3414	2156	582	655	21			

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	H	O	0	0	0
			45	12	22	11			
3	J	2	Total	C	H	O	0	0	0
			45	12	22	11			

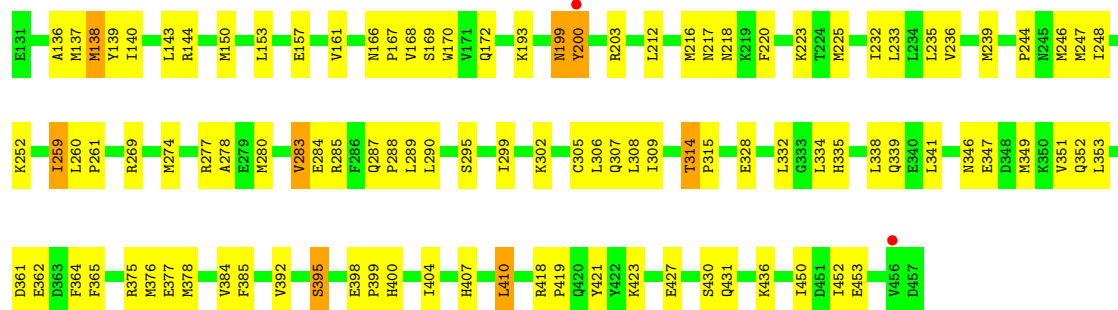
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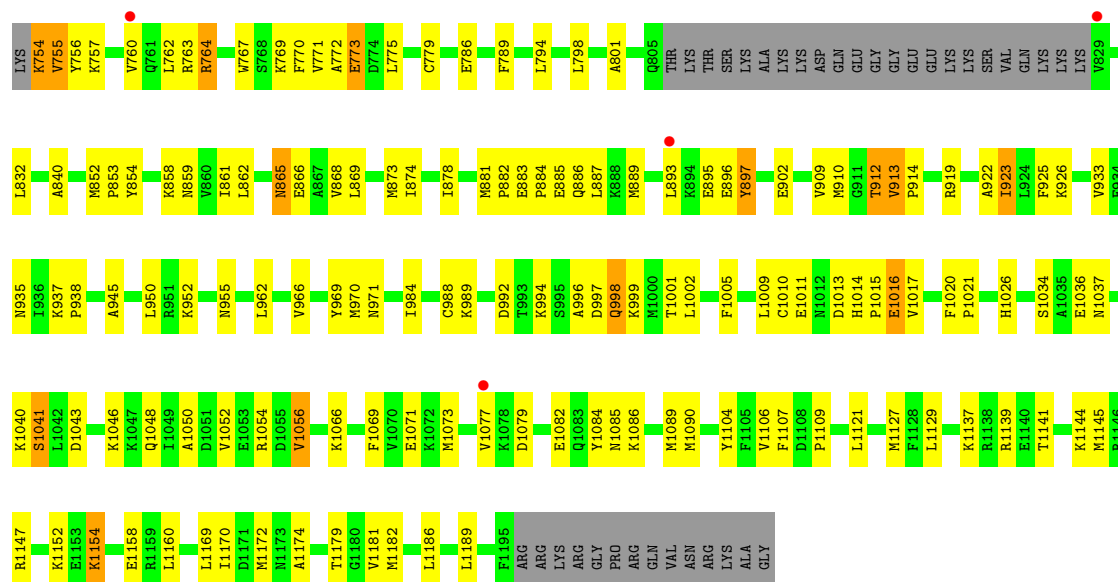
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	2	Total 45	C 12	H 22	O 11	0	0	0
3	L	2	Total 45	C 12	H 22	O 11	0	0	0
3	M	2	Total 45	C 12	H 22	O 11	0	0	0
3	N	2	Total 45	C 12	H 22	O 11	0	0	0
3	O	2	Total 45	C 12	H 22	O 11	0	0	0
3	P	2	Total 45	C 12	H 22	O 11	0	0	0



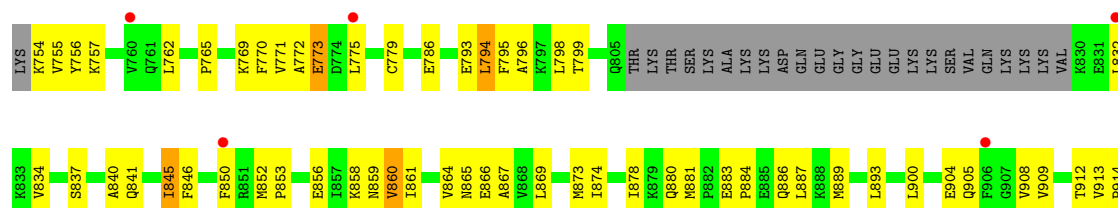
• Molecule 1: Protein diaphanous homolog 1

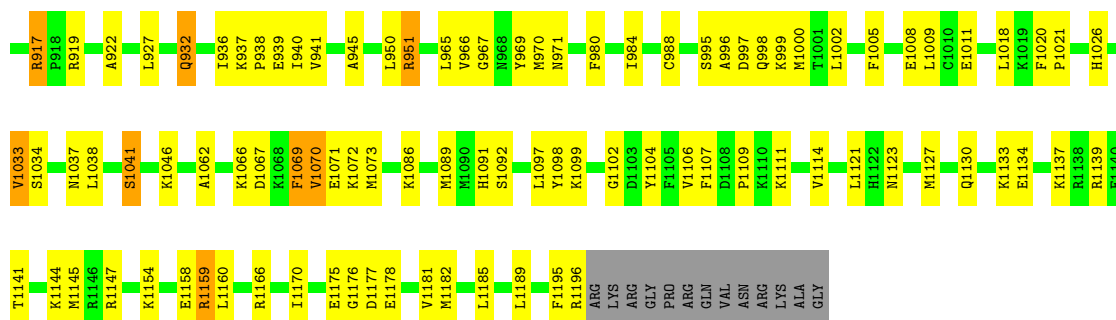


• Molecule 2: Protein diaphanous homolog 1

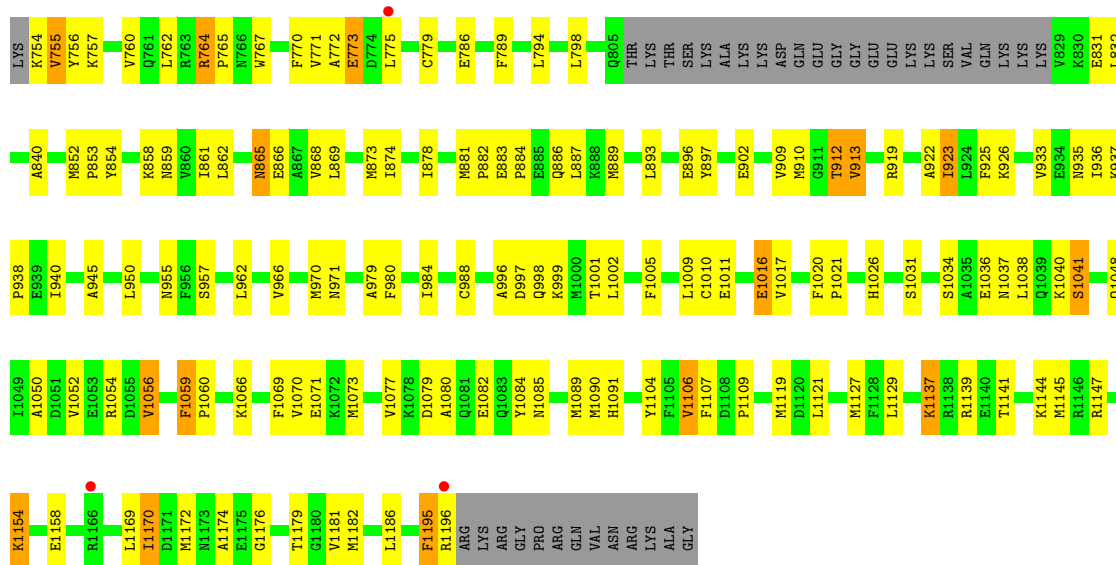


• Molecule 2: Protein diaphanous homolog 1

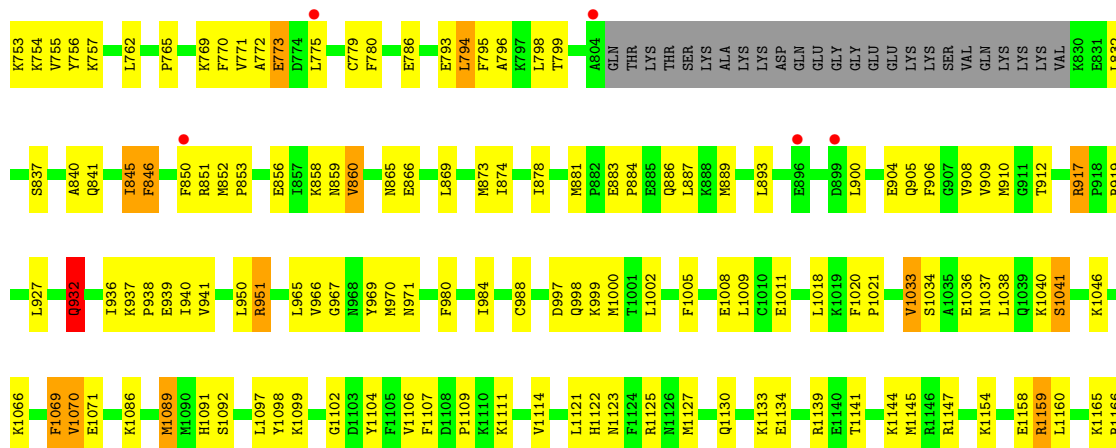


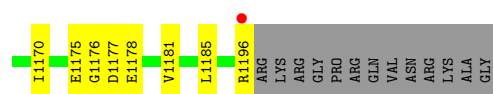


• Molecule 2: Protein diaphanous homolog 1



• Molecule 2: Protein diaphanous homolog 1





- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain I: 100%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain J: 50% 50%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain K: 100%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain L: 100%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain M: 50% 50%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain N: 100%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain O: 50% 50%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain P:

50%

50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.93Å 208.52Å 131.52Å 90.00° 102.74° 90.00°	Depositor
Resolution (Å)	29.95 – 2.75 29.95 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.95-2.75) 95.8 (29.95-2.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.199 , 0.261 0.196 , 0.259	Depositor DCC
R_{free} test set	1800 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 82.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24400	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: FRU, GLC

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	0.66	0/2626	0.95	4/3536 (0.1%)
1	B	0.58	0/2607	0.94	4/3510 (0.1%)
1	C	0.74	0/2626	1.00	3/3536 (0.1%)
1	D	0.67	0/2669	0.97	4/3594 (0.1%)
2	E	0.50	0/3462	0.86	7/4641 (0.2%)
2	F	0.55	2/3466 (0.1%)	0.84	0/4645
2	G	0.50	1/3473 (0.0%)	0.86	8/4655 (0.2%)
2	H	0.56	2/3466 (0.1%)	0.86	0/4644
All	All	0.59	5/24395 (0.0%)	0.91	30/32761 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	932	GLN	CD-NE2	-9.49	1.13	1.33
2	F	932	GLN	CD-NE2	-9.15	1.14	1.33
2	F	932	GLN	CD-OE1	-6.89	1.10	1.23
2	H	932	GLN	CD-OE1	-6.83	1.10	1.23
2	G	1195	PHE	CA-C	5.18	1.55	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	ASN	N-CA-C	7.13	120.09	108.26
1	C	196	THR	N-CA-C	6.93	117.42	108.34
2	E	913	VAL	CA-C-N	6.59	126.35	119.76
2	E	913	VAL	C-N-CA	6.59	126.35	119.76
2	E	755	VAL	N-CA-C	6.17	116.72	108.27
1	A	149	ASP	CB-CA-C	-6.04	109.60	116.54
1	C	199	ASN	N-CA-C	6.03	120.31	107.70
2	E	935	ASN	N-CA-C	-5.90	106.06	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	913	VAL	CA-C-N	5.85	125.61	119.76
2	G	913	VAL	C-N-CA	5.85	125.61	119.76
2	G	935	ASN	N-CA-C	-5.79	106.19	113.72
1	B	440	ASP	CA-C-N	5.76	125.72	119.78
1	B	440	ASP	C-N-CA	5.76	125.72	119.78
2	E	764	ARG	CA-C-N	5.61	126.85	119.84
2	E	764	ARG	C-N-CA	5.61	126.85	119.84
1	A	166	ASN	CA-C-N	5.56	125.46	119.85
1	A	166	ASN	C-N-CA	5.56	125.46	119.85
2	G	755	VAL	N-CA-C	5.54	115.86	108.27
1	B	421	TYR	N-CA-C	-5.41	105.28	111.07
1	B	295	SER	N-CA-C	5.40	120.28	111.37
1	A	199	ASN	N-CA-C	5.37	119.79	107.48
2	G	764	ARG	CA-C-N	5.29	126.45	119.84
2	G	764	ARG	C-N-CA	5.29	126.45	119.84
1	C	296	GLY	N-CA-C	5.20	120.05	113.24
1	D	314	THR	N-CA-C	5.14	120.59	113.45
2	E	897	TYR	N-CA-C	5.11	117.51	111.33
2	G	1059	PHE	CA-C-N	5.11	125.04	119.78
2	G	1059	PHE	C-N-CA	5.11	125.04	119.78
1	D	421	TYR	N-CA-C	-5.08	105.39	111.03
1	D	295	SER	N-CA-C	5.07	119.73	111.37

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2589	0	2594	80	0
1	B	2571	0	2584	98	0
1	C	2589	0	2594	83	0
1	D	2632	0	2637	100	0
2	E	3410	0	3416	143	0
2	F	3414	0	3420	170	0
2	G	3421	0	3429	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	3414	0	3425	158	0
3	I	23	22	16	0	0
3	J	23	22	14	3	0
3	K	23	22	15	0	0
3	L	23	22	15	0	0
3	M	23	22	15	2	0
3	N	23	22	15	5	0
3	O	23	22	16	1	0
3	P	23	22	16	4	0
All	All	24224	176	24221	872	0

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

All (872) 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:G:966:VAL:HG12	2:G:970:MET:HE2	1.28	1.14
2:G:771:VAL:H	2:G:775:LEU:HD12	1.13	1.10
2:E:966:VAL:HG12	2:E:970:MET:HE2	1.25	1.09
2:F:771:VAL:H	2:F:775:LEU:HD12	1.14	1.07
1:D:375:ARG:HH22	3:P:1:GLC:H61	1.12	1.07
2:H:771:VAL:H	2:H:775:LEU:HD12	1.12	1.06
2:E:771:VAL:H	2:E:775:LEU:HD12	1.19	1.05
1:C:375:ARG:HH22	3:N:1:GLC:H61	1.23	1.04
2:H:852:MET:HE2	2:H:856:GLU:HB3	1.42	1.01
2:G:754:LYS:HG3	2:G:755:VAL:H	1.25	1.00
2:E:937:LYS:HE3	2:E:1090:MET:HE1	1.43	1.00
2:G:937:LYS:HE3	2:G:1090:MET:HE1	1.42	1.00
2:E:919:ARG:O	2:E:923:ILE:HG13	1.61	0.99
2:E:754:LYS:HG3	2:E:755:VAL:H	1.23	0.99
2:F:852:MET:HE2	2:F:856:GLU:HB3	1.42	0.99
2:F:832:LEU:HD21	2:F:840:ALA:CB	1.94	0.98
2:E:1147:ARG:NH1	1:B:376:MET:HG3	1.78	0.97
2:H:771:VAL:H	2:H:775:LEU:CD1	1.77	0.97
2:F:771:VAL:H	2:F:775:LEU:CD1	1.78	0.96
2:G:919:ARG:O	2:G:923:ILE:HG13	1.65	0.94
2:G:1147:ARG:NH1	1:D:376:MET:HG3	1.83	0.92
2:F:869:LEU:HD23	2:F:873:MET:CE	1.99	0.92
2:H:869:LEU:HD23	2:H:873:MET:CE	2.00	0.91
1:D:375:ARG:HH22	3:P:1:GLC:C6	1.84	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LEU:HD13	1:A:332:LEU:HB3	1.54	0.90
1:C:290:LEU:HD13	1:C:332:LEU:HB3	1.53	0.90
1:B:216:MET:HE1	1:B:225:MET:HG2	1.55	0.89
2:H:771:VAL:N	2:H:775:LEU:HD12	1.88	0.89
2:E:858:LYS:NZ	2:E:912:THR:HG21	1.89	0.87
2:F:771:VAL:N	2:F:775:LEU:HD12	1.88	0.87
2:G:1154:LYS:O	2:G:1158:GLU:HG2	1.75	0.86
2:H:883:GLU:HG3	2:H:884:PRO:HD2	1.56	0.86
2:F:883:GLU:HG3	2:F:884:PRO:HD2	1.55	0.86
2:E:881:MET:CE	2:E:887:LEU:HD11	2.07	0.85
1:C:418:ARG:HB3	1:C:419:PRO:HD3	1.56	0.85
1:D:216:MET:HE1	1:D:225:MET:HG2	1.58	0.85
1:C:430:SER:HA	1:D:407:HIS:CD2	2.12	0.85
2:F:1170:ILE:HD12	2:F:1181:VAL:HG13	1.58	0.84
1:C:431:GLN:HE22	1:C:451:ASP:H	1.25	0.84
2:E:754:LYS:HG3	2:E:755:VAL:N	1.90	0.84
1:A:418:ARG:HB3	1:A:419:PRO:HD3	1.58	0.84
2:F:859:ASN:ND2	2:F:1066:LYS:HD3	1.93	0.83
2:G:881:MET:CE	2:G:887:LEU:HD11	2.08	0.83
2:E:1154:LYS:O	2:E:1158:GLU:HG2	1.76	0.83
1:B:392:VAL:O	1:B:395:SER:HB3	1.78	0.83
2:G:858:LYS:NZ	2:G:912:THR:HG21	1.93	0.83
2:H:859:ASN:ND2	2:H:1066:LYS:HD3	1.93	0.82
1:C:377:GLU:OE1	2:H:1144:LYS:HE2	1.79	0.82
1:B:290:LEU:CD1	1:B:332:LEU:HB3	2.09	0.82
2:G:754:LYS:HG3	2:G:755:VAL:N	1.94	0.81
1:D:375:ARG:NH2	3:P:1:GLC:H61	1.94	0.81
1:D:290:LEU:CD1	1:D:332:LEU:HB3	2.11	0.81
1:C:375:ARG:HH22	3:N:1:GLC:C6	1.95	0.80
1:A:398:GLU:HB3	1:A:399:PRO:HD3	1.61	0.80
2:H:1165:LYS:HD3	2:H:1196:ARG:HD2	1.63	0.80
2:H:1020:PHE:CD2	2:H:1021:PRO:HD3	2.17	0.80
2:H:853:PRO:HG2	2:H:856:GLU:HG3	1.64	0.80
1:B:216:MET:CE	1:B:225:MET:HG2	2.12	0.79
2:F:832:LEU:HD21	2:F:840:ALA:HB2	1.64	0.79
2:G:1169:LEU:HD13	1:D:259:ILE:CG2	2.12	0.79
2:G:909:VAL:O	2:G:912:THR:HB	1.84	0.78
1:C:398:GLU:HB3	1:C:399:PRO:HD3	1.64	0.78
1:C:430:SER:HA	1:D:407:HIS:HD2	1.48	0.78
2:G:1176:GLY:O	1:D:168:VAL:HG21	1.84	0.78
2:F:853:PRO:HG2	2:F:856:GLU:HG3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:937:LYS:O	2:H:941:VAL:HG23	1.82	0.78
2:H:1170:ILE:HD12	2:H:1181:VAL:HG13	1.66	0.77
1:D:216:MET:CE	1:D:225:MET:HG2	2.14	0.77
2:F:937:LYS:O	2:F:941:VAL:HG23	1.84	0.77
1:D:244:PRO:O	1:D:248:ILE:HG13	1.85	0.77
2:F:881:MET:HE1	2:F:887:LEU:HD11	1.66	0.77
1:A:377:GLU:OE1	2:F:1144:LYS:HE2	1.85	0.77
2:E:909:VAL:O	2:E:912:THR:HB	1.84	0.77
1:A:430:SER:HA	1:B:407:HIS:CD2	2.20	0.76
2:F:770:PHE:HA	2:F:775:LEU:HD13	1.68	0.76
2:G:1016:GLU:H	2:G:1016:GLU:CD	1.93	0.76
1:A:199:ASN:CG	1:A:201:ASP:HB2	2.10	0.76
2:F:881:MET:CE	2:F:887:LEU:HD11	2.15	0.76
2:E:865:ASN:OD1	2:E:868:VAL:HG23	1.85	0.76
2:G:1037:ASN:O	2:G:1041:SER:HB3	1.86	0.76
2:H:770:PHE:HA	2:H:775:LEU:HD13	1.66	0.75
1:B:216:MET:HE1	1:B:225:MET:HE2	1.66	0.75
2:E:1037:ASN:O	2:E:1041:SER:HB3	1.87	0.75
2:G:771:VAL:N	2:G:775:LEU:HD12	1.98	0.75
2:F:883:GLU:HG3	2:F:884:PRO:CD	2.16	0.75
2:H:883:GLU:HG3	2:H:884:PRO:CD	2.16	0.75
2:E:1169:LEU:HD13	1:B:259:ILE:CG2	2.17	0.75
1:D:166:ASN:HB3	1:D:167:PRO:HD2	1.69	0.75
2:E:1182:MET:HB3	1:B:217:ASN:HA	1.67	0.74
2:G:883:GLU:H	2:G:886:GLN:HE21	1.35	0.74
2:G:865:ASN:OD1	2:G:868:VAL:HG23	1.86	0.74
1:A:431:GLN:HE22	1:A:451:ASP:H	1.33	0.74
2:E:922:ALA:HB1	2:E:1073:MET:HE2	1.70	0.74
2:E:1147:ARG:HH12	1:B:376:MET:HG3	1.51	0.73
2:F:1020:PHE:CD2	2:F:1021:PRO:HD3	2.22	0.73
2:G:922:ALA:HB1	2:G:1073:MET:HE2	1.70	0.73
1:C:375:ARG:NH2	3:N:1:GLC:H61	2.03	0.73
2:E:1016:GLU:CD	2:E:1016:GLU:H	1.97	0.73
1:D:302:LYS:HB3	1:D:349:MET:HE1	1.70	0.73
2:E:883:GLU:H	2:E:886:GLN:HE21	1.36	0.72
2:H:951:ARG:HG3	2:H:951:ARG:HH11	1.54	0.72
2:G:771:VAL:O	2:G:775:LEU:HB2	1.89	0.72
2:G:858:LYS:HE3	2:G:912:THR:CG2	2.18	0.72
2:H:832:LEU:HD21	2:H:840:ALA:CB	2.19	0.72
2:H:881:MET:CE	2:H:887:LEU:HD11	2.19	0.72
1:B:302:LYS:HB3	1:B:349:MET:HE1	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:951:ARG:HG3	2:F:951:ARG:HH11	1.54	0.71
1:D:392:VAL:O	1:D:395:SER:HB3	1.89	0.71
2:H:881:MET:HE1	2:H:887:LEU:HD11	1.72	0.71
1:A:199:ASN:OD1	1:A:201:ASP:HB2	1.91	0.71
2:E:881:MET:HE2	2:E:887:LEU:HD11	1.72	0.71
2:G:881:MET:HE2	2:G:887:LEU:HD11	1.73	0.70
1:D:216:MET:HE1	1:D:225:MET:HE2	1.72	0.70
2:H:845:ILE:HG22	2:H:846:PHE:N	2.07	0.70
2:H:856:GLU:O	2:H:860:VAL:HG23	1.92	0.69
2:F:997:ASP:O	2:F:999:LYS:N	2.24	0.69
2:H:869:LEU:HD23	2:H:873:MET:HE1	1.74	0.69
2:F:869:LEU:HD23	2:F:873:MET:HE1	1.73	0.69
2:E:966:VAL:CG1	2:E:970:MET:HE2	2.14	0.69
1:B:212:LEU:O	1:B:216:MET:HG2	1.92	0.69
2:G:858:LYS:CE	2:G:912:THR:HG21	2.22	0.69
1:D:212:LEU:O	1:D:216:MET:HG2	1.92	0.69
2:E:858:LYS:HE3	2:E:912:THR:CG2	2.23	0.69
1:C:283:VAL:HG12	1:C:284:GLU:N	2.07	0.69
1:C:392:VAL:O	1:C:395:SER:HB3	1.93	0.69
2:H:859:ASN:HD21	2:H:1066:LYS:HD3	1.58	0.69
2:E:771:VAL:O	2:E:775:LEU:HB2	1.92	0.68
2:F:859:ASN:HD21	2:F:1066:LYS:HD3	1.57	0.68
1:B:244:PRO:O	1:B:248:ILE:HG13	1.93	0.68
2:F:771:VAL:O	2:F:775:LEU:HB2	1.93	0.68
2:F:856:GLU:O	2:F:860:VAL:HG23	1.93	0.68
1:A:367:LEU:HD23	1:A:434:LEU:HD23	1.74	0.68
1:B:248:ILE:O	1:B:252:LYS:HG3	1.94	0.68
1:B:306:LEU:HD21	1:B:353:LEU:HD23	1.76	0.68
2:G:966:VAL:CG1	2:G:970:MET:HE2	2.17	0.67
2:G:1147:ARG:HH12	1:D:376:MET:HG3	1.57	0.67
2:E:852:MET:HG2	2:E:853:PRO:HD2	1.76	0.67
1:A:367:LEU:CD2	1:A:434:LEU:HD23	2.25	0.67
2:G:1050:ALA:O	2:G:1054:ARG:HG2	1.94	0.67
2:G:1182:MET:HB3	1:D:217:ASN:HA	1.77	0.67
1:A:430:SER:HA	1:B:407:HIS:HD2	1.59	0.67
1:B:278:ALA:HB2	1:B:285:ARG:HA	1.77	0.66
2:G:859:ASN:ND2	2:G:1066:LYS:HD3	2.11	0.66
2:E:1050:ALA:O	2:E:1054:ARG:HG2	1.95	0.66
2:E:1141:THR:HG22	2:E:1145:MET:HE2	1.77	0.66
2:G:970:MET:HE1	2:G:1002:LEU:HD22	1.76	0.66
2:G:1141:THR:HG22	2:G:1145:MET:HE2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:858:LYS:HE3	2:G:912:THR:HG21	1.77	0.66
2:G:1020:PHE:CD2	2:G:1021:PRO:HD3	2.30	0.66
2:G:764:ARG:HD2	2:H:971:ASN:OD1	1.96	0.66
2:G:771:VAL:H	2:G:775:LEU:CD1	2.00	0.66
2:H:771:VAL:O	2:H:775:LEU:HB2	1.96	0.66
2:H:988:CYS:SG	2:H:1127:MET:HE3	2.36	0.66
2:H:852:MET:HE2	2:H:856:GLU:CB	2.24	0.65
2:E:859:ASN:ND2	2:E:1066:LYS:HD3	2.11	0.65
2:F:1141:THR:HG22	2:F:1145:MET:HE2	1.78	0.65
1:B:299:ILE:HG21	1:B:346:ASN:ND2	2.10	0.65
1:D:278:ALA:HB2	1:D:285:ARG:HA	1.78	0.65
2:H:853:PRO:CG	2:H:856:GLU:HG3	2.27	0.65
1:A:392:VAL:O	1:A:395:SER:HB3	1.97	0.65
2:F:869:LEU:HD22	2:F:874:ILE:HD11	1.78	0.65
1:B:163:LEU:HD23	1:B:171:VAL:HG22	1.78	0.65
2:F:853:PRO:CG	2:F:856:GLU:HG3	2.26	0.65
2:G:970:MET:HE1	2:G:1002:LEU:CD2	2.27	0.65
2:E:858:LYS:HZ2	2:E:912:THR:HG21	1.62	0.65
1:B:190:HIS:CD2	1:B:205:GLN:NE2	2.64	0.65
2:F:869:LEU:HA	2:F:873:MET:CE	2.27	0.65
2:E:858:LYS:CE	2:E:912:THR:HG21	2.26	0.64
2:H:1141:THR:HG22	2:H:1145:MET:HE2	1.78	0.64
2:E:832:LEU:HD21	2:E:840:ALA:CB	2.26	0.64
1:B:216:MET:CE	1:B:225:MET:HE2	2.27	0.64
2:F:845:ILE:HG22	2:F:846:PHE:N	2.12	0.64
2:E:1020:PHE:CD2	2:E:1021:PRO:HD3	2.32	0.64
2:H:881:MET:HE1	2:H:887:LEU:HD21	1.77	0.64
2:H:997:ASP:O	2:H:999:LYS:N	2.23	0.64
1:D:299:ILE:HG21	1:D:346:ASN:ND2	2.11	0.64
2:G:852:MET:HG2	2:G:853:PRO:HD2	1.78	0.64
1:D:302:LYS:HB3	1:D:349:MET:CE	2.28	0.63
1:B:302:LYS:HD3	1:B:341:LEU:CD2	2.27	0.63
1:B:456:VAL:HG12	1:B:457:ASP:N	2.12	0.63
1:D:169:SER:HA	1:D:172:GLN:HG3	1.78	0.63
2:H:869:LEU:HA	2:H:873:MET:CE	2.28	0.63
2:H:869:LEU:HD22	2:H:874:ILE:HD11	1.80	0.63
2:E:771:VAL:N	2:E:775:LEU:HD12	2.04	0.63
2:E:771:VAL:H	2:E:775:LEU:CD1	2.06	0.63
2:E:970:MET:HE1	2:E:1002:LEU:CD2	2.29	0.63
2:E:970:MET:HE1	2:E:1002:LEU:HD22	1.81	0.63
2:F:988:CYS:SG	2:F:1127:MET:HE3	2.39	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:762:LEU:HD11	2:H:969:TYR:HE2	1.64	0.63
2:G:770:PHE:HA	2:G:775:LEU:HD13	1.79	0.63
1:A:283:VAL:HG12	1:A:284:GLU:N	2.14	0.63
1:B:233:LEU:HD12	1:B:233:LEU:O	1.99	0.63
2:F:966:VAL:HG12	2:F:970:MET:HE2	1.79	0.63
2:H:1037:ASN:O	2:H:1041:SER:HB2	1.99	0.63
1:A:431:GLN:HE22	1:A:451:ASP:N	1.98	0.62
1:C:290:LEU:CD1	1:C:332:LEU:HB3	2.28	0.62
1:B:378:MET:HB3	1:B:384:VAL:HG22	1.81	0.62
1:D:248:ILE:O	1:D:252:LYS:HG3	1.99	0.62
1:C:199:ASN:ND2	1:C:201:ASP:HB2	2.14	0.62
1:A:375:ARG:HH22	3:J:1:GLC:H61	1.65	0.62
1:A:287:GLN:HB3	1:A:288:PRO:HD3	1.81	0.62
1:D:378:MET:HB3	1:D:384:VAL:HG22	1.81	0.61
1:B:335:HIS:HE1	1:B:339:GLN:HE21	1.48	0.61
2:G:881:MET:CE	2:G:882:PRO:HD2	2.31	0.61
1:D:335:HIS:CE1	1:D:339:GLN:HE21	2.18	0.61
2:H:966:VAL:HG12	2:H:970:MET:HE2	1.82	0.61
1:C:367:LEU:HD23	1:C:434:LEU:HD23	1.83	0.61
2:H:869:LEU:HA	2:H:873:MET:HE1	1.81	0.61
1:D:150:MET:HE1	1:D:203:ARG:NH2	2.16	0.61
1:A:427:GLU:HG3	3:J:1:GLC:O3	2.01	0.61
1:B:335:HIS:CE1	1:B:339:GLN:HE21	2.18	0.61
1:D:200:TYR:CD2	1:D:203:ARG:NH2	2.69	0.61
2:E:881:MET:HE3	2:E:882:PRO:HD2	1.81	0.60
1:D:306:LEU:HD21	1:D:353:LEU:HD23	1.81	0.60
1:D:398:GLU:HB3	1:D:399:PRO:HD3	1.81	0.60
2:F:881:MET:HE1	2:F:887:LEU:HD21	1.83	0.60
1:D:335:HIS:HE1	1:D:339:GLN:HE21	1.48	0.60
1:A:290:LEU:CD1	1:A:332:LEU:HB3	2.30	0.60
1:D:364:PHE:CD1	1:D:436:LYS:HA	2.36	0.60
2:E:1147:ARG:NH1	1:B:376:MET:CG	2.59	0.60
2:F:869:LEU:HA	2:F:873:MET:HE1	1.83	0.60
2:G:1169:LEU:HD13	1:D:259:ILE:HG23	1.82	0.60
2:E:874:ILE:O	2:E:878:ILE:HG13	2.02	0.60
2:F:1170:ILE:HG13	2:F:1185:LEU:HD21	1.84	0.60
1:A:138:MET:HE2	1:A:138:MET:HA	1.84	0.60
2:F:904:GLU:O	2:F:908:VAL:HG23	2.02	0.60
2:H:1170:ILE:HG13	2:H:1185:LEU:HD21	1.83	0.60
2:E:881:MET:CE	2:E:882:PRO:HD2	2.32	0.59
2:F:852:MET:HE2	2:F:856:GLU:CB	2.24	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:988:CYS:HB3	2:F:1127:MET:HE1	1.84	0.59
2:F:997:ASP:C	2:F:999:LYS:H	2.11	0.59
2:H:1033:VAL:CG1	2:H:1034:SER:N	2.65	0.59
2:F:917:ARG:HH11	2:F:917:ARG:HB2	1.67	0.59
1:D:216:MET:CE	1:D:225:MET:HE2	2.33	0.59
1:B:302:LYS:HD3	1:B:341:LEU:HD22	1.83	0.59
1:C:137:MET:HE2	1:C:138:MET:CE	2.32	0.59
2:G:762:LEU:HD11	2:H:969:TYR:CE2	2.36	0.59
1:A:216:MET:HE2	1:A:225:MET:HE2	1.83	0.59
2:G:912:THR:HG22	2:G:913:VAL:N	2.17	0.59
1:A:374:ILE:HD12	1:B:410:LEU:HD13	1.84	0.59
2:H:883:GLU:H	2:H:886:GLN:NE2	2.01	0.59
1:D:153:LEU:O	1:D:157:GLU:HG3	2.03	0.59
2:H:1123:ASN:O	2:H:1127:MET:HG3	2.02	0.59
2:E:754:LYS:CG	2:E:755:VAL:N	2.65	0.59
2:E:883:GLU:HG3	2:E:884:PRO:HD2	1.84	0.59
1:C:431:GLN:NE2	1:C:451:ASP:H	1.97	0.59
2:G:881:MET:HE3	2:G:882:PRO:HD2	1.85	0.59
2:E:858:LYS:HE3	2:E:912:THR:HG21	1.85	0.58
1:B:364:PHE:CD1	1:B:436:LYS:HA	2.38	0.58
1:D:302:LYS:HD3	1:D:341:LEU:HD22	1.84	0.58
1:A:219:LYS:HE3	2:F:1178:GLU:OE1	2.03	0.58
2:G:874:ILE:O	2:G:878:ILE:HG13	2.04	0.58
2:F:883:GLU:H	2:F:886:GLN:NE2	2.01	0.58
2:F:1008:GLU:HG3	2:F:1139:ARG:NH1	2.18	0.58
1:D:302:LYS:HD3	1:D:341:LEU:CD2	2.32	0.58
2:H:832:LEU:HD21	2:H:840:ALA:HB2	1.85	0.58
1:A:166:ASN:HD22	1:A:170:TRP:CG	2.22	0.58
2:F:1037:ASN:O	2:F:1041:SER:HB2	2.04	0.58
2:F:1033:VAL:CG1	2:F:1034:SER:N	2.67	0.58
1:A:239:MET:HA	1:A:247:MET:HG3	1.86	0.57
2:E:910:MET:C	2:E:912:THR:H	2.12	0.57
1:B:216:MET:HE1	1:B:225:MET:CE	2.34	0.57
1:B:302:LYS:HB3	1:B:349:MET:CE	2.34	0.57
1:C:367:LEU:CD2	1:C:434:LEU:HD23	2.34	0.57
1:B:290:LEU:CD1	1:B:332:LEU:CB	2.82	0.57
1:B:314:THR:HB	1:B:315:PRO:HD3	1.86	0.57
2:E:1144:LYS:HE2	1:B:377:GLU:OE1	2.05	0.57
2:G:779:CYS:HB2	2:H:1104:TYR:O	2.05	0.57
2:G:866:GLU:OE2	2:G:926:LYS:HE3	2.05	0.57
1:D:314:THR:HB	1:D:315:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:917:ARG:HH11	2:H:917:ARG:HB2	1.68	0.57
1:A:393:LYS:HA	1:A:398:GLU:OE1	2.04	0.57
2:E:779:CYS:HB2	2:F:1104:TYR:O	2.04	0.57
2:E:854:TYR:O	2:E:909:VAL:HG11	2.04	0.57
1:C:341:LEU:HD22	1:C:349:MET:HE3	1.85	0.57
1:D:172:GLN:HA	1:D:220:PHE:CE2	2.39	0.57
1:B:190:HIS:CD2	1:B:205:GLN:HE21	2.22	0.57
1:C:138:MET:HE2	1:C:138:MET:HA	1.85	0.57
1:B:153:LEU:O	1:B:157:GLU:HG3	2.04	0.57
2:G:1147:ARG:NH1	1:D:376:MET:CG	2.65	0.57
2:G:1147:ARG:HH11	1:D:376:MET:HG3	1.65	0.57
2:H:1154:LYS:O	2:H:1158:GLU:HG2	2.04	0.57
1:D:450:ILE:HG22	1:D:452:ILE:HG23	1.87	0.57
2:H:937:LYS:N	2:H:938:PRO:CD	2.67	0.57
2:H:997:ASP:C	2:H:999:LYS:H	2.11	0.57
2:G:980:PHE:HZ	2:H:753:LYS:HB3	1.70	0.57
1:D:290:LEU:CD1	1:D:332:LEU:CB	2.83	0.57
2:E:789:PHE:HB2	2:F:965:LEU:HD22	1.87	0.56
2:G:754:LYS:CG	2:G:755:VAL:N	2.67	0.56
2:H:1008:GLU:HG3	2:H:1139:ARG:NH1	2.19	0.56
2:E:1169:LEU:HD13	1:B:259:ILE:HG23	1.85	0.56
2:F:988:CYS:CB	2:F:1127:MET:HE1	2.35	0.56
2:E:754:LYS:HB2	2:E:786:GLU:CD	2.31	0.56
1:B:239:MET:HA	1:B:247:MET:HG3	1.86	0.56
2:H:1020:PHE:CG	2:H:1021:PRO:HD3	2.39	0.56
1:A:431:GLN:NE2	1:A:451:ASP:H	2.01	0.56
2:G:754:LYS:HB2	2:G:786:GLU:CD	2.31	0.56
2:G:858:LYS:HE3	2:G:912:THR:HG22	1.87	0.56
2:G:910:MET:C	2:G:912:THR:H	2.13	0.56
2:E:997:ASP:O	2:E:999:LYS:N	2.34	0.56
1:C:199:ASN:CG	1:C:201:ASP:HB2	2.30	0.56
1:D:233:LEU:HD12	1:D:233:LEU:O	2.05	0.56
2:H:1159:ARG:CG	2:H:1160:LEU:N	2.68	0.56
1:C:287:GLN:HB3	1:C:288:PRO:HD3	1.86	0.56
2:E:770:PHE:HA	2:E:775:LEU:HD13	1.87	0.56
2:E:1170:ILE:HD11	2:E:1181:VAL:HG13	1.87	0.56
2:F:1123:ASN:O	2:F:1127:MET:HG3	2.06	0.56
1:B:140:ILE:O	1:B:144:ARG:HG3	2.06	0.56
1:B:150:MET:HE1	1:B:203:ARG:NH2	2.21	0.56
2:F:1159:ARG:CG	2:F:1160:LEU:N	2.68	0.56
2:G:971:ASN:ND2	2:H:765:PRO:HD2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASN:ND2	1:A:201:ASP:HB2	2.21	0.56
1:A:261:PRO:HG3	2:F:1166:ARG:O	2.05	0.56
2:E:866:GLU:OE2	2:E:926:LYS:HE3	2.05	0.56
1:A:136:ALA:HB2	1:A:170:TRP:CE2	2.41	0.55
1:B:453:GLU:OE1	1:C:295:SER:O	2.24	0.55
1:C:216:MET:HE2	1:C:225:MET:HE2	1.88	0.55
2:G:869:LEU:HA	2:G:873:MET:HE2	1.88	0.55
2:H:1107:PHE:O	2:H:1109:PRO:HD3	2.06	0.55
2:E:858:LYS:HE3	2:E:912:THR:HG22	1.88	0.55
2:E:1085:ASN:O	2:E:1089:MET:HG2	2.06	0.55
2:G:883:GLU:HG3	2:G:884:PRO:HD2	1.88	0.55
2:G:1085:ASN:O	2:G:1089:MET:HG2	2.05	0.55
2:H:883:GLU:HB2	2:H:886:GLN:HE21	1.71	0.55
1:C:374:ILE:HD12	1:D:410:LEU:HD13	1.88	0.55
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.71	0.55
1:B:457:ASP:HB3	1:C:245:ASN:HD21	1.72	0.55
1:C:136:ALA:HB2	1:C:170:TRP:CE2	2.41	0.55
1:C:239:MET:HA	1:C:247:MET:HG3	1.89	0.55
2:H:858:LYS:HE3	2:H:912:THR:HB	1.89	0.55
2:H:950:LEU:HD13	2:H:1121:LEU:HD21	1.89	0.55
2:F:756:TYR:O	2:F:757:LYS:HG3	2.06	0.55
2:F:771:VAL:N	2:F:775:LEU:CD1	2.57	0.55
2:E:852:MET:HG2	2:E:853:PRO:CD	2.36	0.55
2:F:1154:LYS:O	2:F:1158:GLU:HG2	2.07	0.55
2:G:1170:ILE:HD11	2:G:1181:VAL:HG13	1.89	0.55
1:B:334:LEU:HD11	1:B:338:LEU:HD21	1.88	0.55
2:H:859:ASN:HD21	2:H:1066:LYS:CE	2.20	0.55
1:B:398:GLU:HB3	1:B:399:PRO:HD3	1.89	0.55
2:F:883:GLU:HB2	2:F:886:GLN:HE21	1.72	0.55
2:H:756:TYR:O	2:H:757:LYS:HG3	2.07	0.55
1:C:237:ARG:CZ	1:C:280:MET:HE1	2.38	0.54
1:A:201:ASP:O	1:A:202:SER:C	2.49	0.54
2:F:859:ASN:HD21	2:F:1066:LYS:CE	2.21	0.54
2:F:869:LEU:HD23	2:F:873:MET:HE3	1.88	0.54
1:C:201:ASP:O	1:C:202:SER:C	2.50	0.54
2:G:854:TYR:O	2:G:909:VAL:HG11	2.06	0.54
2:G:859:ASN:HD22	2:G:1066:LYS:HD3	1.72	0.54
2:E:1147:ARG:HH11	1:B:376:MET:CG	2.17	0.54
1:D:140:ILE:O	1:D:144:ARG:HG3	2.07	0.54
2:H:859:ASN:HD21	2:H:1066:LYS:CD	2.20	0.54
2:G:1005:PHE:CE1	2:H:798:LEU:HD13	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:966:VAL:O	2:H:970:MET:HG3	2.08	0.54
1:A:237:ARG:CZ	1:A:280:MET:HE1	2.37	0.53
2:E:881:MET:HE1	2:E:887:LEU:HD11	1.90	0.53
2:E:988:CYS:SG	2:E:1127:MET:HE3	2.48	0.53
2:E:1052:VAL:HG12	2:E:1077:VAL:CG2	2.38	0.53
2:G:980:PHE:CZ	2:H:753:LYS:HB3	2.43	0.53
2:F:859:ASN:HD21	2:F:1066:LYS:CD	2.20	0.53
2:G:852:MET:HG2	2:G:853:PRO:CD	2.38	0.53
2:E:962:LEU:HD11	2:E:1009:LEU:HD13	1.91	0.53
2:H:1176:GLY:C	2:H:1178:GLU:H	2.16	0.53
2:G:955:ASN:OD1	2:G:1016:GLU:HB2	2.09	0.53
2:G:1104:TYR:O	2:H:779:CYS:HB2	2.08	0.53
2:E:859:ASN:HD22	2:E:1066:LYS:HD3	1.74	0.53
2:F:937:LYS:N	2:F:938:PRO:CD	2.71	0.53
2:H:858:LYS:HE3	2:H:912:THR:CB	2.39	0.53
2:E:897:TYR:C	2:E:897:TYR:CD2	2.87	0.53
2:E:994:LYS:HB2	2:E:998:GLN:OE1	2.09	0.53
2:F:860:VAL:HG13	2:F:865:ASN:HB3	1.91	0.53
2:F:966:VAL:O	2:F:970:MET:HG3	2.09	0.53
2:F:1176:GLY:C	2:F:1178:GLU:H	2.16	0.53
1:D:423:LYS:O	1:D:427:GLU:HG3	2.08	0.53
2:H:860:VAL:HG13	2:H:865:ASN:HB3	1.91	0.53
1:B:138:MET:CE	1:B:138:MET:HA	2.39	0.53
1:C:283:VAL:CG1	1:C:284:GLU:N	2.72	0.53
2:G:754:LYS:HB2	2:G:786:GLU:OE2	2.09	0.53
2:G:925:PHE:CE1	2:G:1048:GLN:HB3	2.43	0.53
1:B:161:VAL:O	1:B:165:ASN:HB2	2.09	0.52
2:H:937:LYS:N	2:H:938:PRO:HD2	2.24	0.52
2:F:793:GLU:O	2:F:796:ALA:HB3	2.10	0.52
2:H:793:GLU:O	2:H:796:ALA:HB3	2.08	0.52
2:E:925:PHE:CE1	2:E:1048:GLN:HB3	2.44	0.52
1:C:431:GLN:HE22	1:C:451:ASP:N	2.01	0.52
2:G:1147:ARG:HH11	1:D:376:MET:CG	2.20	0.52
2:H:905:GLN:O	2:H:909:VAL:HG23	2.10	0.52
2:F:905:GLN:O	2:F:909:VAL:HG23	2.09	0.52
1:C:245:ASN:N	1:C:245:ASN:HD22	2.07	0.52
2:G:1195:PHE:O	2:G:1196:ARG:C	2.51	0.52
2:H:869:LEU:HD23	2:H:873:MET:HE3	1.91	0.52
2:H:1000:MET:HE3	2:H:1005:PHE:HB2	1.91	0.52
2:E:762:LEU:HD11	2:F:969:TYR:HE2	1.75	0.52
2:F:1008:GLU:HG3	2:F:1139:ARG:HH12	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ASN:ND2	1:C:170:TRP:CE2	2.78	0.52
2:G:858:LYS:HZ2	2:G:912:THR:HG21	1.71	0.52
2:G:1021:PRO:HG2	2:G:1129:LEU:HD21	1.91	0.52
2:G:937:LYS:HB3	2:G:938:PRO:HD3	1.92	0.52
2:G:979:ALA:HA	2:H:769:LYS:HD2	1.90	0.52
2:H:1008:GLU:HG3	2:H:1139:ARG:HH12	1.73	0.52
2:F:1175:GLU:HB3	2:F:1178:GLU:HG3	1.92	0.52
2:E:754:LYS:HB2	2:E:786:GLU:OE2	2.10	0.52
1:B:274:MET:HE1	1:B:289:LEU:HD12	1.91	0.52
1:B:289:LEU:HD21	1:B:308:LEU:HD23	1.92	0.52
2:G:798:LEU:HD21	2:H:966:VAL:HG13	1.91	0.52
2:G:962:LEU:HD11	2:G:1009:LEU:HD13	1.90	0.52
1:D:138:MET:HA	1:D:138:MET:CE	2.39	0.52
1:A:293:LEU:HD22	1:A:341:LEU:HD11	1.92	0.52
1:C:393:LYS:HA	1:C:398:GLU:OE1	2.09	0.52
2:H:889:MET:O	2:H:893:LEU:HD13	2.10	0.52
2:F:858:LYS:HE3	2:F:912:THR:HB	1.91	0.52
1:A:302:LYS:HD3	1:A:341:LEU:CD2	2.40	0.51
2:F:988:CYS:CB	2:F:1127:MET:CE	2.88	0.51
2:F:1107:PHE:O	2:F:1109:PRO:HD3	2.10	0.51
1:A:433:VAL:CG1	1:B:410:LEU:HB3	2.40	0.51
1:C:302:LYS:HD3	1:C:341:LEU:CD2	2.40	0.51
1:C:377:GLU:CD	2:H:1147:ARG:HH21	2.18	0.51
1:C:293:LEU:HD22	1:C:341:LEU:HD11	1.92	0.51
1:D:375:ARG:NH2	3:P:1:GLC:C6	2.62	0.51
2:H:1175:GLU:HB3	2:H:1178:GLU:HG3	1.93	0.51
2:E:955:ASN:OD1	2:E:1016:GLU:HB2	2.10	0.51
2:F:754:LYS:CG	2:F:755:VAL:H	2.24	0.51
2:G:897:TYR:C	2:G:897:TYR:CD2	2.88	0.51
2:F:762:LEU:HD21	2:F:799:THR:HG23	1.93	0.51
2:F:837:SER:O	2:F:841:GLN:HG3	2.11	0.51
2:H:859:ASN:HD21	2:H:1066:LYS:HE2	1.76	0.51
2:H:988:CYS:SG	2:H:1127:MET:CE	2.99	0.51
2:H:883:GLU:H	2:H:886:GLN:HE21	1.59	0.51
1:B:456:VAL:CG1	1:B:457:ASP:N	2.74	0.50
2:G:889:MET:O	2:G:893:LEU:HD13	2.11	0.50
1:D:136:ALA:HB2	1:D:170:TRP:CE2	2.46	0.50
1:D:239:MET:HA	1:D:247:MET:HG3	1.93	0.50
2:E:764:ARG:HD2	2:F:971:ASN:OD1	2.12	0.50
2:E:772:ALA:N	2:F:980:PHE:CD2	2.80	0.50
2:H:881:MET:HE2	2:H:887:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:969:TYR:CD1	2:F:795:PHE:CD2	2.98	0.50
2:E:937:LYS:HB3	2:E:938:PRO:HD3	1.93	0.50
2:G:988:CYS:SG	2:G:1127:MET:HE3	2.51	0.50
1:D:290:LEU:HD11	1:D:332:LEU:CB	2.42	0.50
2:F:1130:GLN:O	2:F:1134:GLU:HG3	2.12	0.50
1:D:283:VAL:HG12	1:D:284:GLU:H	1.76	0.50
2:F:937:LYS:N	2:F:938:PRO:HD2	2.27	0.50
1:C:192:GLU:HA	1:C:195:GLU:OE1	2.11	0.50
1:C:418:ARG:HB3	1:C:419:PRO:CD	2.36	0.50
1:D:274:MET:HE1	1:D:289:LEU:HD12	1.93	0.50
2:G:756:TYR:O	2:G:757:LYS:HG3	2.12	0.50
2:G:1052:VAL:HG12	2:G:1077:VAL:CG2	2.42	0.50
1:A:245:ASN:N	1:A:245:ASN:HD22	2.10	0.49
2:E:1104:TYR:O	2:F:779:CYS:HB2	2.12	0.49
1:B:290:LEU:HD11	1:B:332:LEU:CB	2.42	0.49
2:F:1020:PHE:CG	2:F:1021:PRO:HD3	2.46	0.49
2:G:925:PHE:CZ	2:G:1048:GLN:HB3	2.47	0.49
2:H:951:ARG:HG3	2:H:951:ARG:NH1	2.25	0.49
2:E:852:MET:CG	2:E:853:PRO:HD2	2.41	0.49
2:F:859:ASN:HD21	2:F:1066:LYS:HE2	1.77	0.49
2:F:881:MET:HE2	2:F:887:LEU:HD11	1.92	0.49
2:G:997:ASP:O	2:G:999:LYS:N	2.36	0.49
1:D:290:LEU:HD13	1:D:332:LEU:HB3	1.93	0.49
2:E:1021:PRO:HG2	2:E:1129:LEU:HD21	1.94	0.49
1:C:433:VAL:CG1	1:D:410:LEU:HB3	2.42	0.49
2:H:754:LYS:CG	2:H:755:VAL:H	2.25	0.49
2:F:1086:LYS:O	2:F:1089:MET:HB2	2.12	0.49
1:C:193:LYS:HD2	1:C:205:GLN:HE22	1.78	0.49
2:G:997:ASP:C	2:G:999:LYS:H	2.21	0.49
2:G:1069:PHE:O	2:G:1071:GLU:N	2.46	0.49
1:D:334:LEU:HD11	1:D:338:LEU:HD21	1.93	0.49
1:D:347:GLU:O	1:D:351:VAL:HG23	2.13	0.49
2:H:837:SER:O	2:H:841:GLN:HG3	2.12	0.49
2:F:869:LEU:HA	2:F:873:MET:HE2	1.95	0.49
1:C:433:VAL:HG11	1:D:407:HIS:O	2.13	0.49
2:G:945:ALA:HB3	2:G:1026:HIS:CD2	2.48	0.49
2:H:1086:LYS:O	2:H:1089:MET:HB2	2.13	0.49
1:A:259:ILE:HG13	2:F:1189:LEU:HD21	1.95	0.49
2:H:771:VAL:N	2:H:775:LEU:CD1	2.57	0.49
2:H:904:GLU:O	2:H:908:VAL:HG23	2.13	0.49
2:F:917:ARG:HB2	2:F:917:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1000:MET:HE3	2:F:1005:PHE:HB2	1.94	0.49
2:H:988:CYS:CB	2:H:1127:MET:HE1	2.43	0.49
2:E:889:MET:O	2:E:893:LEU:HD13	2.11	0.49
2:F:889:MET:O	2:F:893:LEU:HD13	2.12	0.49
2:G:1010:CYS:SG	2:G:1017:VAL:HG11	2.52	0.49
2:F:950:LEU:HD13	2:F:1121:LEU:HD21	1.94	0.49
1:C:342:ARG:NH2	1:C:357:ASP:OD1	2.46	0.49
2:G:852:MET:CG	2:G:853:PRO:HD2	2.42	0.49
3:N:1:GLC:O6	3:N:2:FRU:H61	2.13	0.48
2:F:858:LYS:HE3	2:F:912:THR:CB	2.43	0.48
1:C:374:ILE:HD12	1:D:410:LEU:CD1	2.43	0.48
1:C:430:SER:HB2	1:D:407:HIS:NE2	2.27	0.48
2:H:1130:GLN:O	2:H:1134:GLU:HG3	2.13	0.48
2:E:858:LYS:CE	2:E:912:THR:CG2	2.88	0.48
2:F:883:GLU:H	2:F:886:GLN:HE21	1.60	0.48
2:G:754:LYS:CB	2:G:786:GLU:OE1	2.61	0.48
1:D:328:GLU:CD	3:O:1:GLC:H61	2.38	0.48
2:E:767:TRP:CH2	2:F:967:GLY:HA3	2.49	0.48
1:C:375:ARG:NH2	3:N:1:GLC:C6	2.71	0.48
1:D:216:MET:HE1	1:D:225:MET:CE	2.40	0.48
1:D:299:ILE:HG21	1:D:346:ASN:HD21	1.78	0.48
1:B:218:ASN:ND2	1:B:220:PHE:HB3	2.29	0.48
2:F:1133:LYS:HB2	2:F:1133:LYS:HE3	1.61	0.48
1:C:338:LEU:O	1:C:342:ARG:HG3	2.14	0.48
2:G:1021:PRO:CG	2:G:1129:LEU:HD21	2.43	0.48
2:E:869:LEU:HA	2:E:873:MET:HE2	1.95	0.48
2:F:988:CYS:SG	2:F:1127:MET:CE	3.02	0.48
2:F:1069:PHE:O	2:F:1070:VAL:C	2.56	0.48
2:G:1144:LYS:HE2	1:D:377:GLU:OE1	2.13	0.48
2:E:910:MET:C	2:E:912:THR:N	2.72	0.48
2:E:969:TYR:CE1	2:F:795:PHE:CD2	3.02	0.48
2:E:997:ASP:C	2:E:999:LYS:H	2.20	0.48
1:C:199:ASN:HD21	1:C:201:ASP:HB2	1.78	0.48
2:G:957:SER:HB3	2:H:780:PHE:CE1	2.48	0.48
2:H:794:LEU:C	2:H:794:LEU:CD2	2.87	0.48
2:E:859:ASN:ND2	2:E:1066:LYS:CD	2.76	0.47
2:F:999:LYS:O	2:F:999:LYS:HG2	2.13	0.47
1:C:233:LEU:O	1:C:237:ARG:HG3	2.13	0.47
2:G:859:ASN:ND2	2:G:1066:LYS:CD	2.75	0.47
2:G:997:ASP:OD2	2:G:999:LYS:HB3	2.14	0.47
1:A:259:ILE:CG1	2:F:1189:LEU:HD21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:945:ALA:HB3	2:E:1026:HIS:CD2	2.49	0.47
1:C:446:ARG:HA	1:C:446:ARG:HD2	1.67	0.47
2:H:858:LYS:HE3	2:H:912:THR:HG21	1.95	0.47
2:H:937:LYS:HB3	2:H:938:PRO:HD3	1.96	0.47
2:H:762:LEU:HD21	2:H:799:THR:HG23	1.94	0.47
2:H:917:ARG:HB2	2:H:917:ARG:NH1	2.29	0.47
2:H:1170:ILE:CG1	2:H:1185:LEU:HD21	2.43	0.47
2:E:754:LYS:CB	2:E:786:GLU:OE1	2.62	0.47
1:B:283:VAL:HG12	1:B:284:GLU:H	1.79	0.47
1:D:289:LEU:HD21	1:D:308:LEU:HD23	1.96	0.47
2:E:912:THR:HG22	2:E:913:VAL:N	2.27	0.47
2:F:1170:ILE:CG1	2:F:1185:LEU:HD21	2.43	0.47
2:G:789:PHE:HB2	2:H:965:LEU:HD22	1.96	0.47
1:A:341:LEU:HD22	1:A:349:MET:HE3	1.96	0.47
2:E:971:ASN:ND2	2:F:765:PRO:HD2	2.29	0.47
2:F:932:GLN:O	2:F:936:ILE:HG13	2.15	0.47
2:H:850:PHE:HE1	2:H:873:MET:HG3	1.79	0.47
2:E:1079:ASP:O	2:E:1082:GLU:HB3	2.15	0.47
2:G:772:ALA:O	2:G:773:GLU:O	2.32	0.47
2:G:881:MET:HE1	2:G:887:LEU:HD11	1.92	0.47
1:C:199:ASN:OD1	1:C:201:ASP:HB2	2.15	0.47
2:G:862:LEU:HD21	2:G:913:VAL:HG13	1.96	0.47
2:G:910:MET:C	2:G:912:THR:N	2.72	0.47
1:D:193:LYS:HA	1:D:199:ASN:ND2	2.30	0.47
2:E:1010:CYS:SG	2:E:1017:VAL:HG11	2.54	0.47
2:E:1020:PHE:N	2:E:1021:PRO:CD	2.78	0.47
1:C:261:PRO:HG3	2:H:1166:ARG:O	2.15	0.47
1:C:285:ARG:NH1	3:M:2:FRU:H62	2.30	0.47
1:A:217:ASN:HA	2:F:1182:MET:HB3	1.96	0.47
2:E:772:ALA:O	2:E:773:GLU:O	2.33	0.47
2:G:1107:PHE:O	2:G:1109:PRO:HD3	2.15	0.47
2:F:988:CYS:CA	2:F:1127:MET:HE1	2.45	0.46
2:G:1020:PHE:CG	2:G:1021:PRO:HD3	2.50	0.46
1:B:232:ILE:HD12	1:B:269:ARG:HD2	1.96	0.46
2:F:794:LEU:C	2:F:794:LEU:CD2	2.88	0.46
2:F:794:LEU:C	2:F:794:LEU:HD23	2.40	0.46
2:G:1036:GLU:CG	2:G:1040:LYS:HE2	2.45	0.46
2:G:1069:PHE:C	2:G:1071:GLU:N	2.70	0.46
1:A:233:LEU:O	1:A:237:ARG:HG3	2.15	0.46
2:E:1069:PHE:C	2:E:1071:GLU:N	2.72	0.46
1:D:168:VAL:O	1:D:172:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ASN:ND2	1:D:220:PHE:HB3	2.31	0.46
2:H:794:LEU:C	2:H:794:LEU:HD23	2.40	0.46
1:A:430:SER:HB2	1:B:407:HIS:NE2	2.31	0.46
2:E:1107:PHE:O	2:E:1109:PRO:HD3	2.15	0.46
1:C:412:ARG:NH1	1:C:412:ARG:HG2	2.31	0.46
1:A:418:ARG:HB3	1:A:419:PRO:CD	2.38	0.46
2:G:754:LYS:HB3	2:G:786:GLU:OE1	2.16	0.46
2:E:869:LEU:HD23	2:E:873:MET:CE	2.45	0.46
1:C:423:LYS:HB2	1:D:400:HIS:NE2	2.31	0.46
2:G:869:LEU:HD23	2:G:873:MET:CE	2.46	0.46
2:H:988:CYS:HB3	2:H:1127:MET:HE1	1.97	0.46
1:A:374:ILE:HD12	1:B:410:LEU:CD1	2.45	0.46
2:E:925:PHE:CZ	2:E:1048:GLN:HB3	2.51	0.46
1:B:302:LYS:HD3	1:B:341:LEU:HD21	1.98	0.46
2:F:1170:ILE:CD1	2:F:1181:VAL:HG13	2.38	0.46
2:G:957:SER:HB3	2:H:780:PHE:HE1	1.80	0.46
2:G:1034:SER:HB3	2:G:1037:ASN:HB2	1.98	0.46
2:H:754:LYS:CG	2:H:755:VAL:N	2.79	0.46
2:H:932:GLN:O	2:H:936:ILE:HG13	2.14	0.46
1:A:278:ALA:HB2	1:A:285:ARG:HA	1.98	0.46
1:A:377:GLU:CD	2:F:1147:ARG:HH21	2.23	0.46
2:E:756:TYR:O	2:E:757:LYS:HG3	2.15	0.46
2:E:772:ALA:HB2	2:F:980:PHE:CZ	2.51	0.46
1:B:347:GLU:O	1:B:351:VAL:HG23	2.15	0.46
1:C:166:ASN:ND2	1:C:170:TRP:CD2	2.72	0.46
2:H:1133:LYS:HB2	2:H:1133:LYS:HE3	1.66	0.46
1:A:375:ARG:NH2	3:J:1:GLC:H61	2.29	0.46
2:F:772:ALA:O	2:F:773:GLU:C	2.59	0.46
2:G:1169:LEU:CD1	1:D:259:ILE:HG23	2.45	0.46
1:D:398:GLU:N	1:D:399:PRO:CD	2.79	0.46
1:A:153:LEU:HB2	1:A:204:ASN:OD1	2.15	0.46
1:A:160:ARG:HD3	1:A:210:ARG:HB3	1.98	0.46
1:A:166:ASN:HD22	1:A:170:TRP:CD1	2.33	0.46
2:E:772:ALA:HB2	2:F:980:PHE:CE2	2.50	0.46
2:G:1079:ASP:O	2:G:1082:GLU:HB3	2.16	0.46
2:H:1033:VAL:HG13	2:H:1034:SER:N	2.30	0.46
2:E:862:LEU:HD21	2:E:913:VAL:HG13	1.98	0.45
2:G:1016:GLU:CD	2:G:1016:GLU:N	2.68	0.45
2:G:1020:PHE:N	2:G:1021:PRO:CD	2.78	0.45
1:A:283:VAL:CG1	1:A:284:GLU:N	2.79	0.45
2:E:1020:PHE:CG	2:E:1021:PRO:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:850:PHE:HE1	2:F:873:MET:HG3	1.81	0.45
2:G:950:LEU:HD13	2:G:1121:LEU:HD21	1.98	0.45
1:A:152:LEU:HD12	1:A:152:LEU:O	2.16	0.45
1:A:215:PHE:O	1:A:221:GLY:HA3	2.16	0.45
2:F:1195:PHE:C	2:F:1196:ARG:HG3	2.42	0.45
2:H:940:ILE:HD13	2:H:1091:HIS:HB2	1.97	0.45
2:E:1021:PRO:CG	2:E:1129:LEU:HD21	2.47	0.45
2:F:1154:LYS:HE3	2:F:1154:LYS:HB2	1.86	0.45
2:F:997:ASP:OD2	2:F:999:LYS:HB3	2.16	0.45
2:F:1069:PHE:O	2:F:1071:GLU:N	2.49	0.45
1:D:347:GLU:HA	1:D:347:GLU:OE1	2.16	0.45
2:H:858:LYS:HE3	2:H:912:THR:CG2	2.47	0.45
2:H:900:LEU:HD22	2:H:904:GLU:OE2	2.16	0.45
2:E:762:LEU:HD11	2:F:969:TYR:CE2	2.51	0.45
2:E:1147:ARG:HH11	1:B:376:MET:HG3	1.64	0.45
2:F:1020:PHE:N	2:F:1021:PRO:CD	2.79	0.45
2:H:874:ILE:O	2:H:878:ILE:HG13	2.16	0.45
2:H:1020:PHE:N	2:H:1021:PRO:CD	2.80	0.45
2:H:1122:HIS:CE1	2:H:1125:ARG:HH21	2.34	0.45
1:A:278:ALA:HB1	1:A:283:VAL:O	2.17	0.45
2:F:754:LYS:CG	2:F:755:VAL:N	2.79	0.45
2:F:970:MET:HE1	2:F:1002:LEU:CD2	2.47	0.45
2:H:754:LYS:HB2	2:H:786:GLU:CD	2.42	0.45
2:F:1033:VAL:HG13	2:F:1034:SER:N	2.31	0.45
2:G:767:TRP:CH2	2:H:967:GLY:HA3	2.52	0.45
1:D:232:ILE:HD12	1:D:269:ARG:HD2	1.98	0.45
2:H:1011:GLU:CD	2:H:1139:ARG:HH22	2.25	0.45
1:B:299:ILE:HG21	1:B:346:ASN:HD21	1.79	0.45
1:B:347:GLU:HA	1:B:347:GLU:OE1	2.17	0.45
2:G:869:LEU:HA	2:G:873:MET:CE	2.46	0.45
2:G:1021:PRO:CB	2:G:1129:LEU:HD21	2.47	0.45
2:H:1175:GLU:CG	2:H:1178:GLU:HG3	2.47	0.45
2:F:832:LEU:HD21	2:F:840:ALA:HB3	1.93	0.44
2:F:846:PHE:CG	2:F:880:GLN:HG3	2.52	0.44
2:G:832:LEU:HD11	2:G:840:ALA:CB	2.47	0.44
1:D:139:TYR:O	1:D:143:LEU:HG	2.17	0.44
2:H:970:MET:HE1	2:H:1002:LEU:CD2	2.47	0.44
2:E:913:VAL:HA	2:E:914:PRO:HD3	1.78	0.44
2:E:997:ASP:OD2	2:E:999:LYS:HB3	2.18	0.44
1:B:457:ASP:HB3	1:C:245:ASN:ND2	2.32	0.44
2:F:922:ALA:HB1	2:F:1073:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1175:GLU:CG	2:F:1178:GLU:HG3	2.47	0.44
1:A:450:ILE:HD13	1:A:450:ILE:N	2.33	0.44
2:E:801:ALA:O	2:F:995:SER:HB2	2.18	0.44
2:F:754:LYS:HB2	2:F:786:GLU:OE2	2.18	0.44
2:F:1011:GLU:CD	2:F:1139:ARG:HH22	2.25	0.44
2:H:845:ILE:O	2:H:846:PHE:C	2.60	0.44
2:E:1069:PHE:O	2:E:1071:GLU:N	2.51	0.44
1:B:239:MET:CA	1:B:247:MET:HG3	2.47	0.44
1:C:450:ILE:HG12	1:D:450:ILE:HD12	2.00	0.44
2:G:1052:VAL:HG11	2:G:1073:MET:CE	2.47	0.44
1:A:407:HIS:CD2	1:B:430:SER:HA	2.52	0.44
2:F:852:MET:O	2:F:853:PRO:C	2.61	0.44
1:C:215:PHE:O	1:C:221:GLY:HA3	2.17	0.44
1:C:385:PHE:CZ	1:D:385:PHE:HB2	2.53	0.44
1:C:407:HIS:CD2	1:D:430:SER:HA	2.53	0.44
2:H:951:ARG:HH11	2:H:951:ARG:CG	2.28	0.44
2:H:1069:PHE:O	2:H:1070:VAL:C	2.59	0.44
1:A:412:ARG:NH1	1:A:412:ARG:HG2	2.32	0.44
2:E:1005:PHE:CE1	2:F:798:LEU:HD13	2.53	0.44
2:G:772:ALA:N	2:H:980:PHE:CD2	2.85	0.44
1:D:277:ARG:O	1:D:280:MET:HG2	2.17	0.44
2:H:1000:MET:HE3	2:H:1005:PHE:CA	2.48	0.44
1:A:433:VAL:HG11	1:B:410:LEU:HB3	1.99	0.44
1:B:302:LYS:CD	1:B:341:LEU:HD22	2.48	0.44
2:F:900:LEU:HD22	2:F:904:GLU:OE2	2.17	0.44
2:F:951:ARG:HG3	2:F:951:ARG:NH1	2.25	0.44
1:C:278:ALA:HB2	1:C:285:ARG:HA	1.99	0.44
2:G:1069:PHE:C	2:G:1071:GLU:H	2.25	0.44
1:A:433:VAL:HG11	1:B:407:HIS:O	2.18	0.44
2:E:798:LEU:HD21	2:F:966:VAL:HG13	2.00	0.44
1:B:233:LEU:HD12	1:B:233:LEU:C	2.41	0.44
2:H:772:ALA:O	2:H:773:GLU:C	2.60	0.44
1:A:134:ARG:HG3	1:A:134:ARG:NH1	2.33	0.44
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.79	0.44
1:A:204:ASN:O	1:A:208:ILE:HG13	2.18	0.44
2:E:883:GLU:HG3	2:E:884:PRO:CD	2.48	0.44
1:A:219:LYS:O	1:A:223:LYS:HG3	2.17	0.43
2:E:754:LYS:HB3	2:E:786:GLU:OE1	2.18	0.43
2:E:763:ARG:NH2	2:F:996:ALA:HA	2.33	0.43
2:E:794:LEU:HD11	2:F:1009:LEU:HD11	2.00	0.43
2:E:1169:LEU:CD1	1:B:259:ILE:HG23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ASN:O	1:B:208:ILE:HG13	2.18	0.43
1:C:278:ALA:HB1	1:C:283:VAL:O	2.18	0.43
2:H:869:LEU:HA	2:H:873:MET:HE2	1.99	0.43
1:A:398:GLU:HB3	1:A:399:PRO:CD	2.42	0.43
1:A:450:ILE:HG12	1:B:450:ILE:HD12	2.00	0.43
2:E:1034:SER:HB3	2:E:1037:ASN:HB2	2.00	0.43
2:F:845:ILE:O	2:F:846:PHE:C	2.62	0.43
2:F:939:GLU:HB3	2:F:1033:VAL:HG22	2.00	0.43
2:F:1102:GLY:HA2	2:F:1107:PHE:CE2	2.53	0.43
1:D:400:HIS:O	1:D:404:ILE:HG13	2.18	0.43
1:A:342:ARG:NH2	1:A:357:ASP:OD1	2.49	0.43
2:E:1056:VAL:O	2:E:1056:VAL:CG1	2.67	0.43
2:H:999:LYS:O	2:H:999:LYS:HG2	2.17	0.43
1:C:137:MET:HE2	1:C:138:MET:HE3	2.00	0.43
1:C:240:ASP:OD1	1:C:240:ASP:C	2.61	0.43
2:H:858:LYS:NZ	2:H:912:THR:HG21	2.34	0.43
1:C:219:LYS:O	1:C:223:LYS:HG3	2.19	0.43
2:G:1137:LYS:HD2	2:G:1137:LYS:HA	1.65	0.43
2:F:795:PHE:N	2:F:795:PHE:CD1	2.87	0.43
2:F:937:LYS:HB3	2:F:938:PRO:HD3	2.01	0.43
2:G:1011:GLU:CD	2:G:1139:ARG:HH22	2.27	0.43
1:B:138:MET:HA	1:B:138:MET:HE3	1.99	0.43
1:B:290:LEU:HD12	1:B:332:LEU:HD13	2.01	0.43
2:H:1098:TYR:CD2	2:H:1114:VAL:HG22	2.53	0.43
2:E:1016:GLU:O	2:E:1017:VAL:C	2.60	0.43
1:B:290:LEU:HD13	1:B:332:LEU:HB3	1.93	0.43
2:F:852:MET:HG2	2:F:853:PRO:HD2	2.01	0.43
2:G:1106:VAL:HB	2:H:770:PHE:CE1	2.52	0.43
1:D:290:LEU:HD11	1:D:332:LEU:HB2	2.01	0.43
1:A:423:LYS:HB2	1:B:400:HIS:NE2	2.34	0.43
2:E:1021:PRO:CB	2:E:1129:LEU:HD21	2.49	0.43
1:B:236:VAL:HG12	1:B:277:ARG:HD2	2.01	0.43
2:F:1099:LYS:O	2:F:1099:LYS:HD3	2.19	0.43
2:H:1046:LYS:HE3	2:H:1046:LYS:HB2	1.86	0.43
2:E:861:ILE:HD12	2:E:910:MET:HE1	2.01	0.42
2:E:1152:LYS:HE3	2:E:1152:LYS:HB2	1.91	0.42
2:H:853:PRO:HB2	2:H:856:GLU:HG3	2.01	0.42
2:F:1137:LYS:HD2	2:F:1137:LYS:HA	1.81	0.42
2:H:967:GLY:HA2	2:H:970:MET:CE	2.49	0.42
2:F:864:VAL:HG12	2:F:864:VAL:O	2.18	0.42
2:F:1069:PHE:O	2:F:1072:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:ARG:CZ	3:M:2:FRU:H62	2.49	0.42
1:C:430:SER:CA	1:D:407:HIS:CD2	2.96	0.42
2:G:936:ILE:HG23	2:G:1038:LEU:HD22	2.00	0.42
2:G:1056:VAL:O	2:G:1056:VAL:CG1	2.67	0.42
1:D:431:GLN:HG3	1:D:450:ILE:HG23	2.01	0.42
2:E:1036:GLU:CG	2:E:1040:LYS:HE2	2.49	0.42
2:F:1175:GLU:HG2	2:F:1178:GLU:HG3	2.01	0.42
1:C:398:GLU:N	1:C:399:PRO:CD	2.82	0.42
2:H:754:LYS:HB2	2:H:786:GLU:OE2	2.19	0.42
2:H:769:LYS:HG3	2:H:770:PHE:N	2.34	0.42
2:H:1036:GLU:CG	2:H:1040:LYS:HE2	2.49	0.42
1:A:149:ASP:OD1	1:A:200:TYR:HE1	2.02	0.42
1:A:306:LEU:HD12	1:A:306:LEU:HA	1.74	0.42
2:E:1069:PHE:C	2:E:1071:GLU:H	2.27	0.42
1:B:275:THR:O	1:B:278:ALA:HB3	2.19	0.42
2:F:754:LYS:HB2	2:F:786:GLU:CD	2.44	0.42
1:C:284:GLU:HG3	1:C:332:LEU:HD21	2.02	0.42
2:F:861:ILE:HG22	2:F:919:ARG:HD2	2.02	0.42
2:G:1016:GLU:O	2:G:1017:VAL:C	2.63	0.42
1:D:138:MET:HA	1:D:138:MET:HE2	2.01	0.42
1:D:332:LEU:HD23	1:D:332:LEU:HA	1.88	0.42
2:H:939:GLU:HB3	2:H:1033:VAL:HG22	2.01	0.42
2:H:1122:HIS:ND1	2:H:1125:ARG:NH2	2.56	0.42
2:H:1159:ARG:HG3	2:H:1160:LEU:N	2.34	0.42
2:E:1016:GLU:CD	2:E:1016:GLU:N	2.72	0.42
2:E:1052:VAL:HG11	2:E:1073:MET:CE	2.50	0.42
2:E:1137:LYS:HA	2:E:1137:LYS:HD2	1.65	0.42
1:C:283:VAL:HG12	1:C:284:GLU:H	1.83	0.42
1:C:287:GLN:HB3	1:C:288:PRO:CD	2.50	0.42
2:G:1059:PHE:HA	2:G:1060:PRO:HD3	1.87	0.42
2:H:852:MET:O	2:H:853:PRO:C	2.59	0.42
2:H:1033:VAL:HG13	2:H:1034:SER:H	1.85	0.42
2:E:1015:PRO:O	2:E:1016:GLU:C	2.63	0.42
2:E:1043:ASP:O	2:E:1046:LYS:HB3	2.20	0.42
1:B:206:HIS:HA	1:B:246:MET:HG3	2.01	0.42
1:B:290:LEU:HD11	1:B:332:LEU:HB2	2.02	0.42
2:F:769:LYS:HG3	2:F:770:PHE:N	2.35	0.42
2:F:945:ALA:HB1	2:F:1026:HIS:ND1	2.35	0.42
1:D:365:PHE:CD2	1:D:365:PHE:C	2.97	0.42
1:A:172:GLN:HA	1:A:220:PHE:CE2	2.54	0.42
2:E:950:LEU:HD13	2:E:1121:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1169:LEU:O	2:E:1170:ILE:HG12	2.20	0.42
2:F:756:TYR:C	2:F:757:LYS:HG3	2.45	0.42
2:F:852:MET:CG	2:F:853:PRO:HD2	2.49	0.42
2:F:865:ASN:OD1	2:F:867:ALA:HB3	2.20	0.42
2:F:940:ILE:HD13	2:F:1091:HIS:HB2	2.01	0.42
2:F:951:ARG:HG3	2:F:951:ARG:O	2.20	0.42
2:G:794:LEU:HD11	2:H:1009:LEU:HD11	2.02	0.42
2:G:1036:GLU:HG2	2:G:1040:LYS:HE2	2.01	0.42
2:H:769:LYS:CG	2:H:770:PHE:N	2.82	0.42
2:E:1186:LEU:HD22	1:B:252:LYS:HB3	2.02	0.42
1:B:235:LEU:HD12	1:B:235:LEU:HA	1.85	0.42
1:B:260:LEU:HA	1:B:261:PRO:HD3	1.86	0.42
1:B:423:LYS:O	1:B:427:GLU:HG3	2.20	0.42
2:F:1097:LEU:HA	2:F:1097:LEU:HD23	1.83	0.42
2:F:1159:ARG:HG3	2:F:1160:LEU:N	2.35	0.42
1:D:218:ASN:HD22	1:D:220:PHE:H	1.67	0.42
1:A:287:GLN:CB	1:A:288:PRO:HD3	2.49	0.41
2:E:754:LYS:HB2	2:E:786:GLU:OE1	2.19	0.41
2:E:1011:GLU:CD	2:E:1139:ARG:HH22	2.27	0.41
2:F:1062:ALA:HB1	2:F:1067:ASP:HB3	2.02	0.41
1:C:297:THR:OG1	1:C:302:LYS:NZ	2.53	0.41
2:H:919:ARG:HG3	2:H:1069:PHE:CD1	2.55	0.41
2:F:913:VAL:HA	2:F:914:PRO:HD3	1.88	0.41
2:F:988:CYS:HA	2:F:1127:MET:CE	2.50	0.41
1:C:289:LEU:HD21	1:C:308:LEU:HD23	2.02	0.41
2:G:861:ILE:HD12	2:G:910:MET:HE1	2.02	0.41
1:D:450:ILE:HG22	1:D:452:ILE:CG2	2.51	0.41
2:F:1038:LEU:HD12	2:F:1038:LEU:HA	1.94	0.41
1:D:233:LEU:HD12	1:D:233:LEU:C	2.44	0.41
1:D:233:LEU:O	1:D:236:VAL:HB	2.20	0.41
1:D:247:MET:HE2	1:D:305:CYS:SG	2.60	0.41
2:H:906:PHE:O	2:H:910:MET:HG2	2.20	0.41
2:H:1154:LYS:HE3	2:H:1154:LYS:HB2	1.88	0.41
1:A:303:VAL:HG23	1:A:349:MET:HE2	2.01	0.41
1:A:398:GLU:N	1:A:399:PRO:CD	2.84	0.41
2:E:893:LEU:C	2:E:895:GLU:H	2.27	0.41
1:B:218:ASN:HD22	1:B:220:PHE:H	1.67	0.41
2:F:1046:LYS:HE3	2:F:1046:LYS:HB2	1.83	0.41
2:G:1080:ALA:C	2:G:1082:GLU:H	2.27	0.41
1:D:418:ARG:HB3	1:D:419:PRO:HD3	2.01	0.41
2:H:850:PHE:O	2:H:851:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1175:GLU:HG2	2:H:1178:GLU:HG3	2.01	0.41
1:A:290:LEU:CD1	1:A:332:LEU:CB	2.98	0.41
2:E:769:LYS:CG	2:E:770:PHE:N	2.82	0.41
2:E:789:PHE:HB2	2:F:965:LEU:CD2	2.51	0.41
2:E:858:LYS:HZ1	2:E:912:THR:HG21	1.81	0.41
1:B:218:ASN:ND2	1:B:221:GLY:H	2.18	0.41
2:F:853:PRO:HB2	2:F:856:GLU:HG3	2.02	0.41
1:C:418:ARG:N	1:C:419:PRO:CD	2.82	0.41
1:D:157:GLU:O	1:D:161:VAL:HG23	2.20	0.41
2:E:952:LYS:HG2	2:E:952:LYS:O	2.20	0.41
1:D:361:ASP:O	1:D:362:GLU:C	2.63	0.41
1:A:240:ASP:C	1:A:240:ASP:OD1	2.63	0.41
1:A:338:LEU:O	1:A:342:ARG:HG3	2.21	0.41
2:E:1086:LYS:O	2:E:1089:MET:HB2	2.21	0.41
2:F:769:LYS:CG	2:F:770:PHE:N	2.83	0.41
2:F:874:ILE:O	2:F:878:ILE:HG13	2.20	0.41
1:C:172:GLN:HA	1:C:220:PHE:CE2	2.56	0.41
1:C:219:LYS:HE3	2:H:1178:GLU:OE1	2.21	0.41
2:G:754:LYS:HB2	2:G:786:GLU:OE1	2.20	0.41
1:D:260:LEU:HA	1:D:261:PRO:HD3	1.90	0.41
1:A:193:LYS:HD2	1:A:199:ASN:HD22	1.85	0.41
1:B:277:ARG:O	1:B:280:MET:HG2	2.21	0.41
1:B:395:SER:C	1:B:397:ALA:H	2.29	0.41
2:F:919:ARG:HG3	2:F:1069:PHE:CD1	2.56	0.41
2:F:1098:TYR:CD2	2:F:1114:VAL:HG22	2.56	0.41
1:C:442:ASP:C	1:C:442:ASP:OD1	2.63	0.41
2:G:883:GLU:HG3	2:G:884:PRO:CD	2.50	0.41
1:D:236:VAL:HG12	1:D:277:ARG:HD2	2.02	0.41
2:H:1176:GLY:C	2:H:1178:GLU:N	2.79	0.41
2:E:989:LYS:O	2:E:992:ASP:HB2	2.21	0.41
2:E:1084:TYR:CD2	2:E:1084:TYR:C	2.99	0.41
2:E:1189:LEU:HD21	1:B:259:ILE:HG12	2.02	0.41
1:B:233:LEU:O	1:B:236:VAL:HB	2.21	0.41
1:B:365:PHE:CD2	1:B:365:PHE:C	2.98	0.41
2:F:858:LYS:HE3	2:F:912:THR:HG21	2.03	0.41
2:G:1084:TYR:CD2	2:G:1084:TYR:C	2.99	0.41
2:H:858:LYS:CE	2:H:912:THR:HG21	2.50	0.41
2:H:970:MET:HE1	2:H:1002:LEU:HD22	2.03	0.41
2:H:1069:PHE:O	2:H:1071:GLU:N	2.54	0.41
2:H:1099:LYS:O	2:H:1099:LYS:HD3	2.21	0.41
1:C:159:LEU:O	1:C:160:ARG:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:GLN:O	1:C:409:LEU:HB2	2.21	0.41
2:G:1031:SER:HB2	2:G:1119:MET:HA	2.03	0.41
1:A:442:ASP:OD1	1:A:442:ASP:C	2.63	0.40
2:E:1013:ASP:C	2:E:1014:HIS:CG	2.99	0.40
1:B:139:TYR:O	1:B:143:LEU:HG	2.21	0.40
1:B:389:LEU:HD23	1:B:389:LEU:HA	1.81	0.40
2:F:853:PRO:CB	2:F:856:GLU:HG3	2.51	0.40
2:G:764:ARG:HA	2:G:765:PRO:HD3	1.86	0.40
2:H:1038:LEU:HD12	2:H:1038:LEU:HA	1.93	0.40
1:A:259:ILE:HD13	1:A:259:ILE:HA	1.78	0.40
1:B:287:GLN:N	1:B:288:PRO:CD	2.84	0.40
2:F:858:LYS:NZ	2:F:912:THR:HG21	2.37	0.40
2:H:1102:GLY:HA2	2:H:1107:PHE:CE2	2.56	0.40
2:E:861:ILE:CD1	2:E:910:MET:HE1	2.52	0.40
1:B:190:HIS:HD2	1:B:205:GLN:NE2	2.18	0.40
2:F:970:MET:HE1	2:F:1002:LEU:HD22	2.03	0.40
1:D:307:GLN:HB2	1:D:352:GLN:CD	2.46	0.40
2:H:852:MET:HG2	2:H:853:PRO:HD2	2.03	0.40
1:B:307:GLN:HB2	1:B:352:GLN:CD	2.46	0.40
1:C:152:LEU:O	1:C:152:LEU:HD12	2.21	0.40
2:G:1169:LEU:O	2:G:1170:ILE:HG12	2.21	0.40
2:H:795:PHE:N	2:H:795:PHE:CD1	2.88	0.40
1:A:418:ARG:N	1:A:419:PRO:CD	2.85	0.40
1:C:226:LEU:HD21	1:C:257:LEU:HD22	2.04	0.40
2:G:940:ILE:HD13	2:G:1091:HIS:HB2	2.03	0.40
2:G:1186:LEU:HD22	1:D:252:LYS:HB3	2.02	0.40
1:D:287:GLN:N	1:D:288:PRO:CD	2.85	0.40
2:H:1097:LEU:HA	2:H:1097:LEU:HD23	1.89	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	320/327 (98%)	311 (97%)	9 (3%)	0	100	100
1	B	315/327 (96%)	300 (95%)	15 (5%)	0	100	100
1	C	320/327 (98%)	309 (97%)	11 (3%)	0	100	100
1	D	325/327 (99%)	313 (96%)	12 (4%)	0	100	100
2	E	415/457 (91%)	375 (90%)	33 (8%)	7 (2%)	7	14
2	F	415/457 (91%)	368 (89%)	37 (9%)	10 (2%)	4	9
2	G	416/457 (91%)	376 (90%)	32 (8%)	8 (2%)	6	12
2	H	415/457 (91%)	366 (88%)	39 (9%)	10 (2%)	4	9
All	All	2941/3136 (94%)	2718 (92%)	188 (6%)	35 (1%)	10	20

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	773	GLU
2	E	996	ALA
2	F	773	GLU
2	G	773	GLU
2	H	773	GLU
2	E	1174	ALA
2	F	998	GLN
2	F	1070	VAL
2	G	996	ALA
2	G	1174	ALA
2	H	998	GLN
2	E	865	ASN
2	F	845	ILE
2	G	865	ASN
2	H	845	ILE
2	H	1070	VAL
2	H	1177	ASP
2	E	998	GLN
2	E	1172	MET
2	F	1177	ASP
2	G	998	GLN
2	G	1172	MET
2	H	1018	LEU
2	F	1018	LEU
2	F	1069	PHE
2	H	846	PHE
2	F	984	ILE

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Mol	Chain	Res	Type
2	H	1069	PHE
2	G	1070	VAL
2	E	1106	VAL
2	F	834	VAL
2	F	1106	VAL
2	G	1106	VAL
2	H	984	ILE
2	H	1106	VAL

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	292/297 (98%)	286 (98%)	6 (2%)	47	67
1	B	290/297 (98%)	278 (96%)	12 (4%)	27	49
1	C	292/297 (98%)	285 (98%)	7 (2%)	43	65
1	D	297/297 (100%)	285 (96%)	12 (4%)	28	50
2	E	378/410 (92%)	362 (96%)	16 (4%)	26	49
2	F	378/410 (92%)	367 (97%)	11 (3%)	37	61
2	G	379/410 (92%)	363 (96%)	16 (4%)	26	49
2	H	378/410 (92%)	365 (97%)	13 (3%)	32	57
All	All	2684/2828 (95%)	2591 (96%)	93 (4%)	32	56

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	A	245	ASN
1	A	309	ILE
1	A	314	THR
1	A	395	SER
1	A	450	ILE
2	E	754	LYS

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Mol	Chain	Res	Type
2	E	760	VAL
2	E	885	GLU
2	E	896	GLU
2	E	902	GLU
2	E	912	THR
2	E	923	ILE
2	E	933	VAL
2	E	984	ILE
2	E	1001	THR
2	E	1016	GLU
2	E	1041	SER
2	E	1056	VAL
2	E	1154	LYS
2	E	1160	LEU
2	E	1179	THR
1	B	138	MET
1	B	155	CYS
1	B	223	LYS
1	B	235	LEU
1	B	246	MET
1	B	259	ILE
1	B	283	VAL
1	B	309	ILE
1	B	395	SER
1	B	448	LEU
1	B	452	ILE
1	B	453	GLU
2	F	794	LEU
2	F	860	VAL
2	F	866	GLU
2	F	917	ARG
2	F	927	LEU
2	F	951	ARG
2	F	1033	VAL
2	F	1041	SER
2	F	1092	SER
2	F	1111	LYS
2	F	1159	ARG
1	C	172	GLN
1	C	197	SER
1	C	245	ASN
1	C	309	ILE

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Mol	Chain	Res	Type
1	C	314	THR
1	C	395	SER
1	C	452	ILE
2	G	760	VAL
2	G	831	GLU
2	G	896	GLU
2	G	902	GLU
2	G	912	THR
2	G	923	ILE
2	G	933	VAL
2	G	984	ILE
2	G	1001	THR
2	G	1016	GLU
2	G	1041	SER
2	G	1056	VAL
2	G	1137	LYS
2	G	1154	LYS
2	G	1170	ILE
2	G	1179	THR
1	D	137	MET
1	D	138	MET
1	D	200	TYR
1	D	223	LYS
1	D	235	LEU
1	D	246	MET
1	D	259	ILE
1	D	283	VAL
1	D	309	ILE
1	D	395	SER
1	D	410	LEU
1	D	453	GLU
2	H	794	LEU
2	H	860	VAL
2	H	866	GLU
2	H	917	ARG
2	H	927	LEU
2	H	932	GLN
2	H	951	ARG
2	H	1033	VAL
2	H	1041	SER
2	H	1089	MET
2	H	1092	SER

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Mol	Chain	Res	Type
2	H	1111	LYS
2	H	1159	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	HIS
1	A	218	ASN
1	A	245	ASN
1	A	262	GLN
1	A	420	GLN
1	A	431	GLN
2	E	761	GLN
2	E	859	ASN
2	E	876	ASN
2	E	886	GLN
2	E	1026	HIS
2	E	1039	GLN
2	E	1173	ASN
1	B	172	GLN
1	B	190	HIS
1	B	204	ASN
1	B	205	GLN
1	B	218	ASN
1	B	262	GLN
1	B	335	HIS
1	B	435	HIS
1	B	437	ASN
2	F	842	ASN
2	F	859	ASN
2	F	876	ASN
2	F	880	GLN
2	F	886	GLN
2	F	1014	HIS
2	F	1039	GLN
1	C	165	ASN
1	C	172	GLN
1	C	190	HIS
1	C	205	GLN
1	C	218	ASN
1	C	245	ASN
1	C	262	GLN

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Mol	Chain	Res	Type
1	C	420	GLN
1	C	431	GLN
2	G	761	GLN
2	G	859	ASN
2	G	876	ASN
2	G	886	GLN
2	G	1026	HIS
2	G	1057	GLN
2	G	1085	ASN
2	G	1168	GLN
2	G	1173	ASN
1	D	172	GLN
1	D	218	ASN
1	D	262	GLN
1	D	335	HIS
1	D	435	HIS
1	D	437	ASN
1	D	447	HIS
2	H	859	ASN
2	H	876	ASN
2	H	886	GLN
2	H	932	GLN
2	H	1014	HIS
2	H	1039	GLN
2	H	1173	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 ⓘ

16 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	GLC	I	1	3	11,11,12	1.13	1 (9%)	15,15,17	3.42	8 (53%)
3	FRU	I	2	3	11,12,12	1.19	1 (9%)	10,18,18	3.28	4 (40%)
3	GLC	J	1	3	11,11,12	1.21	1 (9%)	15,15,17	3.89	9 (60%)
3	FRU	J	2	3	11,12,12	1.15	1 (9%)	10,18,18	3.27	4 (40%)
3	GLC	K	1	3	11,11,12	1.34	1 (9%)	15,15,17	3.19	6 (40%)
3	FRU	K	2	3	11,12,12	1.07	1 (9%)	10,18,18	3.59	5 (50%)
3	GLC	L	1	3	11,11,12	1.42	2 (18%)	15,15,17	3.25	7 (46%)
3	FRU	L	2	3	11,12,12	1.18	1 (9%)	10,18,18	3.28	4 (40%)
3	GLC	M	1	3	11,11,12	1.24	1 (9%)	15,15,17	3.47	7 (46%)
3	FRU	M	2	3	11,12,12	1.33	1 (9%)	10,18,18	3.33	4 (40%)
3	GLC	N	1	3	11,11,12	1.48	1 (9%)	15,15,17	3.67	9 (60%)
3	FRU	N	2	3	11,12,12	1.15	1 (9%)	10,18,18	3.33	4 (40%)
3	GLC	O	1	3	11,11,12	1.32	1 (9%)	15,15,17	2.56	4 (26%)
3	FRU	O	2	3	11,12,12	1.25	1 (9%)	10,18,18	3.27	4 (40%)
3	GLC	P	1	3	11,11,12	1.59	2 (18%)	15,15,17	2.97	7 (46%)
3	FRU	P	2	3	11,12,12	1.24	1 (9%)	10,18,18	3.33	4 (40%)

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	GLC	I	1	3	2/2/5/5	0/2/19/22	0/1/1/1
3	FRU	I	2	3	2/2/4/4	3/5/24/24	0/1/1/1
3	GLC	J	1	3	3/3/5/5	1/2/19/22	0/1/1/1
3	FRU	J	2	3	2/2/4/4	3/5/24/24	0/1/1/1
3	GLC	K	1	3	2/2/5/5	1/2/19/22	0/1/1/1
3	FRU	K	2	3	2/2/4/4	3/5/24/24	0/1/1/1
3	GLC	L	1	3	2/2/5/5	0/2/19/22	0/1/1/1
3	FRU	L	2	3	2/2/4/4	3/5/24/24	0/1/1/1
3	GLC	M	1	3	2/2/5/5	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FRU	M	2	3	2/2/4/4	4/5/24/24	0/1/1/1
3	GLC	N	1	3	3/3/5/5	0/2/19/22	0/1/1/1
3	FRU	N	2	3	2/2/4/4	3/5/24/24	0/1/1/1
3	GLC	O	1	3	2/2/5/5	0/2/19/22	0/1/1/1
3	FRU	O	2	3	2/2/4/4	5/5/24/24	0/1/1/1
3	GLC	P	1	3	3/3/5/5	0/2/19/22	0/1/1/1
3	FRU	P	2	3	2/2/4/4	2/5/24/24	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	GLC	O3-C3	-2.84	1.35	1.43
3	P	1	GLC	O3-C3	-2.83	1.36	1.43
3	M	1	GLC	O3-C3	-2.72	1.36	1.43
3	L	1	GLC	O3-C3	-2.68	1.36	1.43
3	K	1	GLC	O3-C3	-2.68	1.36	1.43
3	O	1	GLC	O3-C3	-2.67	1.36	1.43
3	M	2	FRU	O3-C3	-2.64	1.37	1.42
3	L	2	FRU	O3-C3	-2.57	1.37	1.42
3	O	2	FRU	O3-C3	-2.56	1.37	1.42
3	P	2	FRU	O3-C3	-2.56	1.37	1.42
3	N	2	FRU	O3-C3	-2.54	1.37	1.42
3	J	1	GLC	O3-C3	-2.50	1.36	1.43
3	I	2	FRU	O3-C3	-2.47	1.37	1.42
3	J	2	FRU	O3-C3	-2.41	1.38	1.42
3	I	1	GLC	O3-C3	-2.41	1.37	1.43
3	P	1	GLC	O4-C4	-2.18	1.37	1.43
3	L	1	GLC	O4-C4	-2.17	1.37	1.43
3	K	2	FRU	O3-C3	-2.14	1.38	1.42

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1	GLC	C1-C2-C3	8.14	121.50	109.64
3	I	1	GLC	O2-C2-C3	7.07	124.79	110.15
3	J	1	GLC	O2-C2-C3	6.81	124.25	110.15
3	N	2	FRU	O5-C5-C6	6.65	127.03	108.89
3	L	2	FRU	O5-C5-C6	6.59	126.85	108.89
3	P	2	FRU	O5-C5-C6	6.55	126.76	108.89
3	O	1	GLC	C1-C2-C3	6.51	119.12	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	2	FRU	O5-C5-C6	6.41	126.36	108.89
3	L	1	GLC	O2-C2-C3	6.40	123.41	110.15
3	N	1	GLC	O2-C2-C3	6.29	123.18	110.15
3	J	2	FRU	O5-C5-C6	6.22	125.86	108.89
3	L	1	GLC	C2-C3-C4	5.99	121.40	110.86
3	I	1	GLC	C2-C3-C4	5.94	121.31	110.86
3	K	2	FRU	O4-C4-C5	5.89	128.01	111.08
3	K	1	GLC	C2-C3-C4	5.81	121.08	110.86
3	K	1	GLC	O2-C2-C3	5.77	122.10	110.15
3	M	2	FRU	O4-C4-C5	5.66	127.35	111.08
3	I	1	GLC	O2-C2-C1	5.52	121.86	109.22
3	I	2	FRU	O5-C5-C6	5.51	123.92	108.89
3	J	1	GLC	O2-C2-C1	5.49	121.80	109.22
3	I	2	FRU	O4-C4-C5	5.44	126.70	111.08
3	J	1	GLC	C2-C3-C4	5.40	120.36	110.86
3	O	2	FRU	O5-C5-C6	5.35	123.46	108.89
3	K	2	FRU	O4-C4-C3	5.33	128.13	112.16
3	N	1	GLC	O3-C3-C2	5.29	120.86	110.05
3	O	2	FRU	O4-C4-C5	5.29	126.27	111.08
3	N	1	GLC	O4-C4-C5	5.27	122.31	109.32
3	M	1	GLC	O5-C5-C6	5.20	117.78	107.66
3	N	2	FRU	O4-C4-C5	5.18	125.95	111.08
3	P	1	GLC	C2-C3-C4	5.17	119.95	110.86
3	M	2	FRU	O5-C5-C6	5.11	122.83	108.89
3	M	1	GLC	O5-C5-C4	5.10	123.25	110.83
3	O	1	GLC	O2-C2-C3	5.10	120.72	110.15
3	J	1	GLC	O5-C5-C6	5.10	117.58	107.66
3	K	1	GLC	C1-C2-C3	5.05	117.00	109.64
3	J	2	FRU	O4-C4-C5	4.98	125.37	111.08
3	P	2	FRU	O4-C4-C5	4.96	125.32	111.08
3	M	2	FRU	O4-C4-C3	4.91	126.89	112.16
3	P	1	GLC	O4-C4-C5	4.88	121.35	109.32
3	O	2	FRU	O4-C4-C3	4.88	126.80	112.16
3	N	1	GLC	O2-C2-C1	4.86	120.34	109.22
3	L	2	FRU	O4-C4-C5	4.85	125.02	111.08
3	J	2	FRU	O4-C4-C3	4.83	126.66	112.16
3	L	2	FRU	O4-C4-C3	4.83	126.65	112.16
3	J	1	GLC	O3-C3-C2	4.79	119.83	110.05
3	J	1	GLC	C1-O5-C5	-4.75	105.81	112.19
3	M	2	FRU	C6-C5-C4	4.74	126.28	115.10
3	P	2	FRU	O4-C4-C3	4.73	126.35	112.16
3	N	2	FRU	O4-C4-C3	4.64	126.07	112.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	GLC	O2-C2-C1	4.54	119.63	109.22
3	J	1	GLC	O5-C5-C4	4.52	121.82	110.83
3	P	1	GLC	O4-C4-C3	4.50	120.99	110.38
3	P	1	GLC	O3-C3-C2	4.50	119.24	110.05
3	I	2	FRU	O4-C4-C3	4.50	125.65	112.16
3	K	1	GLC	O3-C3-C2	4.49	119.22	110.05
3	M	1	GLC	O2-C2-C3	4.49	119.45	110.15
3	L	1	GLC	O3-C3-C2	4.45	119.13	110.05
3	N	1	GLC	O4-C4-C3	4.45	120.86	110.38
3	I	2	FRU	C6-C5-C4	4.45	125.59	115.10
3	K	1	GLC	O2-C2-C1	4.43	119.37	109.22
3	O	2	FRU	C6-C5-C4	4.39	125.45	115.10
3	N	1	GLC	C2-C3-C4	4.36	118.54	110.86
3	L	1	GLC	C1-C2-C3	4.28	115.88	109.64
3	N	1	GLC	O3-C3-C4	3.99	119.79	110.38
3	I	1	GLC	O3-C3-C4	3.94	119.67	110.38
3	I	1	GLC	O3-C3-C2	3.89	118.00	110.05
3	P	1	GLC	O3-C3-C4	3.79	119.32	110.38
3	O	1	GLC	O2-C2-C1	3.79	117.91	109.22
3	N	1	GLC	C1-C2-C3	3.74	115.08	109.64
3	P	2	FRU	C6-C5-C4	3.67	123.76	115.10
3	N	2	FRU	C6-C5-C4	3.63	123.65	115.10
3	J	2	FRU	C6-C5-C4	3.62	123.63	115.10
3	K	1	GLC	O3-C3-C4	3.59	118.85	110.38
3	J	1	GLC	O3-C3-C4	3.52	118.68	110.38
3	K	2	FRU	C6-C5-C4	3.41	123.14	115.10
3	P	1	GLC	C3-C4-C5	3.38	116.36	110.23
3	M	1	GLC	O2-C2-C1	3.35	116.90	109.22
3	L	2	FRU	C6-C5-C4	3.35	123.00	115.10
3	L	1	GLC	O3-C3-C4	3.29	118.13	110.38
3	M	1	GLC	C1-O5-C5	3.18	116.45	112.19
3	N	1	GLC	C3-C4-C5	3.00	115.68	110.23
3	I	1	GLC	C1-O5-C5	-2.96	108.21	112.19
3	M	1	GLC	C2-C3-C4	2.60	115.43	110.86
3	J	1	GLC	C6-C5-C4	2.52	119.20	113.02
3	P	1	GLC	O5-C5-C6	2.47	112.46	107.66
3	K	2	FRU	O3-C3-C4	2.46	121.93	113.25
3	O	1	GLC	C1-O5-C5	-2.12	109.34	112.19
3	I	1	GLC	C3-C4-C5	2.06	113.97	110.23
3	L	1	GLC	O5-C5-C6	2.05	111.66	107.66
3	I	1	GLC	O5-C1-C2	2.05	115.68	110.79

All (35) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	1	GLC	C3
3	I	1	GLC	C2
3	I	2	FRU	C5
3	I	2	FRU	C4
3	J	1	GLC	C3
3	J	1	GLC	C5
3	J	1	GLC	C2
3	J	2	FRU	C5
3	J	2	FRU	C4
3	K	1	GLC	C3
3	K	1	GLC	C2
3	K	2	FRU	C5
3	K	2	FRU	C4
3	L	1	GLC	C3
3	L	1	GLC	C2
3	L	2	FRU	C5
3	L	2	FRU	C4
3	M	1	GLC	C2
3	M	1	GLC	C3
3	M	2	FRU	C5
3	M	2	FRU	C4
3	N	1	GLC	C3
3	N	1	GLC	C2
3	N	1	GLC	C4
3	N	2	FRU	C5
3	N	2	FRU	C4
3	O	1	GLC	C2
3	O	1	GLC	C3
3	O	2	FRU	C5
3	O	2	FRU	C4
3	P	1	GLC	C2
3	P	1	GLC	C3
3	P	1	GLC	C4
3	P	2	FRU	C5
3	P	2	FRU	C4

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	2	FRU	O1-C1-C2-C3
3	O	2	FRU	O1-C1-C2-O2
3	L	2	FRU	O5-C5-C6-O6
3	I	2	FRU	C4-C5-C6-O6

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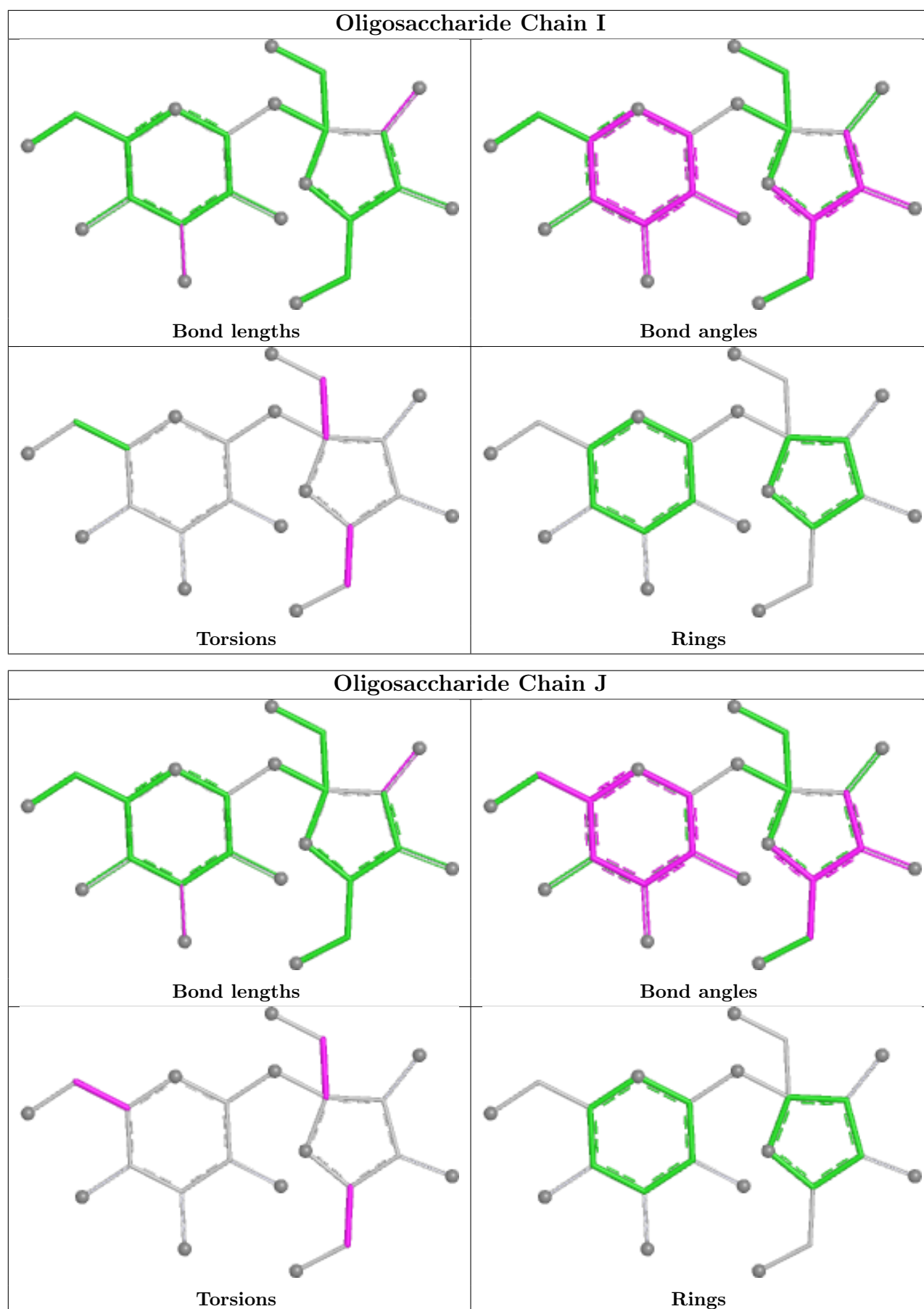
Mol	Chain	Res	Type	Atoms
3	K	2	FRU	C4-C5-C6-O6
3	M	2	FRU	C4-C5-C6-O6
3	N	2	FRU	C4-C5-C6-O6
3	O	2	FRU	C4-C5-C6-O6
3	M	1	GLC	O5-C5-C6-O6
3	J	2	FRU	O5-C5-C6-O6
3	N	2	FRU	O5-C5-C6-O6
3	O	2	FRU	O5-C5-C6-O6
3	J	1	GLC	O5-C5-C6-O6
3	I	2	FRU	O5-C5-C6-O6
3	P	2	FRU	O5-C5-C6-O6
3	M	2	FRU	O5-C5-C6-O6
3	O	2	FRU	O1-C1-C2-O5
3	J	2	FRU	C4-C5-C6-O6
3	K	2	FRU	O5-C5-C6-O6
3	K	1	GLC	O5-C5-C6-O6
3	L	2	FRU	C4-C5-C6-O6
3	M	2	FRU	O1-C1-C2-O2
3	M	2	FRU	O1-C1-C2-C3
3	I	2	FRU	O1-C1-C2-C3
3	K	2	FRU	O1-C1-C2-C3
3	L	2	FRU	O1-C1-C2-C3
3	P	2	FRU	O1-C1-C2-C3
3	J	2	FRU	O1-C1-C2-C3
3	N	2	FRU	O1-C1-C2-C3

There are no ring outliers.

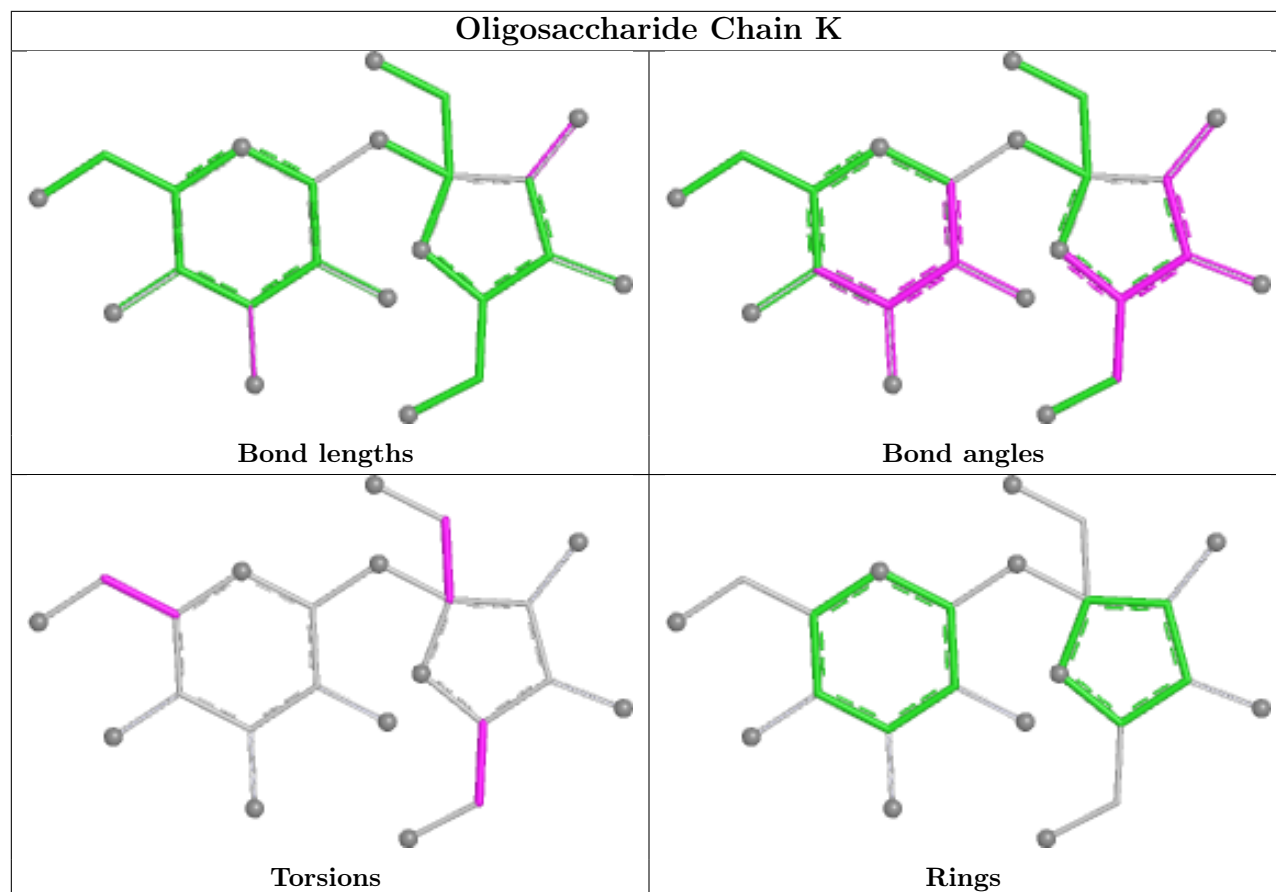
6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	FRU	2	0
3	O	1	GLC	1	0
3	P	1	GLC	4	0
3	J	1	GLC	3	0
3	N	2	FRU	1	0
3	N	1	GLC	5	0

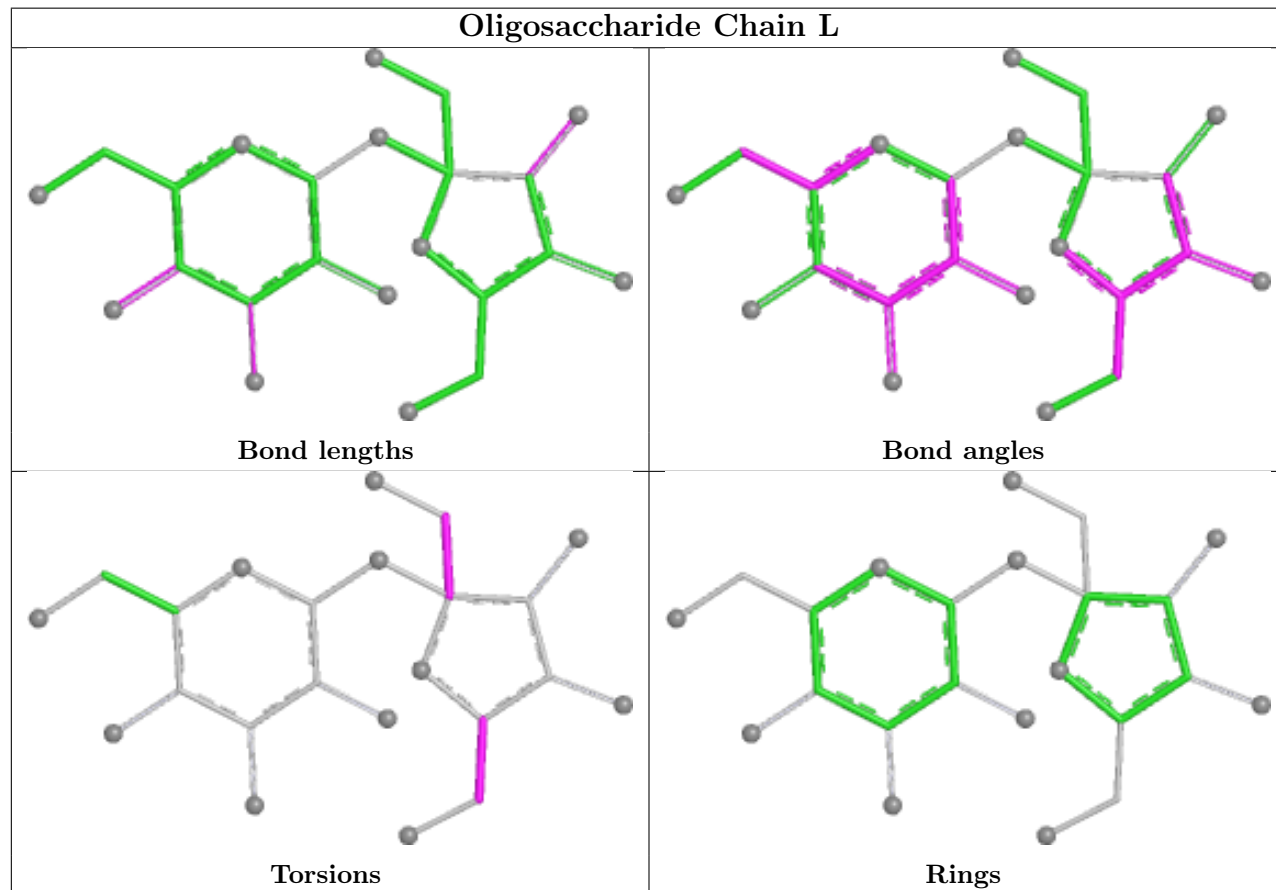
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



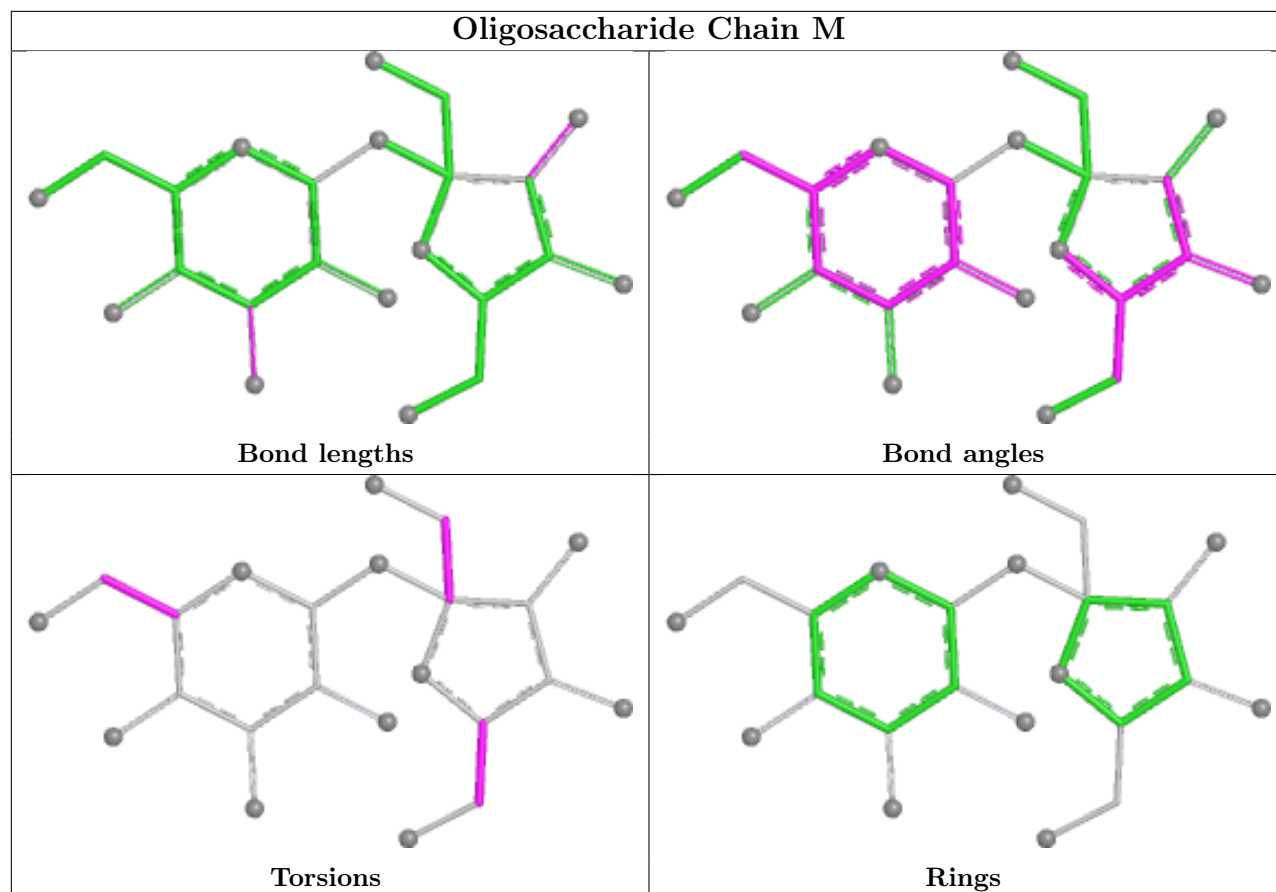
Oligosaccharide Chain K



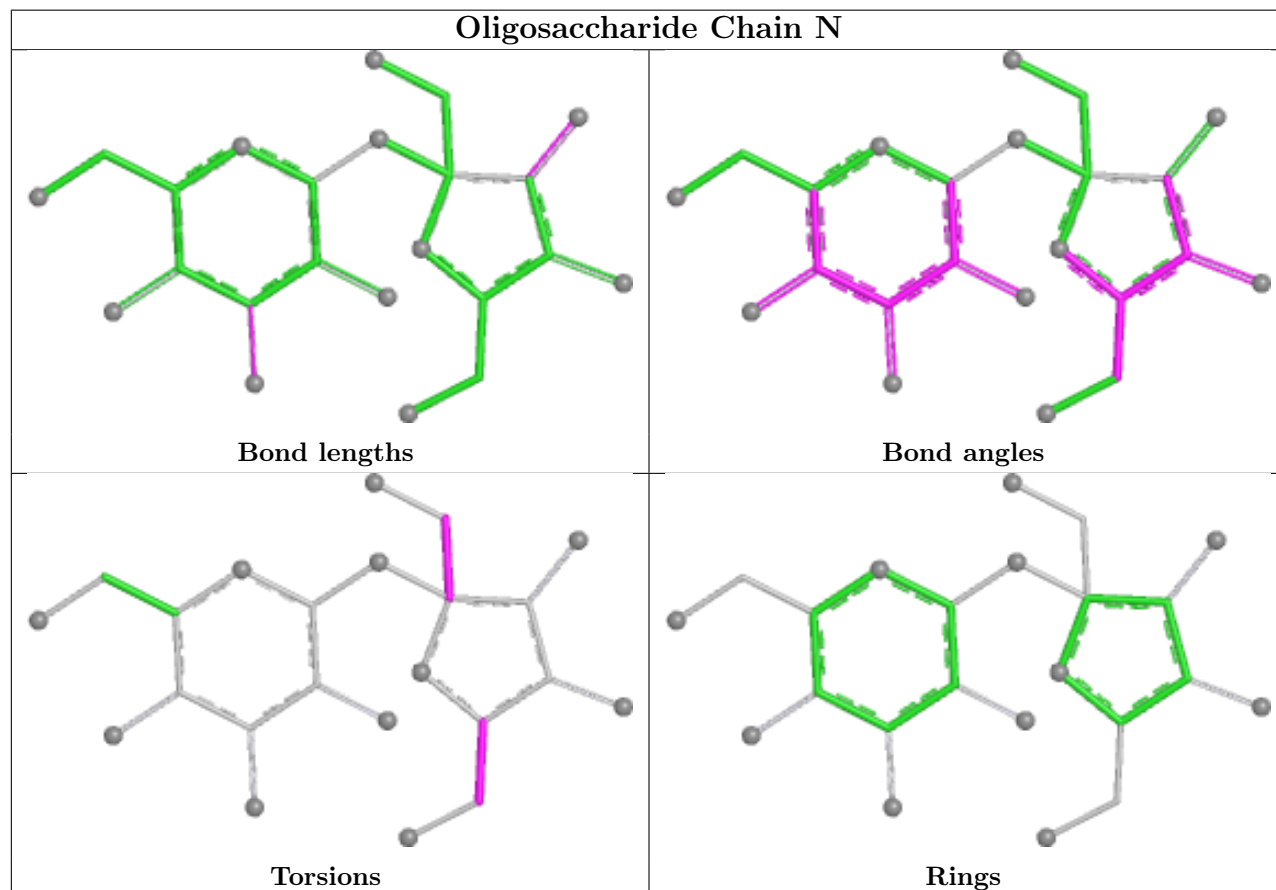
Oligosaccharide Chain L

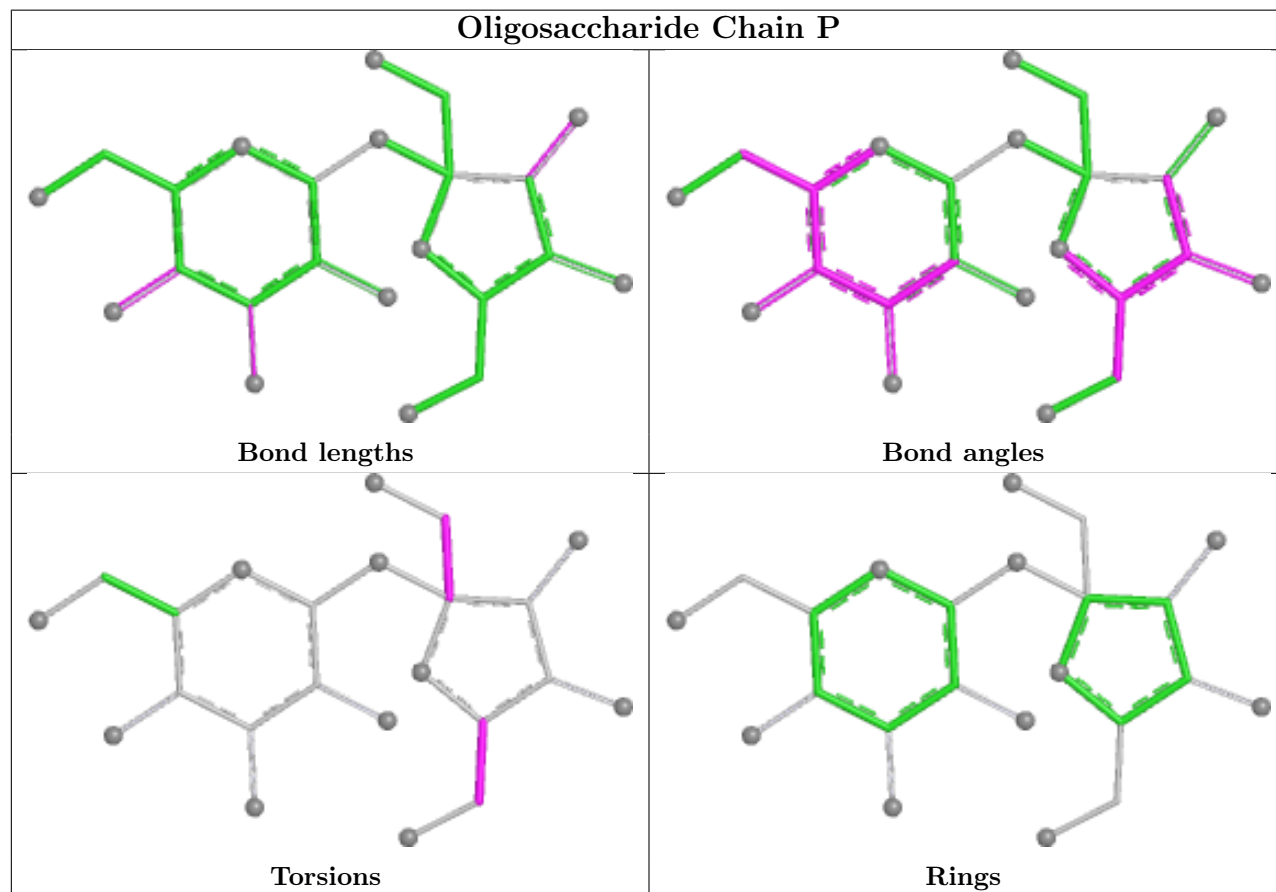
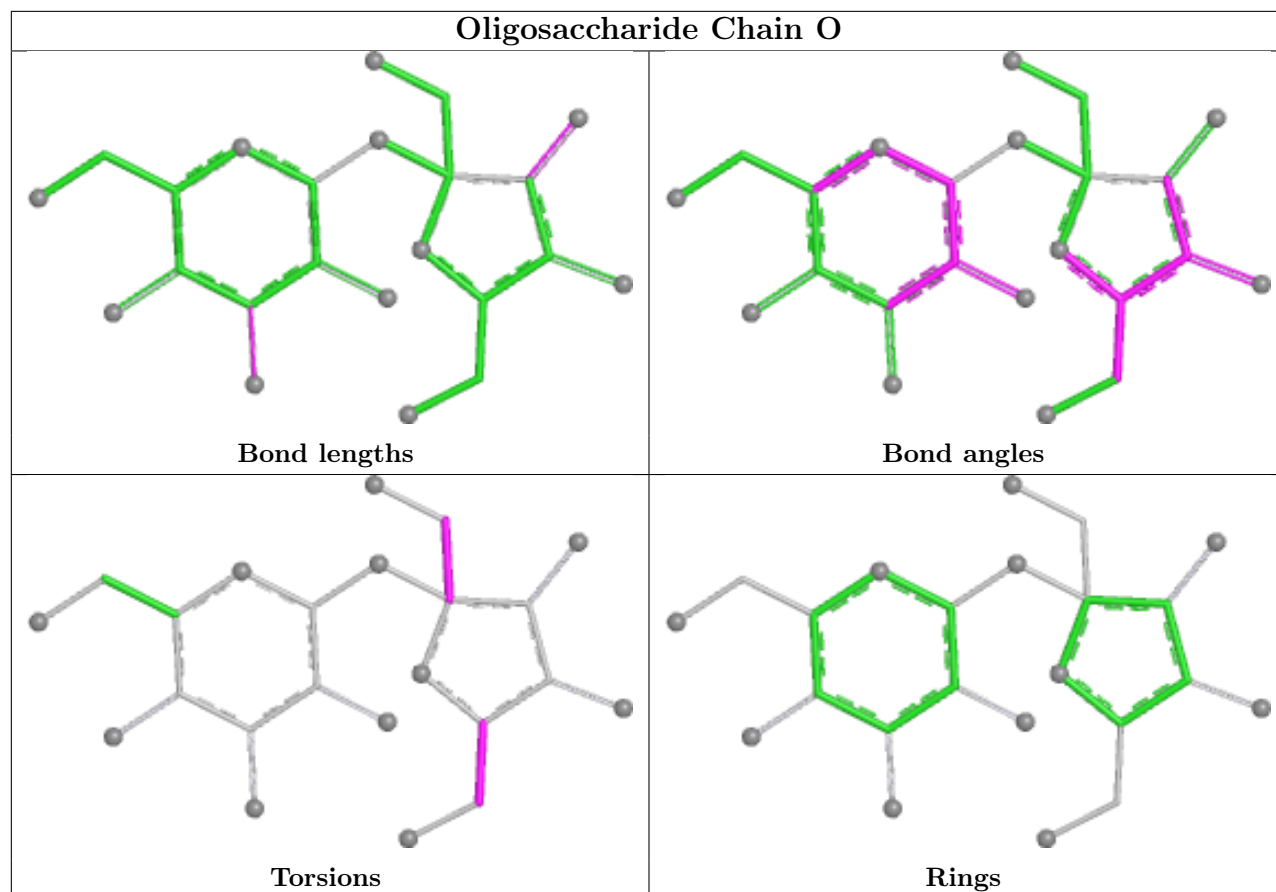


Oligosaccharide Chain M



Oligosaccharide Chain N





5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	322/327 (98%)	-0.57	1 (0%) 90 91	53, 74, 117, 180	0
1	B	319/327 (97%)	-0.37	2 (0%) 85 86	54, 88, 139, 197	0
1	C	322/327 (98%)	-0.52	3 (0%) 81 81	48, 70, 108, 191	0
1	D	327/327 (100%)	-0.37	2 (0%) 85 86	52, 81, 127, 185	0
2	E	419/457 (91%)	-0.06	4 (0%) 79 79	62, 110, 160, 200	0
2	F	419/457 (91%)	-0.05	5 (1%) 76 76	59, 107, 173, 214	0
2	G	420/457 (91%)	-0.09	3 (0%) 84 84	68, 111, 159, 201	0
2	H	419/457 (91%)	-0.05	6 (1%) 73 73	62, 105, 166, 205	0
All	All	2967/3136 (94%)	-0.23	26 (0%) 81 81	48, 96, 157, 214	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	200	TYR	4.3
1	D	456	VAL	4.1
2	H	804	ALA	3.7
1	A	200	TYR	3.7
2	H	896	GLU	3.3
1	D	200	TYR	3.3
2	H	775	LEU	2.8
2	G	1196	ARG	2.7
2	F	906	PHE	2.6
2	F	832	LEU	2.5
1	B	296	GLY	2.5
2	E	829	VAL	2.5
2	G	775	LEU	2.4
2	H	850	PHE	2.4
1	B	200	TYR	2.4
2	F	760	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	1196	ARG	2.3
2	E	1077	VAL	2.3
2	F	850	PHE	2.3
2	F	775	LEU	2.2
1	C	191	ASP	2.2
2	G	1166	ARG	2.1
2	E	893	LEU	2.1
1	C	198	GLY	2.0
2	E	760	VAL	2.0
2	H	899	ASP	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.

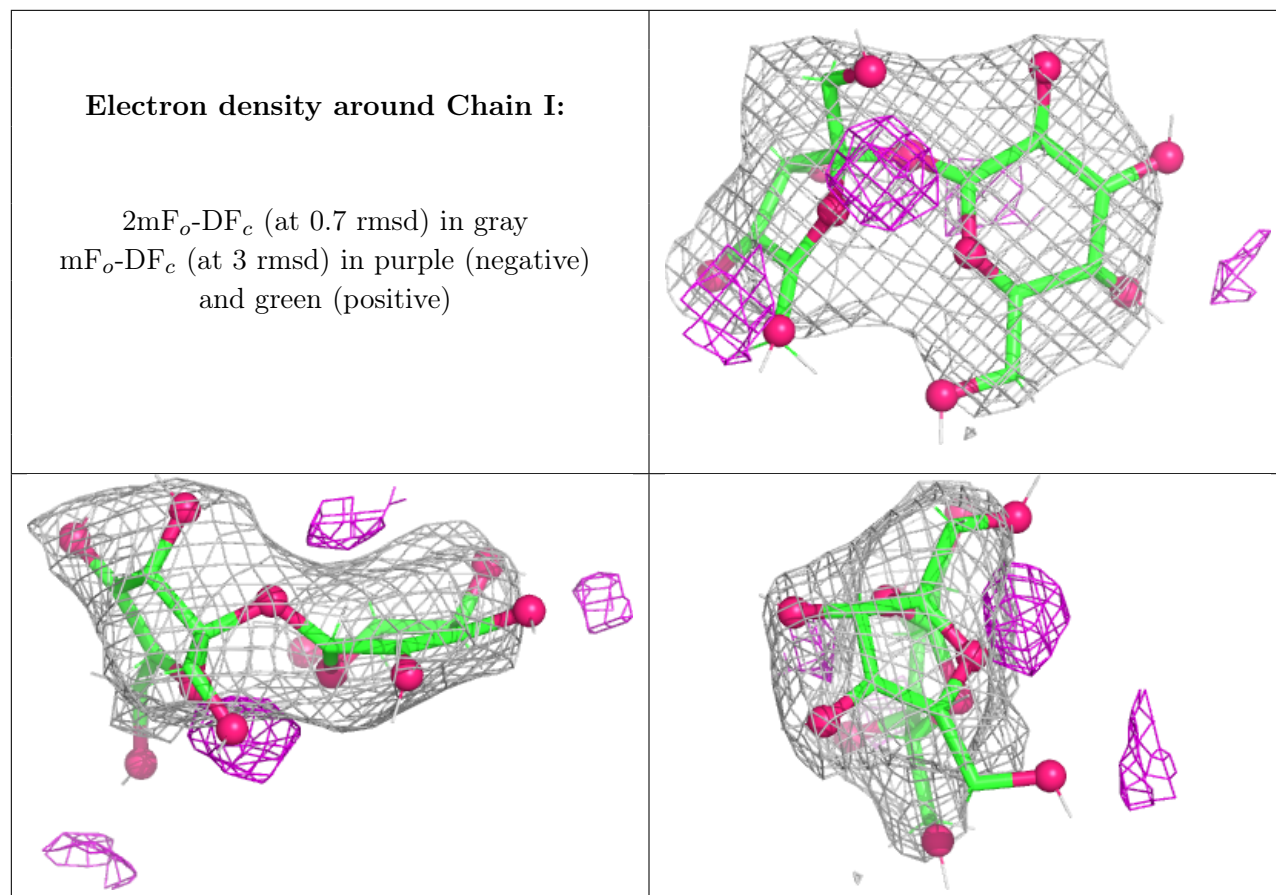
6.3 Carbohydrates [i](#)

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, 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
3	FRU	N	2	12/12	0.46	0.14	186,223,266,269	0
3	FRU	J	2	12/12	0.68	0.13	181,204,244,254	0
3	FRU	K	2	12/12	0.71	0.12	147,171,192,198	0
3	GLC	M	1	11/12	0.73	0.12	173,194,218,225	0
3	GLC	K	1	11/12	0.75	0.11	147,167,190,200	0
3	GLC	O	1	11/12	0.75	0.12	153,178,205,214	0
3	FRU	P	2	12/12	0.75	0.17	173,208,265,286	0
3	FRU	M	2	12/12	0.79	0.13	173,193,232,251	0
3	GLC	I	1	11/12	0.79	0.11	162,181,212,217	0
3	FRU	L	2	12/12	0.80	0.14	179,215,269,298	0
3	FRU	I	2	12/12	0.81	0.11	162,187,204,207	0
3	FRU	O	2	12/12	0.84	0.10	153,176,208,211	0
3	GLC	J	1	11/12	0.87	0.12	181,197,229,237	0
3	GLC	N	1	11/12	0.87	0.15	185,217,256,261	0
3	GLC	L	1	11/12	0.87	0.15	179,215,252,273	0
3	GLC	P	1	11/12	0.88	0.15	173,199,226,239	0

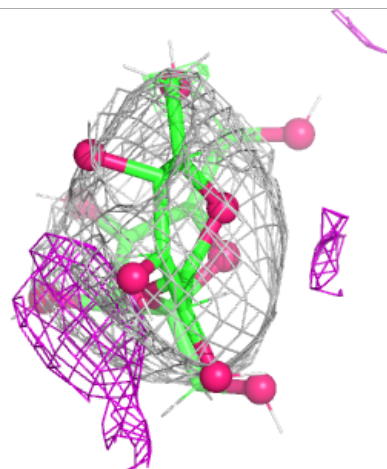
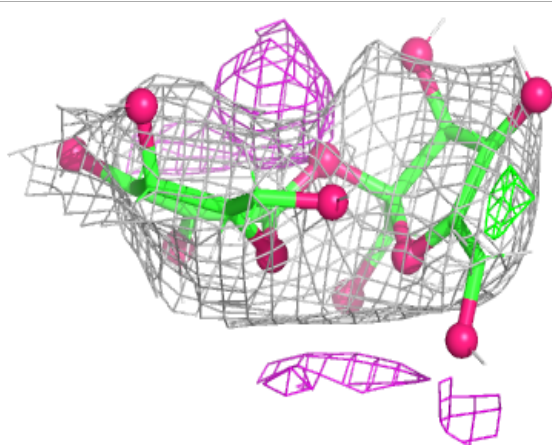
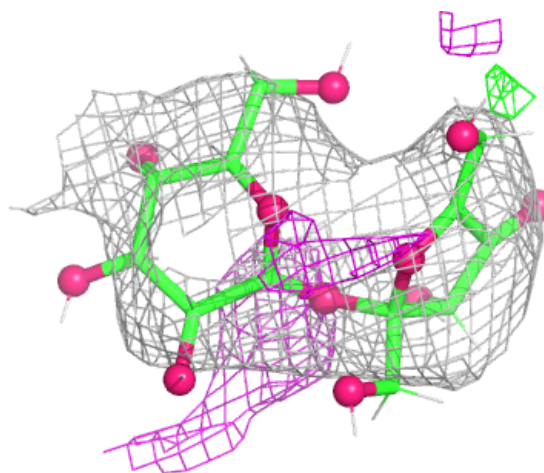
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



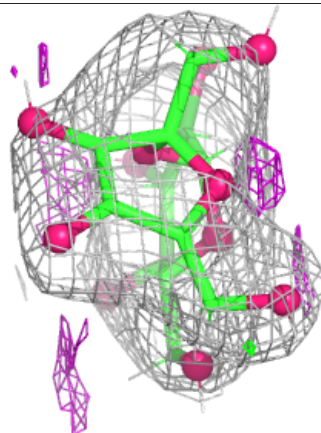
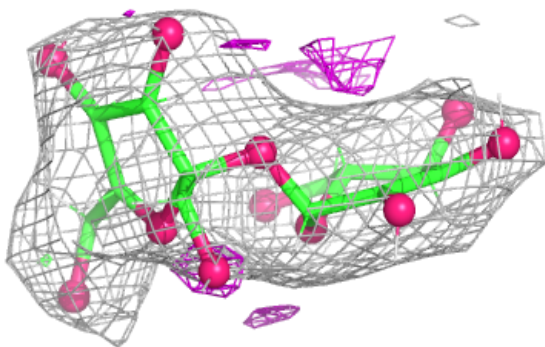
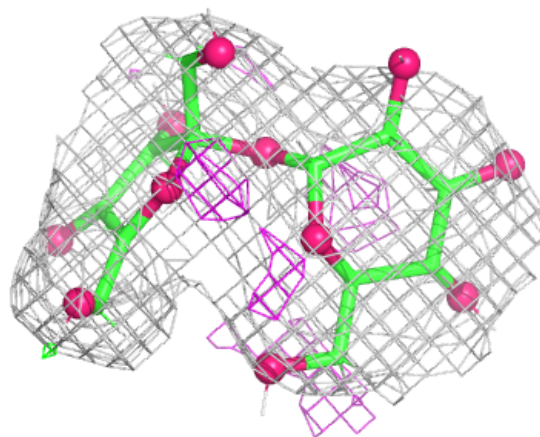
Electron density around Chain J:

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



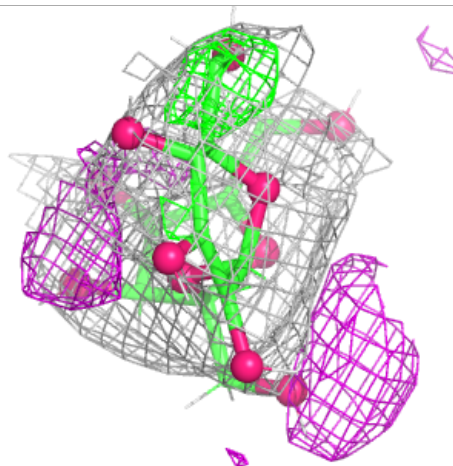
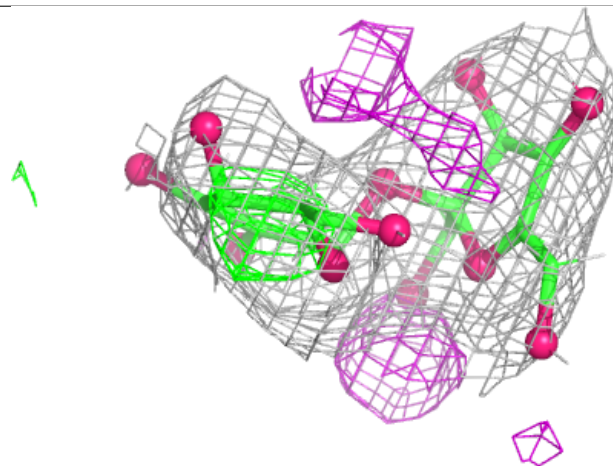
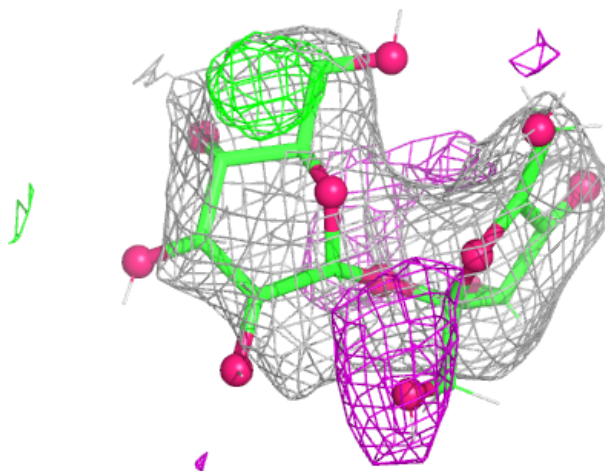
Electron density around Chain K:

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



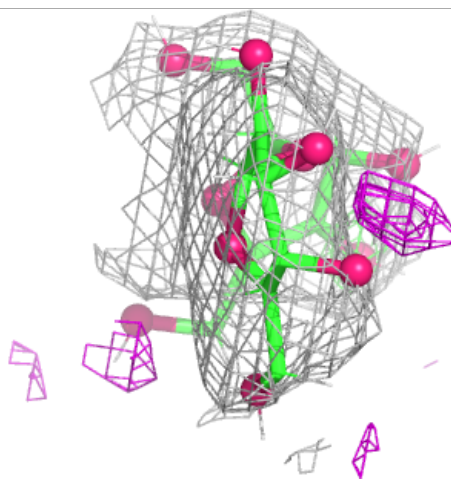
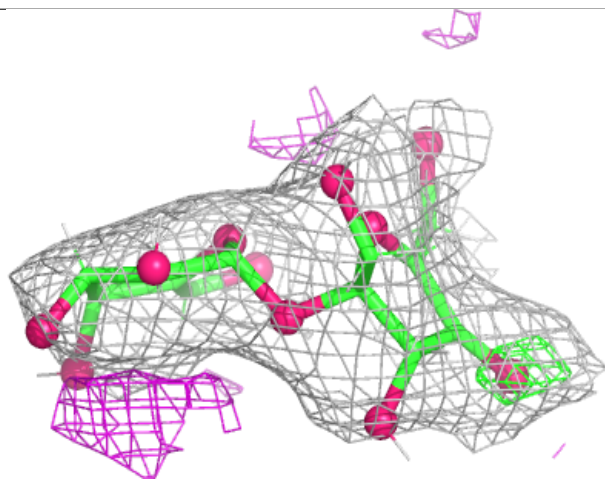
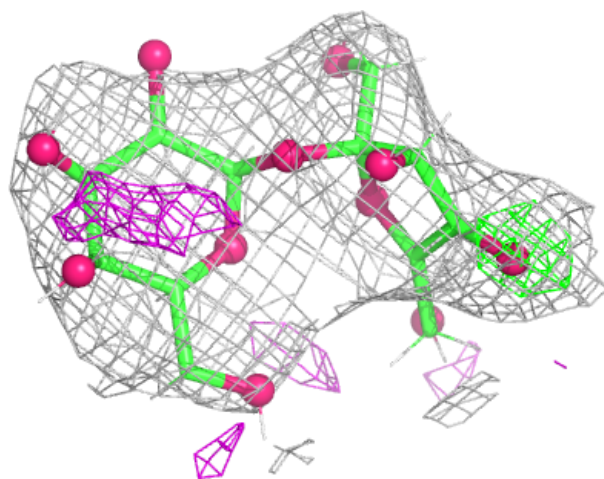
Electron density around Chain L:

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



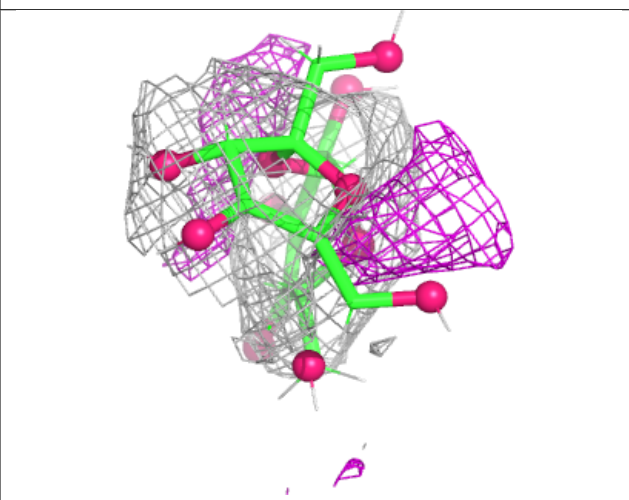
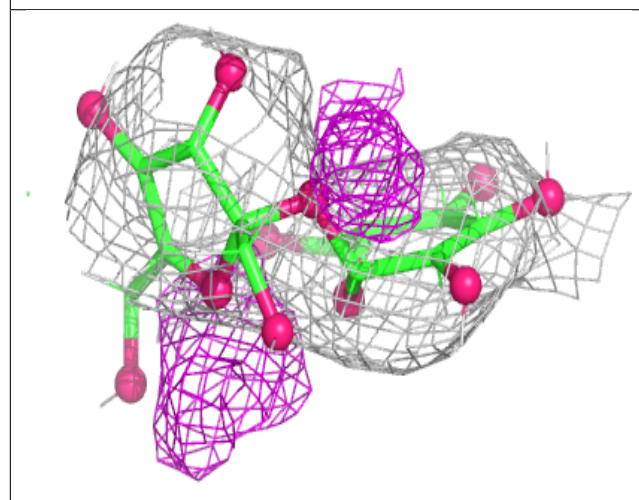
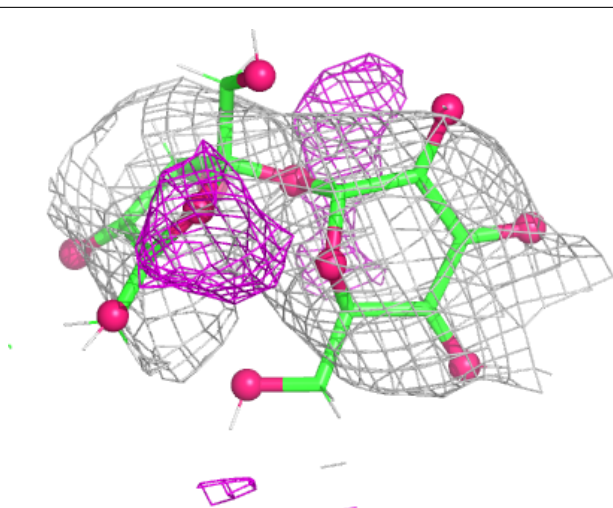
Electron density around Chain M:

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



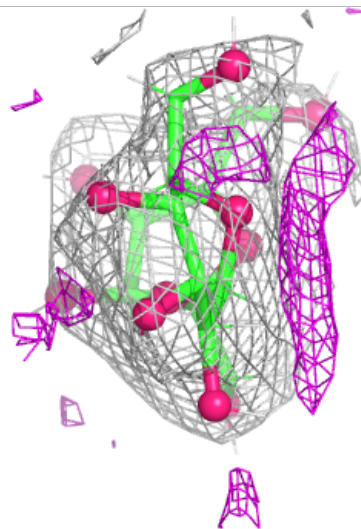
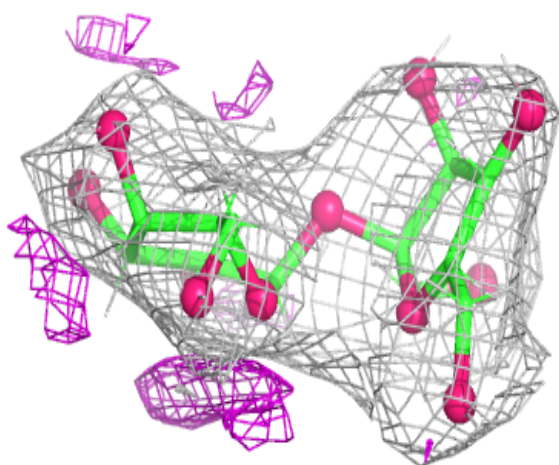
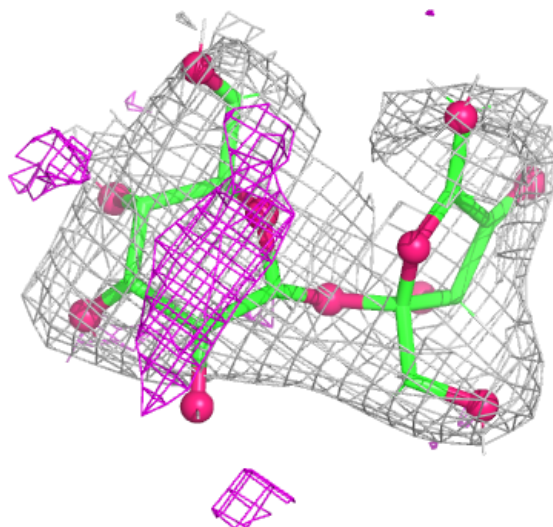
Electron density around Chain N:

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



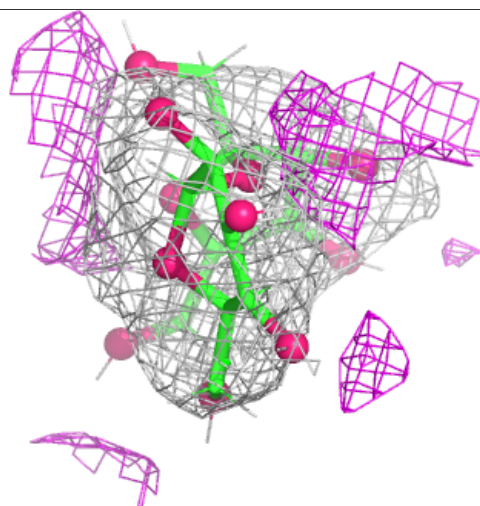
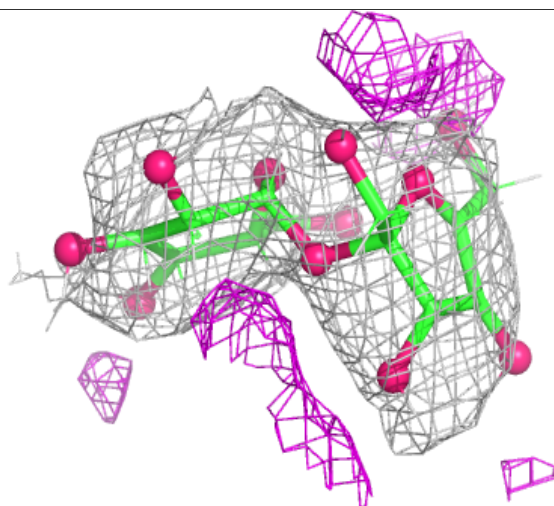
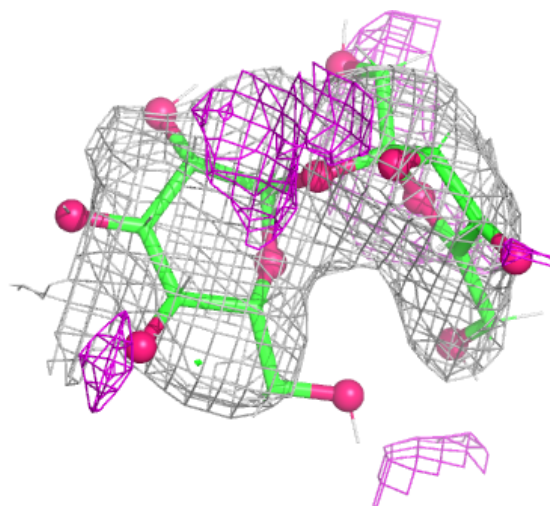
Electron density around Chain O:

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



Electron density around Chain P:

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.