



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:43 AM UTC

PDB ID : 4RES / pdb_00004res
Title : Crystal structure of the Na,K-ATPase E2P-bufalin complex with bound potassium
Authors : Laursen, M.; Yatime, L.; Gregersen, J.L.; Nissen, P.; Fedosova, N.U.
Deposited on : 2014-09-23
Resolution : 3.41 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

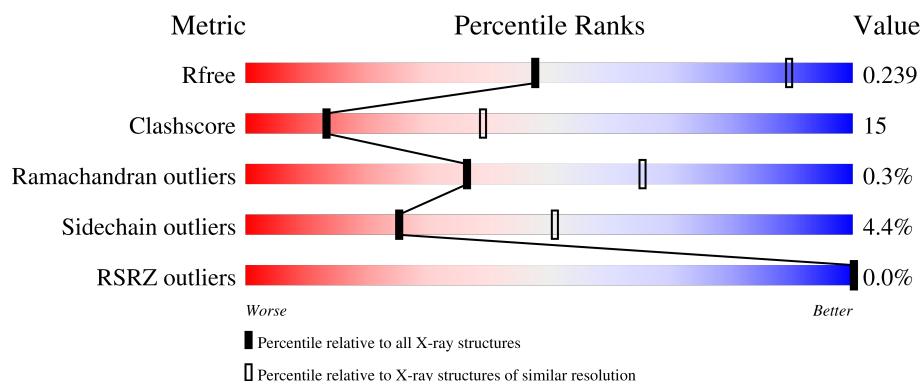
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	1021	
1	C	1021	
2	B	303	
2	D	303	
3	E	65	

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Mol	Chain	Length	Quality of chain
3	G	65	42%6%51%
4	F	2	50%50%
5	H	2	50%50%
5	I	2	100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 20881 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			
1	C	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	288	Total	C	N	O	S	0	0	0
			2357	1525	385	434	13			
2	D	285	Total	C	N	O	S	0	0	0
			2327	1504	380	430	13			

- Molecule 3 is a protein called Na⁺/K⁺ ATPase gamma subunit transcript variant a.

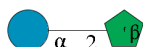
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	32	Total	C	N	O	0	0	0
			255	174	37	44			
3	E	32	Total	C	N	O	0	0	0
			255	174	37	44			

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



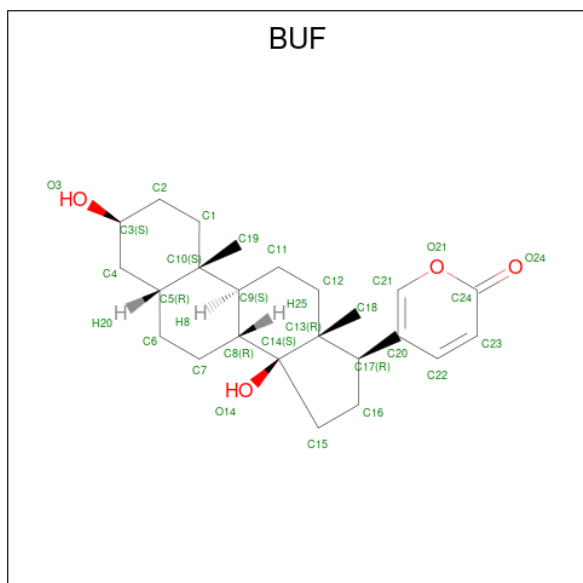
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	H	2	Total	C	O	0	0	0
			23	12	11			
5	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is bufalin (CCD ID: BUF) (formula: $C_{24}H_{34}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			28	24	4		
6	C	1	Total	C	O	0	0
			28	24	4		

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			28	27	1		
7	E	1	Total	C	O	0	0
			28	27	1		

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	K	0	0
			3	3		
8	C	3	Total	K	0	0
			3	3		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

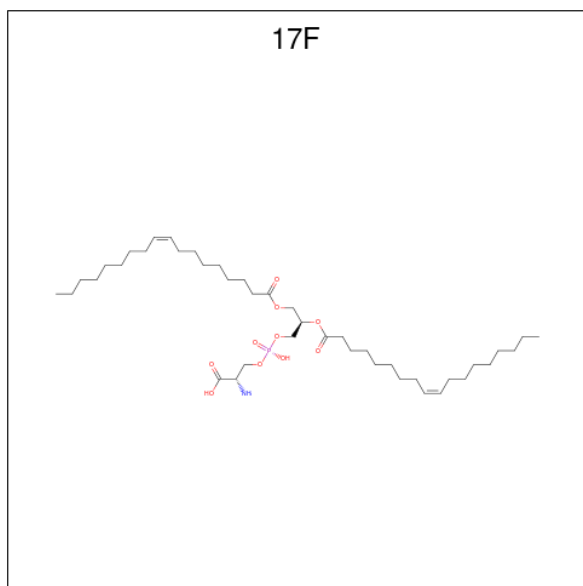
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Mg	0	0
			1	1		
9	C	1	Total	Mg	0	0
			1	1		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 11 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (CCD ID: 17F) (formula: $C_{42}H_{78}NO_{10}P$).

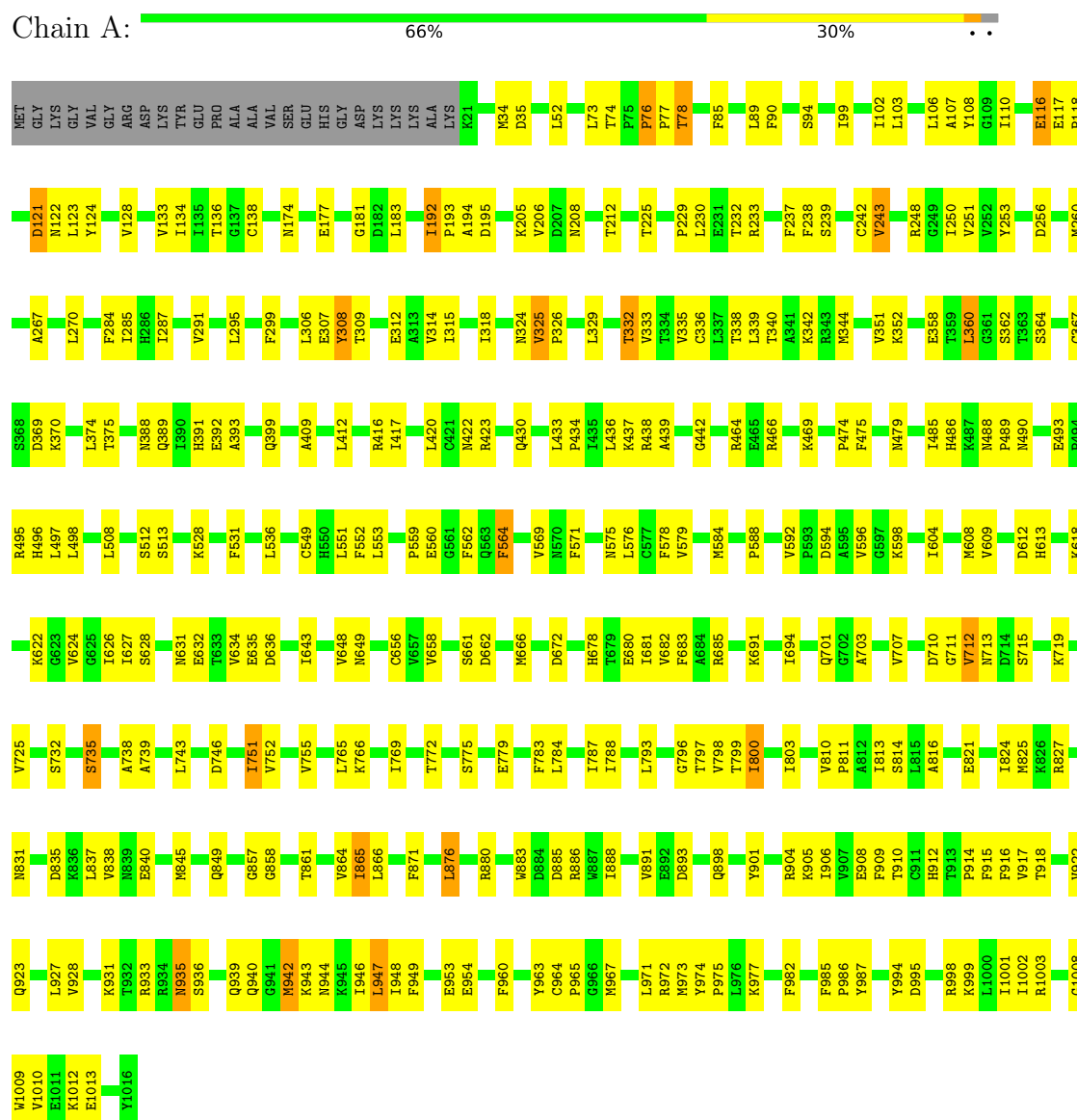


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	G	1	Total	C	N	O	P	0	0
			19	8	1	9	1		

3 Residue-property plots

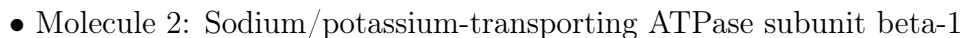
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Sodium/potassium-transporting ATPase subunit alpha-1



- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

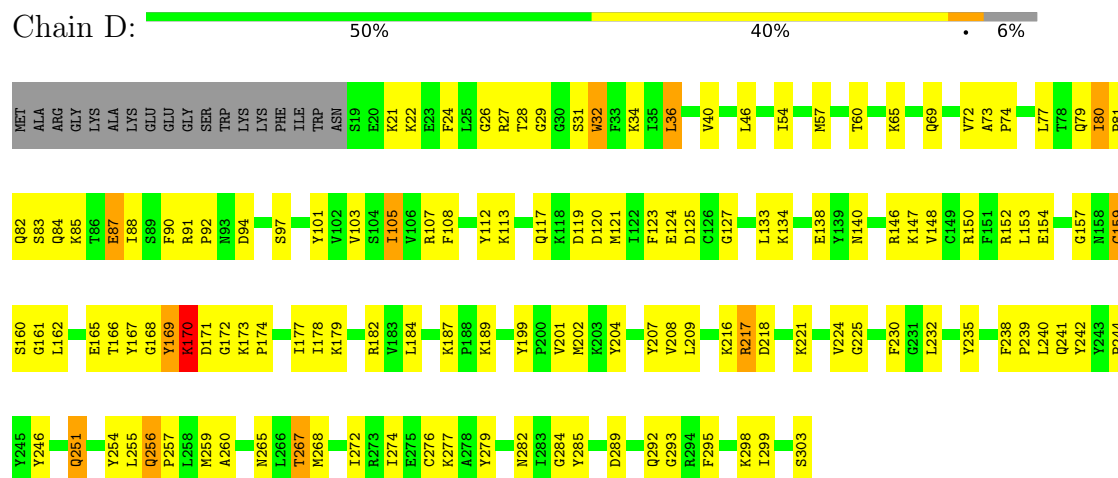
Response	Percentage
Yes	65%
No	30%
Don't know	5%



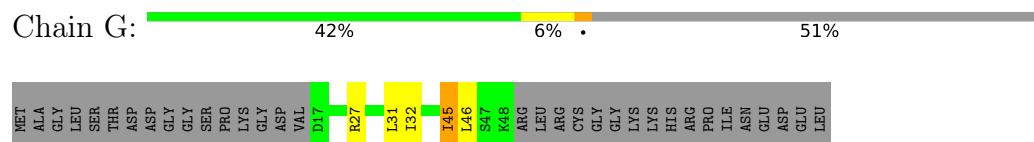
Response	Percentage
Yes, the U.S. should take action to protect the environment	52%
No, the U.S. should not take action to protect the environment	39%
Don't know	5%



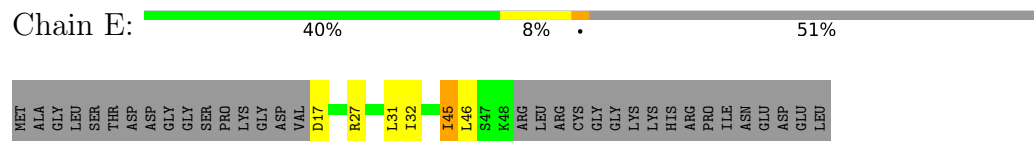
- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



- Molecule 3: Na⁺/K⁺ ATPase gamma subunit transcript variant a



- Molecule 3: Na⁺/K⁺ ATPase gamma subunit transcript variant a



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



- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



GLC1
FR02

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.91Å 240.27Å 152.70Å 90.00° 102.28° 90.00°	Depositor
Resolution (Å)	49.90 – 3.41 49.90 – 3.41	Depositor EDS
% Data completeness (in resolution range)	49.9 (49.90-3.41) 50.4 (49.90-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.245 , 0.288 (Not available) , 0.239	Depositor DCC
R_{free} test set	1634 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å ²)	92.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 100.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.368 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20881	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 17F, K, BUF, FRU, NAG, MG, GLC, CLR, PHD

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	0.44	0/7867	0.91	18/10674 (0.2%)
1	C	0.45	1/7867 (0.0%)	0.91	19/10674 (0.2%)
2	B	0.45	0/2419	0.96	13/3263 (0.4%)
2	D	0.46	0/2387	0.95	13/3218 (0.4%)
3	E	0.40	0/261	0.86	0/354
3	G	0.39	0/261	0.85	0/354
All	All	0.44	1/21062 (0.0%)	0.92	63/28537 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	22	GLU	N-CA	5.02	1.52	1.46

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ILE	CA-C-N	7.38	126.89	118.85
1	A	192	ILE	C-N-CA	7.38	126.89	118.85
1	C	116	GLU	CA-C-N	7.32	128.77	120.06
1	C	116	GLU	C-N-CA	7.32	128.77	120.06
1	C	192	ILE	CA-C-N	7.28	126.79	118.85
1	C	192	ILE	C-N-CA	7.28	126.79	118.85
1	A	116	GLU	CA-C-N	7.23	128.66	120.06
1	A	116	GLU	C-N-CA	7.23	128.66	120.06
2	B	173	LYS	CA-C-N	7.21	126.97	119.76
2	B	173	LYS	C-N-CA	7.21	126.97	119.76
1	A	117	GLU	N-CA-C	7.17	123.47	113.57
1	C	76	PRO	CA-C-N	7.08	126.76	119.82
1	C	76	PRO	C-N-CA	7.08	126.76	119.82
1	C	117	GLU	N-CA-C	7.07	123.33	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	268	MET	N-CA-C	6.97	118.57	110.97
1	A	76	PRO	CA-C-N	6.94	126.62	119.82
1	A	76	PRO	C-N-CA	6.94	126.62	119.82
2	D	268	MET	N-CA-C	6.92	118.51	110.97
2	D	173	LYS	CA-C-N	6.72	126.63	119.85
2	D	173	LYS	C-N-CA	6.72	126.63	119.85
1	C	793	LEU	CA-C-N	6.61	126.06	118.85
1	C	793	LEU	C-N-CA	6.61	126.06	118.85
2	B	209	LEU	CA-C-N	6.59	126.77	120.31
2	B	209	LEU	C-N-CA	6.59	126.77	120.31
1	A	649	ASN	CA-C-N	6.45	126.14	119.56
1	A	649	ASN	C-N-CA	6.45	126.14	119.56
1	C	649	ASN	CA-C-N	6.40	126.08	119.56
1	C	649	ASN	C-N-CA	6.40	126.08	119.56
2	D	209	LEU	CA-C-N	6.31	126.49	120.31
2	D	209	LEU	C-N-CA	6.31	126.49	120.31
2	B	251	GLN	CA-C-N	-6.27	113.82	120.03
2	B	251	GLN	C-N-CA	-6.27	113.82	120.03
1	A	793	LEU	CA-C-N	6.25	125.67	118.85
1	A	793	LEU	C-N-CA	6.25	125.67	118.85
2	D	251	GLN	CA-C-N	-6.22	113.87	120.03
2	D	251	GLN	C-N-CA	-6.22	113.87	120.03
2	D	208	VAL	N-CA-C	5.94	116.19	108.35
2	D	207	TYR	N-CA-C	5.93	120.64	113.17
2	B	90	PHE	N-CA-C	5.88	117.19	108.60
2	B	208	VAL	N-CA-C	5.86	116.08	108.35
2	D	127	GLY	N-CA-C	5.86	118.67	111.93
2	B	127	GLY	N-CA-C	5.81	118.61	111.93
1	A	325	VAL	CA-C-N	5.78	127.07	119.84
1	A	325	VAL	C-N-CA	5.78	127.07	119.84
2	B	207	TYR	N-CA-C	5.78	120.45	113.17
1	C	325	VAL	CA-C-N	5.77	127.05	119.84
1	C	325	VAL	C-N-CA	5.77	127.05	119.84
2	D	90	PHE	N-CA-C	5.61	117.32	108.96
1	A	681	ILE	N-CA-C	5.57	116.50	108.48
1	C	116	GLU	N-CA-C	5.48	117.72	109.23
1	A	116	GLU	N-CA-C	5.48	117.72	109.23
1	C	681	ILE	N-CA-C	5.37	116.22	108.48
2	B	87	GLU	N-CA-C	5.19	116.85	108.34
2	B	170	LYS	N-CA-C	5.17	121.82	110.80
1	A	977	LYS	CA-C-N	5.16	125.45	119.47
1	A	977	LYS	C-N-CA	5.16	125.45	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	87	GLU	N-CA-C	5.15	116.78	108.34
2	D	170	LYS	N-CA-C	5.08	121.63	110.80
1	C	422	ASN	N-CA-C	5.07	117.24	109.07
1	A	308	TYR	N-CA-C	5.04	117.34	110.24
1	C	910	THR	N-CA-C	-5.03	106.93	113.16
1	C	872	LEU	CA-C-N	5.00	125.02	119.32
1	C	872	LEU	C-N-CA	5.00	125.02	119.32

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	7730	0	7776	220	0
1	C	7730	0	7776	227	0
2	B	2357	0	2328	85	0
2	D	2327	0	2301	87	0
3	E	255	0	259	5	0
3	G	255	0	259	4	0
4	F	28	0	25	1	0
5	H	23	0	21	3	0
5	I	23	0	21	2	0
6	A	28	0	34	3	0
6	C	28	0	34	5	0
7	A	28	0	46	4	0
7	E	28	0	46	4	0
8	A	3	0	0	0	0
8	C	3	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	14	0	13	1	0
11	G	19	0	10	0	0
All	All	20881	0	20949	618	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 15.

All (618) 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:B:80:ILE:HG13	2:B:81:PRO:HD3	1.44	0.97
2:D:80:ILE:HG13	2:D:81:PRO:HD3	1.45	0.97
2:B:79:GLN:HB3	2:B:295:PHE:HZ	1.33	0.93
2:D:79:GLN:HB3	2:D:295:PHE:HZ	1.34	0.91
2:D:80:ILE:HD12	2:D:105:ILE:HD12	1.52	0.91
2:B:80:ILE:HD12	2:B:105:ILE:HD12	1.52	0.91
1:A:910:THR:HG22	1:A:974:TYR:HB2	1.54	0.90
1:C:910:THR:HG22	1:C:974:TYR:HB2	1.55	0.88
2:B:165:GLU:HB3	2:B:166:THR:HA	1.60	0.84
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.59	0.83
2:D:165:GLU:HB3	2:D:166:THR:HA	1.60	0.83
1:C:375:THR:HA	1:C:588:PRO:HA	1.60	0.82
1:C:864:VAL:HG22	2:D:57:MET:HG3	1.62	0.81
2:D:94:ASP:HB3	2:D:97:SER:HB2	1.62	0.81
2:B:94:ASP:HB3	2:B:97:SER:HB2	1.63	0.81
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.17	0.80
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.18	0.79
1:C:799:THR:HG22	1:C:973:MET:HE3	1.67	0.77
1:A:375:THR:HA	1:A:588:PRO:HA	1.68	0.76
1:A:612:ASP:OD1	1:A:613:HIS:N	2.18	0.76
1:A:799:THR:HG21	1:A:912:HIS:HB3	1.68	0.76
1:C:612:ASP:OD1	1:C:613:HIS:N	2.19	0.76
1:C:799:THR:HG21	1:C:912:HIS:HB3	1.68	0.76
1:A:800:ILE:HG21	6:A:2001:BUF:H33	1.69	0.75
1:A:799:THR:HG22	1:A:973:MET:HE3	1.69	0.75
1:C:604:ILE:HD11	1:C:755:VAL:HG21	1.67	0.75
1:C:195:ASP:HB2	1:C:253:TYR:HB2	1.70	0.73
1:C:800:ILE:HG21	6:C:1102:BUF:H33	1.70	0.73
2:D:80:ILE:HG12	2:D:177:ILE:HB	1.70	0.73
1:A:604:ILE:HD11	1:A:755:VAL:HG21	1.71	0.72
2:B:80:ILE:HG12	2:B:177:ILE:HB	1.72	0.71
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.72	0.71
1:A:725:VAL:HG11	1:A:751:ILE:HD11	1.71	0.71
2:D:166:THR:HB	2:D:169:TYR:H	1.55	0.71
1:C:901:TYR:HA	1:C:904:ARG:HE	1.55	0.70
1:C:672:ASP:OD1	1:C:701:GLN:NE2	2.24	0.70
2:B:166:THR:HB	2:B:169:TYR:H	1.56	0.70
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ASP:OD1	1:A:701:GLN:NE2	2.25	0.69
2:B:170:LYS:HB2	2:B:174:PRO:HA	1.72	0.69
2:D:170:LYS:HB2	2:D:174:PRO:HA	1.72	0.69
1:A:434:PRO:HG2	1:A:437:LYS:HB2	1.74	0.69
1:A:901:TYR:HA	1:A:904:ARG:HE	1.56	0.69
2:D:171:ASP:OD1	2:D:172:GLY:N	2.24	0.69
1:C:434:PRO:HG2	1:C:437:LYS:HB2	1.74	0.69
1:A:399:GLN:HE21	1:A:436:LEU:HD11	1.56	0.69
1:C:399:GLN:HE21	1:C:436:LEU:HD11	1.57	0.69
2:B:171:ASP:OD1	2:B:172:GLY:N	2.24	0.69
1:C:725:VAL:HG11	1:C:751:ILE:HD11	1.75	0.68
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.58	0.68
1:A:849:GLN:OE1	1:A:994:TYR:OH	2.12	0.67
1:A:609:VAL:HG22	1:A:683:PHE:HD2	1.59	0.67
2:B:80:ILE:HD13	2:B:177:ILE:HD12	1.77	0.67
2:D:80:ILE:HD13	2:D:177:ILE:HD12	1.77	0.67
1:A:118:PRO:HA	1:A:121:ASP:HB2	1.75	0.66
1:C:118:PRO:HA	1:C:121:ASP:HB2	1.76	0.66
1:A:335:VAL:O	1:A:339:LEU:HG	1.96	0.66
1:C:609:VAL:HG22	1:C:683:PHE:HD2	1.61	0.65
2:B:124:GLU:OE2	2:B:134:LYS:NZ	2.29	0.65
1:C:225:THR:HG21	1:C:233:ARG:HD2	1.77	0.65
2:D:124:GLU:OE2	2:D:134:LYS:NZ	2.30	0.65
1:C:909:PHE:HA	1:C:912:HIS:HD2	1.62	0.65
1:A:909:PHE:HA	1:A:912:HIS:HD2	1.62	0.65
1:C:420:LEU:HB3	1:C:486:HIS:HE1	1.63	0.65
2:D:168:GLY:HA3	2:D:171:ASP:HB3	1.78	0.65
2:D:31:SER:HB2	2:D:34:LYS:HD2	1.77	0.64
1:C:849:GLN:OE1	1:C:994:TYR:OH	2.15	0.64
1:C:335:VAL:O	1:C:339:LEU:HG	1.97	0.64
2:D:79:GLN:HG2	2:D:82:GLN:HG2	1.80	0.64
1:A:225:THR:HG21	1:A:233:ARG:HD2	1.78	0.64
1:A:367:CYS:HB2	1:A:707:VAL:HG22	1.79	0.63
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.80	0.63
2:B:168:GLY:HA3	2:B:171:ASP:HB3	1.79	0.63
2:B:65:LYS:HG3	2:B:184:LEU:HD22	1.80	0.62
2:B:79:GLN:HG2	2:B:82:GLN:HG2	1.82	0.62
1:A:420:LEU:HB3	1:A:486:HIS:HE1	1.65	0.62
2:D:113:LYS:HA	2:D:153:LEU:HD11	1.82	0.62
1:A:800:ILE:HD13	6:A:2001:BUF:H33	1.82	0.61
2:D:133:LEU:HG	2:D:240:LEU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:CYS:HB2	1:C:707:VAL:HG22	1.81	0.61
1:A:845:MET:SD	1:A:849:GLN:NE2	2.74	0.61
2:B:31:SER:HB2	2:B:34:LYS:HD2	1.81	0.60
1:A:422:ASN:O	1:A:464:ARG:NH1	2.33	0.60
2:B:276:CYS:HB2	2:B:295:PHE:HB3	1.82	0.60
1:A:284:PHE:HB2	1:A:838:VAL:HB	1.84	0.60
1:C:338:THR:O	1:C:342:LYS:HG2	2.00	0.60
2:D:182:ARG:NH1	2:D:256:GLN:OE1	2.29	0.60
1:A:430:GLN:HG3	1:A:433:LEU:HD12	1.84	0.60
1:C:430:GLN:HG3	1:C:433:LEU:HD12	1.84	0.60
2:B:124:GLU:HB2	2:B:147:LYS:HD3	1.84	0.60
2:D:124:GLU:HB2	2:D:147:LYS:HD3	1.84	0.60
2:B:189:LYS:H	2:B:282:ASN:HB2	1.68	0.59
1:C:691:LYS:HA	1:C:694:ILE:HD12	1.85	0.59
1:C:422:ASN:O	1:C:464:ARG:NH1	2.34	0.59
2:D:202:MET:HB2	2:D:235:TYR:CD2	2.38	0.59
1:C:800:ILE:HD13	6:C:1102:BUF:H33	1.85	0.58
2:D:65:LYS:HG3	2:D:184:LEU:HD22	1.83	0.58
2:D:276:CYS:HB2	2:D:295:PHE:HB3	1.83	0.58
1:C:942:MET:H	5:H:2:FRU:H5	1.68	0.58
1:A:338:THR:O	1:A:342:LYS:HG2	2.03	0.58
2:B:153:LEU:HB2	2:B:162:LEU:HD23	1.84	0.58
1:C:364:SER:OG	1:C:703:ALA:HB1	2.04	0.58
2:B:202:MET:HB2	2:B:235:TYR:CD2	2.38	0.58
1:C:845:MET:SD	1:C:849:GLN:NE2	2.76	0.58
1:C:260:MET:HE2	1:C:712:VAL:HG11	1.84	0.58
1:A:549:CYS:HA	1:A:579:VAL:HG23	1.86	0.58
1:C:284:PHE:HB2	1:C:838:VAL:HB	1.86	0.58
2:D:189:LYS:H	2:D:282:ASN:HB2	1.69	0.58
1:C:116:GLU:HG3	1:C:118:PRO:HD3	1.86	0.58
2:D:153:LEU:HB2	2:D:162:LEU:HD23	1.85	0.58
1:A:116:GLU:HG3	1:A:118:PRO:HD3	1.86	0.58
1:A:943:LYS:HG3	5:I:2:FRU:H61	1.85	0.58
1:C:118:PRO:HB3	1:C:122:ASN:HB2	1.86	0.58
1:A:691:LYS:HA	1:A:694:ILE:HD12	1.86	0.57
1:A:909:PHE:HD1	1:A:912:HIS:CD2	2.22	0.57
1:A:118:PRO:HB3	1:A:122:ASN:HB2	1.86	0.57
2:B:133:LEU:HG	2:B:240:LEU:HB3	1.86	0.57
1:A:766:LYS:HG3	1:A:837:LEU:HD12	1.85	0.57
1:A:89:LEU:HD21	1:A:134:ILE:HA	1.85	0.57
1:A:942:MET:H	5:I:2:FRU:H5	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.87	0.57
1:A:928:VAL:O	1:A:931:LYS:HB3	2.04	0.57
1:A:909:PHE:HD1	1:A:912:HIS:HD2	1.52	0.56
1:A:364:SER:OG	1:A:703:ALA:HB1	2.05	0.56
2:D:230:PHE:HE1	4:F:1:NAG:H81	1.70	0.56
2:D:108:PHE:HZ	2:D:179:LYS:HD3	1.70	0.56
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.88	0.56
1:A:861:THR:HG21	1:A:914:PRO:HB2	1.87	0.56
1:C:89:LEU:HD21	1:C:134:ILE:HA	1.86	0.56
1:C:861:THR:HG21	1:C:914:PRO:HB2	1.87	0.56
2:D:138:GLU:O	2:D:146:ARG:NH2	2.39	0.56
1:C:909:PHE:HD1	1:C:912:HIS:CD2	2.24	0.56
1:C:928:VAL:O	1:C:931:LYS:HB3	2.05	0.56
2:D:91:ARG:H	2:D:97:SER:HG	1.50	0.56
1:A:775:SER:HB3	1:A:923:GLN:NE2	2.20	0.55
2:B:29:GLY:HA2	2:B:32:TRP:CD1	2.40	0.55
1:C:909:PHE:HD1	1:C:912:HIS:HD2	1.53	0.55
1:A:831:ASN:N	1:A:835:ASP:OD2	2.28	0.55
1:A:329:LEU:HD13	1:A:772:THR:HG21	1.87	0.55
1:C:866:LEU:HD13	1:C:876:LEU:HD21	1.89	0.55
1:C:230:LEU:HA	1:C:237:PHE:HZ	1.71	0.55
1:A:360:LEU:O	1:A:755:VAL:HG23	2.07	0.55
1:C:238:PHE:O	1:C:239:SER:OG	2.25	0.55
2:B:17:TRP:CD1	2:B:18:ASN:H	2.24	0.55
1:C:1001:ILE:HG22	1:C:1010:VAL:HG21	1.89	0.55
2:B:119:ASP:O	2:B:123:PHE:HB2	2.07	0.55
2:B:182:ARG:NH1	2:B:256:GLN:OE1	2.34	0.54
1:C:831:ASN:N	1:C:835:ASP:OD2	2.29	0.54
1:A:183:LEU:HD11	1:A:248:ARG:HB3	1.89	0.54
1:C:329:LEU:HD13	1:C:772:THR:HG21	1.89	0.54
2:D:29:GLY:HA2	2:D:32:TRP:CD1	2.42	0.54
1:C:963:TYR:CE2	7:E:101:CLR:H6	2.43	0.54
2:D:216:LYS:HB2	2:D:221:LYS:HG2	1.87	0.54
1:C:183:LEU:HD11	1:C:248:ARG:HB3	1.89	0.54
1:C:909:PHE:HA	1:C:912:HIS:CD2	2.43	0.54
2:D:167:TYR:C	2:D:169:TYR:N	2.64	0.54
1:A:230:LEU:HA	1:A:237:PHE:HZ	1.72	0.54
1:A:909:PHE:HA	1:A:912:HIS:CD2	2.43	0.54
2:B:167:TYR:C	2:B:169:TYR:N	2.65	0.54
1:A:931:LYS:HE2	1:A:947:LEU:HD13	1.88	0.54
2:D:157:GLY:C	2:D:159:CYS:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:166:THR:N	2:D:167:TYR:HA	2.23	0.54
1:A:358:GLU:OE2	1:A:362:SER:OG	2.18	0.54
1:C:420:LEU:HB3	1:C:486:HIS:CE1	2.43	0.54
2:B:146:ARG:HB2	2:B:251:GLN:HG2	1.91	0.53
1:C:549:CYS:HA	1:C:579:VAL:HG23	1.91	0.53
1:C:775:SER:HB3	1:C:923:GLN:NE2	2.23	0.53
2:D:146:ARG:HB2	2:D:251:GLN:HG2	1.91	0.53
2:D:119:ASP:O	2:D:123:PHE:HB2	2.09	0.53
1:A:608:MET:HB3	1:A:682:VAL:HG22	1.88	0.53
1:C:719:LYS:HB2	1:C:738:ALA:HB1	1.91	0.53
2:B:80:ILE:HD11	2:B:177:ILE:H	1.73	0.53
1:C:931:LYS:HE2	1:C:947:LEU:HD13	1.89	0.53
1:A:634:VAL:HG13	1:A:648:VAL:HB	1.91	0.53
2:B:138:GLU:O	2:B:146:ARG:NH2	2.42	0.53
1:C:811:PRO:HB3	1:C:927:LEU:HD13	1.91	0.53
2:B:108:PHE:HZ	2:B:179:LYS:HD3	1.73	0.53
2:B:166:THR:N	2:B:167:TYR:HA	2.24	0.52
1:A:883:TRP:NE1	1:A:908:GLU:OE1	2.43	0.52
2:B:216:LYS:HB2	2:B:221:LYS:HG2	1.89	0.52
1:A:1001:ILE:HG22	1:A:1010:VAL:HG21	1.91	0.52
3:G:45:ILE:HD12	3:G:46:LEU:HG	1.91	0.52
1:A:108:TYR:CE2	1:A:123:LEU:HB2	2.45	0.52
1:A:430:GLN:HG2	1:A:438:ARG:HB2	1.91	0.52
1:C:963:TYR:HE2	7:E:101:CLR:H6	1.74	0.52
2:D:24:PHE:HB3	2:D:28:THR:HA	1.90	0.52
1:C:943:LYS:HG3	5:H:2:FRU:H61	1.91	0.52
2:D:103:VAL:HG12	2:D:107:ARG:HE	1.74	0.52
1:A:118:PRO:HB3	1:A:122:ASN:H	1.74	0.52
1:A:174:ASN:HB3	1:A:177:GLU:HG3	1.92	0.52
2:B:103:VAL:HG12	2:B:107:ARG:HE	1.74	0.52
1:C:766:LYS:HG3	1:C:837:LEU:HD12	1.90	0.52
1:C:887:TRP:CZ2	2:D:85:LYS:HB3	2.45	0.52
3:E:45:ILE:HD12	3:E:46:LEU:HG	1.92	0.52
1:A:880:ARG:HA	1:A:883:TRP:HB3	1.91	0.52
1:C:85:PHE:HE1	1:C:138:CYS:HA	1.75	0.52
1:C:118:PRO:HB3	1:C:122:ASN:H	1.75	0.52
1:C:880:ARG:HA	1:C:883:TRP:HB3	1.91	0.52
1:A:488:ASN:ND2	1:A:490:ASN:HB2	2.25	0.52
1:A:963:TYR:CE2	7:A:2002:CLR:H6	2.45	0.52
2:B:157:GLY:C	2:B:159:CYS:H	2.17	0.52
1:C:108:TYR:CE2	1:C:123:LEU:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:PHE:HB3	2:B:28:THR:HA	1.91	0.51
1:C:99:ILE:HA	1:C:102:ILE:HD12	1.91	0.51
1:A:485:ILE:HB	1:A:498:LEU:HD13	1.92	0.51
1:A:811:PRO:HB3	1:A:927:LEU:HD13	1.93	0.51
1:A:866:LEU:HD13	1:A:876:LEU:HD21	1.93	0.51
1:C:634:VAL:HG13	1:C:648:VAL:HB	1.93	0.51
1:A:85:PHE:HE1	1:A:138:CYS:HA	1.76	0.51
1:C:107:ALA:HB2	1:C:318:ILE:HG21	1.92	0.51
1:C:174:ASN:HB3	1:C:177:GLU:HG3	1.92	0.51
1:A:118:PRO:C	1:A:121:ASP:H	2.18	0.51
1:A:238:PHE:O	1:A:239:SER:OG	2.24	0.51
2:D:80:ILE:HD11	2:D:177:ILE:H	1.75	0.51
1:A:420:LEU:HB3	1:A:486:HIS:CE1	2.45	0.51
1:C:430:GLN:HG2	1:C:438:ARG:HB2	1.93	0.51
1:A:719:LYS:HB2	1:A:738:ALA:HB1	1.93	0.51
1:C:267:ALA:HB2	1:C:715:SER:HB3	1.91	0.51
1:C:485:ILE:HB	1:C:498:LEU:HD13	1.93	0.51
2:B:284:GLY:O	2:B:293:GLY:HA3	2.10	0.51
1:C:551:LEU:HG	1:C:552:PHE:O	2.11	0.51
2:D:32:TRP:CE3	2:D:36:LEU:HD11	2.46	0.51
1:A:551:LEU:HG	1:A:552:PHE:O	2.11	0.51
1:A:594:ASP:O	1:A:598:LYS:HG2	2.10	0.51
1:C:118:PRO:C	1:C:121:ASP:H	2.18	0.51
2:D:284:GLY:O	2:D:293:GLY:HA3	2.10	0.51
2:B:224:VAL:HG11	2:B:267:THR:HG23	1.93	0.50
1:C:949:PHE:HB2	3:E:45:ILE:HG23	1.94	0.50
1:A:99:ILE:HA	1:A:102:ILE:HD12	1.93	0.50
1:C:206:VAL:HG23	1:C:242:CYS:HA	1.93	0.50
1:A:430:GLN:HG2	1:A:439:ALA:H	1.76	0.50
1:C:358:GLU:OE2	1:C:362:SER:OG	2.21	0.50
1:C:594:ASP:O	1:C:598:LYS:HG2	2.11	0.50
1:C:885:ASP:OD1	1:C:888:ILE:HG13	2.11	0.50
1:A:206:VAL:HG23	1:A:242:CYS:HA	1.93	0.50
1:C:352:LYS:NZ	1:C:739:ALA:O	2.43	0.50
1:C:960:PHE:O	1:C:964:CYS:HB2	2.11	0.50
2:B:32:TRP:CE3	2:B:36:LEU:HD11	2.47	0.50
1:C:243:VAL:HG12	1:C:442:GLY:O	2.11	0.50
1:C:389:GLN:HB3	1:C:391:HIS:NE2	2.27	0.50
2:D:224:VAL:HG11	2:D:267:THR:HG23	1.93	0.50
1:A:107:ALA:HB2	1:A:318:ILE:HG21	1.93	0.50
1:A:779:GLU:HB3	1:A:800:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:LEU:O	1:C:755:VAL:HG23	2.12	0.49
1:C:999:LYS:O	1:C:1003:ARG:NE	2.45	0.49
1:A:284:PHE:CD1	1:A:838:VAL:HG21	2.47	0.49
1:A:417:ILE:HD13	1:A:579:VAL:HG21	1.95	0.49
1:C:416:ARG:HH12	1:C:497:LEU:HD21	1.76	0.49
1:C:608:MET:HB3	1:C:682:VAL:HG22	1.92	0.49
1:C:658:VAL:HB	1:C:683:PHE:HD1	1.77	0.49
1:C:488:ASN:ND2	1:C:490:ASN:HB2	2.28	0.49
2:D:177:ILE:HA	2:D:260:ALA:HA	1.94	0.49
1:A:389:GLN:HB3	1:A:391:HIS:NE2	2.28	0.49
1:A:935:ASN:HA	1:A:1003:ARG:HD3	1.94	0.49
1:A:949:PHE:HB2	3:G:45:ILE:HG23	1.95	0.49
1:C:76:PRO:HB2	1:C:78:THR:OG1	2.11	0.49
1:A:632:GLU:HB3	1:A:636:ASP:HB2	1.93	0.49
2:D:242:TYR:CD2	2:D:257:PRO:HG3	2.46	0.49
1:A:885:ASP:OD1	1:A:888:ILE:HG13	2.12	0.49
1:A:935:ASN:ND2	1:A:940:GLN:OE1	2.46	0.49
1:C:430:GLN:HG2	1:C:439:ALA:H	1.78	0.49
1:C:632:GLU:HB3	1:C:636:ASP:HB2	1.94	0.49
1:C:284:PHE:CD1	1:C:838:VAL:HG21	2.48	0.49
1:C:370:LYS:HA	1:C:374:LEU:HD12	1.95	0.49
1:A:370:LYS:HA	1:A:374:LEU:HD12	1.95	0.48
1:A:963:TYR:HE2	7:A:2002:CLR:H6	1.78	0.48
1:A:416:ARG:HH12	1:A:497:LEU:HD21	1.77	0.48
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.96	0.48
2:B:225:GLY:HA2	2:B:265:ASN:O	2.14	0.48
2:B:242:TYR:CD2	2:B:257:PRO:HG3	2.47	0.48
1:C:935:ASN:OD1	1:C:935:ASN:N	2.46	0.48
1:C:964:CYS:HB3	1:C:967:MET:CG	2.43	0.48
1:A:76:PRO:HB2	1:A:78:THR:OG1	2.12	0.48
1:A:512:SER:HB3	1:A:575:ASN:HA	1.94	0.48
1:A:935:ASN:OD1	1:A:935:ASN:N	2.47	0.48
1:C:110:ILE:HB	1:C:315:ILE:HD11	1.95	0.48
1:C:306:LEU:HD12	1:C:308:TYR:HE2	1.79	0.48
2:B:119:ASP:OD2	2:B:121:MET:HB2	2.14	0.48
2:B:230:PHE:HE1	10:B:1001:NAG:H81	1.78	0.48
1:C:287:ILE:O	1:C:291:VAL:HG22	2.14	0.48
1:A:360:LEU:H	1:A:360:LEU:HD22	1.78	0.48
1:A:658:VAL:HB	1:A:683:PHE:HD1	1.78	0.48
1:A:964:CYS:HB3	1:A:967:MET:CG	2.44	0.48
1:C:329:LEU:HD11	1:C:769:ILE:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:935:ASN:ND2	1:C:940:GLN:OE1	2.47	0.48
1:C:417:ILE:HD13	1:C:579:VAL:HG21	1.96	0.48
1:C:886:ARG:HA	1:C:901:TYR:CD1	2.49	0.48
2:D:92:PRO:HD2	2:D:303:SER:HB2	1.96	0.48
1:A:260:MET:HE2	1:A:712:VAL:HG11	1.95	0.48
1:A:287:ILE:O	1:A:291:VAL:HG22	2.14	0.48
1:A:906:ILE:O	1:A:910:THR:HG23	2.13	0.48
1:C:732:SER:OG	1:C:735:SER:OG	2.30	0.48
1:C:941:GLY:HA2	5:H:2:FRU:H12	1.95	0.48
1:C:883:TRP:NE1	1:C:908:GLU:OE1	2.44	0.48
2:D:119:ASP:OD2	2:D:121:MET:HB2	2.14	0.48
2:B:177:ILE:HA	2:B:260:ALA:HA	1.96	0.47
1:C:512:SER:HB3	1:C:575:ASN:HA	1.94	0.47
1:C:784:LEU:O	1:C:788:ILE:HG12	2.14	0.47
2:D:225:GLY:HA2	2:D:265:ASN:O	2.14	0.47
1:A:332:THR:HA	1:A:813:ILE:HD11	1.96	0.47
1:A:94:SER:HB3	1:A:133:VAL:HG13	1.95	0.47
1:A:732:SER:OG	1:A:735:SER:OG	2.31	0.47
1:C:559:PRO:HG2	1:C:562:PHE:HB2	1.96	0.47
1:A:423:ARG:NH1	1:A:474:PRO:HB3	2.29	0.47
1:A:559:PRO:HG2	1:A:562:PHE:HB2	1.96	0.47
1:C:76:PRO:HA	1:C:77:PRO:HD3	1.80	0.47
2:D:289:ASP:HB3	2:D:292:GLN:HB3	1.97	0.47
1:A:755:VAL:HG13	1:A:825:MET:HE1	1.97	0.47
2:D:120:ASP:OD1	2:D:150:ARG:NH2	2.47	0.47
1:A:106:LEU:O	1:A:110:ILE:HG12	2.15	0.47
1:A:124:TYR:O	1:A:128:VAL:HG23	2.15	0.47
1:A:336:CYS:SG	1:A:816:ALA:HB2	2.54	0.47
1:A:824:ILE:HG22	1:A:827:ARG:HH12	1.79	0.47
1:A:866:LEU:HD23	1:A:866:LEU:HA	1.69	0.47
1:A:886:ARG:HA	1:A:901:TYR:CD1	2.49	0.47
1:A:960:PHE:O	1:A:964:CYS:HB2	2.14	0.47
2:B:187:LYS:O	2:B:282:ASN:ND2	2.48	0.47
1:C:332:THR:HA	1:C:813:ILE:HD11	1.97	0.47
1:C:779:GLU:HB3	1:C:800:ILE:HD11	1.97	0.47
1:C:1009:TRP:CH2	1:C:1013:GLU:HG3	2.50	0.47
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.97	0.47
2:D:239:PRO:HB2	2:D:241:GLN:HG2	1.97	0.47
2:B:87:GLU:HA	2:B:298:LYS:O	2.15	0.47
1:C:106:LEU:O	1:C:110:ILE:HG12	2.15	0.47
2:B:74:PRO:O	2:B:292:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ASP:OD1	2:B:150:ARG:NH2	2.48	0.47
2:B:154:GLU:HG3	2:B:162:LEU:HG	1.97	0.47
2:D:88:ILE:HG23	2:D:101:TYR:CE1	2.50	0.47
1:A:181:GLY:N	1:A:251:VAL:O	2.42	0.47
1:A:871:PHE:CE1	1:A:893:ASP:HB3	2.51	0.47
1:A:352:LYS:NZ	1:A:739:ALA:O	2.47	0.46
1:A:466:ARG:HG2	1:A:489:PRO:HB3	1.97	0.46
1:C:423:ARG:NH1	1:C:474:PRO:HB3	2.29	0.46
1:A:306:LEU:HD12	1:A:308:TYR:HE2	1.80	0.46
1:A:865:ILE:HD12	1:A:914:PRO:HG3	1.96	0.46
1:C:508:LEU:HD21	1:C:528:LYS:HE2	1.97	0.46
1:C:551:LEU:HD13	1:C:576:LEU:HA	1.96	0.46
2:B:88:ILE:HG23	2:B:101:TYR:CE1	2.50	0.46
1:C:466:ARG:HG2	1:C:489:PRO:HB3	1.98	0.46
1:C:935:ASN:HA	1:C:1003:ARG:HD3	1.97	0.46
1:A:332:THR:HG22	1:A:813:ILE:HG12	1.96	0.46
1:A:871:PHE:CZ	1:A:893:ASP:HB3	2.50	0.46
2:B:92:PRO:HD2	2:B:303:SER:HB2	1.98	0.46
2:B:160:SER:O	2:B:162:LEU:N	2.49	0.46
1:C:643:ILE:HD11	1:C:648:VAL:HG22	1.97	0.46
2:D:160:SER:O	2:D:162:LEU:N	2.49	0.46
1:A:76:PRO:HA	1:A:77:PRO:HD3	1.80	0.46
1:A:622:LYS:HA	1:A:627:ILE:O	2.16	0.46
1:A:885:ASP:O	1:A:904:ARG:NH2	2.47	0.46
1:C:94:SER:HB3	1:C:133:VAL:HG13	1.96	0.46
1:A:267:ALA:HB2	1:A:715:SER:HB3	1.97	0.46
1:A:643:ILE:HD11	1:A:648:VAL:HG22	1.97	0.46
2:B:153:LEU:H	2:B:153:LEU:HD12	1.81	0.46
1:C:622:LYS:HA	1:C:627:ILE:O	2.16	0.46
2:D:154:GLU:HG3	2:D:162:LEU:HG	1.98	0.46
1:A:592:VAL:O	1:A:596:VAL:HG23	2.16	0.46
1:C:360:LEU:H	1:C:360:LEU:HD22	1.80	0.46
1:C:755:VAL:HG13	1:C:825:MET:HE1	1.97	0.46
1:C:871:PHE:CE1	1:C:893:ASP:HB3	2.51	0.46
1:A:508:LEU:HD21	1:A:528:LYS:HE2	1.98	0.46
1:A:74:THR:HG23	1:A:256:ASP:OD1	2.16	0.46
1:A:230:LEU:HA	1:A:237:PHE:CZ	2.51	0.46
1:A:713:ASN:OD1	1:A:713:ASN:N	2.49	0.46
2:B:148:VAL:HG11	2:B:254:TYR:HA	1.98	0.46
2:D:87:GLU:HA	2:D:298:LYS:O	2.16	0.46
1:A:309:THR:HG22	1:A:312:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LEU:HD13	1:A:576:LEU:HA	1.97	0.45
1:A:803:ILE:HD13	1:A:803:ILE:HA	1.81	0.45
1:A:628:SER:OG	1:A:631:ASN:OD1	2.34	0.45
1:C:34:MET:HE3	1:C:34:MET:HB3	1.82	0.45
1:C:824:ILE:HG22	1:C:827:ARG:HH12	1.81	0.45
1:C:891:VAL:HG21	1:C:904:ARG:NH1	2.31	0.45
2:D:57:MET:O	2:D:60:THR:OG1	2.31	0.45
2:D:167:TYR:C	2:D:169:TYR:H	2.22	0.45
1:A:110:ILE:HB	1:A:315:ILE:HD11	1.98	0.45
2:D:187:LYS:O	2:D:282:ASN:ND2	2.50	0.45
1:A:469:LYS:HA	1:A:486:HIS:CD2	2.52	0.45
1:C:90:PHE:O	1:C:94:SER:HB2	2.17	0.45
1:C:488:ASN:ND2	1:C:493:GLU:O	2.49	0.45
1:A:329:LEU:HD11	1:A:769:ILE:HG12	1.97	0.45
7:A:2002:CLR:H262	7:A:2002:CLR:H231	1.82	0.45
1:C:336:CYS:SG	1:C:816:ALA:HB2	2.56	0.45
1:C:372:GLY:CA	1:C:377:ASN:HB2	2.47	0.45
2:D:148:VAL:HG11	2:D:254:TYR:HA	1.98	0.45
2:D:153:LEU:H	2:D:153:LEU:HD12	1.82	0.45
1:A:192:ILE:HA	1:A:193:PRO:HD3	1.67	0.45
1:A:243:VAL:HG12	1:A:442:GLY:O	2.16	0.45
2:B:239:PRO:HB2	2:B:241:GLN:HG2	1.99	0.45
1:C:885:ASP:O	1:C:904:ARG:NH2	2.48	0.45
1:A:1009:TRP:CH2	1:A:1013:GLU:HG3	2.52	0.45
1:C:208:ASN:HB3	1:C:212:THR:OG1	2.17	0.45
1:C:628:SER:OG	1:C:631:ASN:OD1	2.34	0.45
1:A:295:LEU:HD12	1:A:324:ASN:ND2	2.31	0.45
2:D:83:SER:HB3	2:D:87:GLU:H	1.83	0.45
7:E:101:CLR:H262	7:E:101:CLR:H231	1.81	0.45
1:A:118:PRO:HA	1:A:121:ASP:CB	2.43	0.44
2:B:80:ILE:CD1	2:B:177:ILE:H	2.29	0.44
2:B:167:TYR:C	2:B:169:TYR:H	2.22	0.44
2:B:259:MET:HE3	2:B:259:MET:HB2	1.68	0.44
1:C:181:GLY:N	1:C:251:VAL:O	2.43	0.44
1:C:624:VAL:HG23	1:C:626:ILE:HG13	1.98	0.44
2:B:199:TYR:O	2:B:201:VAL:N	2.50	0.44
1:C:469:LYS:HA	1:C:486:HIS:CD2	2.53	0.44
1:C:965:PRO:HD3	3:E:31:LEU:HD11	1.99	0.44
2:D:199:TYR:O	2:D:201:VAL:N	2.50	0.44
1:A:624:VAL:HG23	1:A:626:ILE:HG13	1.99	0.44
1:C:121:ASP:OD1	6:C:1102:BUF:H11	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:PRO:HD3	3:G:31:LEU:HD11	1.99	0.44
2:D:74:PRO:O	2:D:292:GLN:HG3	2.17	0.44
1:A:584:MET:HE2	1:A:584:MET:HB3	1.91	0.44
1:A:865:ILE:CD1	1:A:914:PRO:HG3	2.48	0.44
1:A:618:LYS:NZ	1:A:636:ASP:OD1	2.46	0.44
1:C:74:THR:HG23	1:C:256:ASP:OD1	2.18	0.44
1:C:309:THR:HG22	1:C:312:GLU:OE1	2.18	0.44
1:C:906:ILE:O	1:C:910:THR:HG23	2.17	0.44
2:D:166:THR:HB	2:D:169:TYR:N	2.27	0.44
2:D:277:LYS:HB3	2:D:279:TYR:CE1	2.53	0.44
1:A:409:ALA:HA	1:A:412:LEU:HD12	1.99	0.44
1:A:909:PHE:CD1	1:A:912:HIS:HD2	2.34	0.44
1:C:118:PRO:HA	1:C:121:ASP:CB	2.44	0.44
1:C:124:TYR:O	1:C:128:VAL:HG23	2.18	0.44
1:C:192:ILE:HA	1:C:193:PRO:HD3	1.67	0.44
1:C:332:THR:HG22	1:C:813:ILE:HG12	1.99	0.44
2:D:259:MET:HE3	2:D:259:MET:HB2	1.70	0.44
1:A:325:VAL:HA	1:A:326:PRO:HD3	1.66	0.43
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.87	0.43
2:B:289:ASP:HB3	2:B:292:GLN:HB3	2.00	0.43
1:C:234:ASN:OD1	1:C:234:ASN:N	2.50	0.43
1:C:779:GLU:HG2	1:C:800:ILE:HG12	2.01	0.43
1:A:52:LEU:O	1:A:183:LEU:HD22	2.18	0.43
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.82	0.43
1:C:230:LEU:HA	1:C:237:PHE:CZ	2.51	0.43
1:C:1009:TRP:CZ2	1:C:1013:GLU:HG3	2.53	0.43
2:D:57:MET:HE3	2:D:57:MET:HB3	1.91	0.43
1:C:803:ILE:HD13	1:C:803:ILE:HA	1.82	0.43
1:A:662:ASP:O	1:A:666:MET:HG3	2.18	0.43
1:A:999:LYS:O	1:A:1003:ARG:NE	2.50	0.43
2:B:26:GLY:HA2	2:B:27:ARG:HA	1.71	0.43
2:B:167:TYR:O	2:B:167:TYR:CG	2.72	0.43
1:C:270:LEU:HD11	1:C:692:LEU:HD22	2.00	0.43
1:A:90:PHE:O	1:A:94:SER:HB2	2.19	0.43
1:A:340:THR:O	1:A:344:MET:HG2	2.19	0.43
1:A:469:LYS:HA	1:A:486:HIS:HD2	1.84	0.43
1:A:710:ASP:CG	1:A:711:GLY:H	2.26	0.43
1:A:825:MET:HA	1:A:825:MET:HE2	2.00	0.43
1:A:1009:TRP:CZ2	1:A:1013:GLU:HG3	2.53	0.43
1:A:656:CYS:SG	1:A:678:HIS:ND1	2.87	0.43
2:B:166:THR:HB	2:B:169:TYR:N	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:O	1:C:183:LEU:HD22	2.18	0.43
1:C:423:ARG:NH2	1:C:474:PRO:HG3	2.34	0.43
1:A:784:LEU:O	1:A:788:ILE:HG12	2.18	0.43
2:B:277:LYS:HB3	2:B:279:TYR:CE1	2.53	0.43
1:C:372:GLY:HA2	1:C:377:ASN:HB2	1.99	0.43
1:C:409:ALA:HA	1:C:412:LEU:HD12	2.00	0.43
1:C:865:ILE:CD1	1:C:914:PRO:HG3	2.49	0.43
2:D:167:TYR:O	2:D:167:TYR:CG	2.72	0.43
2:D:277:LYS:HE2	2:D:285:TYR:CE2	2.54	0.43
1:A:796:GLY:N	1:A:912:HIS:ND1	2.67	0.43
2:B:125:ASP:OD1	2:B:152:ARG:NH1	2.49	0.43
2:B:162:LEU:HB3	2:B:163:ASN:H	1.64	0.43
1:C:369:PHD:OP2	1:C:371:THR:OG1	2.31	0.43
1:A:985:PHE:N	1:A:986:PRO:HD2	2.34	0.43
2:B:69:GLN:O	2:B:72:VAL:HG22	2.19	0.43
1:C:205:LYS:HG3	1:C:475:PHE:CZ	2.54	0.43
1:C:871:PHE:CZ	1:C:893:ASP:HB3	2.54	0.43
1:C:125:LEU:HD22	6:C:1102:BUF:H3	1.99	0.42
1:C:584:MET:HE2	1:C:584:MET:HB3	1.92	0.42
1:C:953:GLU:OE1	1:C:954:GLU:N	2.52	0.42
2:D:244:PRO:HG2	2:D:246:TYR:CE1	2.54	0.42
1:A:488:ASN:ND2	1:A:493:GLU:O	2.52	0.42
2:B:277:LYS:HE2	2:B:285:TYR:CE2	2.54	0.42
1:C:564:PHE:HB2	1:C:571:PHE:CZ	2.54	0.42
1:C:618:LYS:NZ	1:C:636:ASP:OD1	2.47	0.42
1:C:821:GLU:OE1	1:C:933:ARG:HB2	2.19	0.42
1:C:865:ILE:HD12	1:C:914:PRO:HG3	1.99	0.42
1:A:208:ASN:HB3	1:A:212:THR:OG1	2.19	0.42
1:A:798:VAL:HG11	1:A:971:LEU:HD22	2.02	0.42
1:A:975:PRO:HG3	3:G:27:ARG:NH2	2.34	0.42
1:C:121:ASP:CG	6:C:1102:BUF:H11	2.44	0.42
1:C:661:SER:OG	1:C:685:ARG:NH1	2.53	0.42
2:D:80:ILE:CD1	2:D:177:ILE:H	2.31	0.42
1:A:121:ASP:OD1	1:A:797:THR:OG1	2.26	0.42
1:C:469:LYS:HA	1:C:486:HIS:HD2	1.85	0.42
2:D:26:GLY:HA2	2:D:27:ARG:HA	1.72	0.42
1:A:430:GLN:NE2	1:A:439:ALA:HB3	2.34	0.42
1:A:512:SER:OG	1:A:513:SER:N	2.52	0.42
1:A:779:GLU:HG2	1:A:800:ILE:HG12	2.02	0.42
1:C:536:LEU:HD23	1:C:536:LEU:HA	1.88	0.42
1:C:856:LEU:HD11	2:D:46:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:GLN:O	2:D:72:VAL:HG22	2.19	0.42
2:D:83:SER:OG	2:D:87:GLU:O	2.22	0.42
1:A:34:MET:HE3	1:A:34:MET:HB3	1.82	0.42
1:A:103:LEU:HB3	1:A:318:ILE:HG23	2.01	0.42
1:A:982:PHE:HE1	7:A:2002:CLR:H183	1.84	0.42
1:C:430:GLN:HB3	1:C:438:ARG:HB2	2.02	0.42
1:C:814:SER:HB2	1:C:946:ILE:C	2.45	0.42
1:A:898:GLN:NE2	2:B:181:ASN:OD1	2.52	0.42
1:C:810:VAL:HB	1:C:811:PRO:HD3	2.01	0.42
1:A:412:LEU:O	1:A:416:ARG:HG3	2.20	0.42
1:A:752:VAL:O	1:A:755:VAL:HG12	2.19	0.42
1:A:783:PHE:CZ	1:A:787:ILE:HD11	2.55	0.42
1:A:891:VAL:HG21	1:A:904:ARG:NH1	2.34	0.42
2:B:83:SER:OG	2:B:87:GLU:O	2.23	0.42
1:C:181:GLY:HA2	1:C:250:ILE:HG23	2.01	0.42
1:C:392:GLU:HG2	1:C:393:ALA:O	2.19	0.42
2:B:83:SER:HB3	2:B:87:GLU:H	1.85	0.42
1:C:605:LYS:HE2	1:C:607:ILE:HD11	2.01	0.42
1:C:935:ASN:HB3	1:C:939:GLN:OE1	2.20	0.42
1:C:982:PHE:HE1	7:E:101:CLR:H183	1.85	0.42
1:A:205:LYS:HG3	1:A:475:PHE:CZ	2.54	0.42
1:A:417:ILE:CD1	1:A:579:VAL:HG21	2.50	0.42
1:A:423:ARG:NH2	1:A:474:PRO:HG3	2.35	0.42
1:A:430:GLN:HB3	1:A:438:ARG:HB2	2.02	0.42
1:A:915:PHE:O	1:A:918:THR:HB	2.20	0.42
1:A:1008:GLY:O	1:A:1012:LYS:HG2	2.20	0.42
2:B:217:ARG:NH1	2:B:218:ASP:OD2	2.53	0.42
2:D:112:TYR:CE1	2:D:255:LEU:HB3	2.55	0.42
1:A:626:ILE:O	1:A:680:GLU:HB3	2.20	0.41
1:A:803:ILE:HG12	1:A:916:PHE:HD1	1.85	0.41
1:C:412:LEU:O	1:C:416:ARG:HG3	2.20	0.41
1:C:752:VAL:O	1:C:755:VAL:HG12	2.19	0.41
1:C:998:ARG:O	1:C:1002:ILE:HG13	2.20	0.41
1:A:564:PHE:HB2	1:A:571:PHE:CZ	2.55	0.41
1:A:810:VAL:HB	1:A:811:PRO:HD3	2.02	0.41
1:A:840:GLU:H	1:A:840:GLU:CD	2.28	0.41
1:A:936:SER:HB2	1:A:1003:ARG:NH2	2.34	0.41
1:A:944:ASN:O	1:A:948:ILE:HG12	2.20	0.41
1:A:953:GLU:OE1	1:A:954:GLU:N	2.53	0.41
1:C:887:TRP:CD1	2:D:84:GLN:O	2.72	0.41
1:C:936:SER:HB2	1:C:1003:ARG:NH2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:GLY:HA2	1:A:987:TYR:CD2	2.56	0.41
1:C:73:LEU:HD23	1:C:73:LEU:HA	1.83	0.41
1:C:662:ASP:O	1:C:666:MET:HG3	2.20	0.41
1:C:825:MET:HE2	1:C:825:MET:HA	2.02	0.41
1:C:857:GLY:HA2	1:C:987:TYR:CD2	2.55	0.41
1:C:909:PHE:CD1	1:C:912:HIS:HD2	2.37	0.41
1:A:392:GLU:HG2	1:A:393:ALA:O	2.20	0.41
1:C:430:GLN:NE2	1:C:439:ALA:HB3	2.35	0.41
1:C:840:GLU:H	1:C:840:GLU:CD	2.29	0.41
1:A:496:HIS:HB2	1:A:553:LEU:HB2	2.03	0.41
2:B:80:ILE:CG1	2:B:177:ILE:H	2.33	0.41
1:C:496:HIS:HB2	1:C:553:LEU:HB2	2.02	0.41
1:C:592:VAL:O	1:C:596:VAL:HG23	2.21	0.41
1:C:783:PHE:CZ	1:C:787:ILE:HD11	2.56	0.41
1:C:801:LEU:HD23	1:C:801:LEU:HA	1.85	0.41
1:C:858:GLY:HA3	1:C:915:PHE:CZ	2.54	0.41
1:A:194:ALA:HB1	1:A:253:TYR:O	2.20	0.41
1:A:918:THR:O	1:A:922:VAL:HG22	2.21	0.41
1:A:972:ARG:NH2	1:A:974:TYR:OH	2.51	0.41
2:B:51:ILE:O	2:B:55:GLN:HG2	2.20	0.41
2:B:169:TYR:O	2:B:170:LYS:HB3	2.20	0.41
2:B:178:ILE:HG22	2:B:238:PHE:HZ	1.86	0.41
1:C:508:LEU:HD11	1:C:528:LYS:HE2	2.03	0.41
1:C:781:THR:HA	1:C:784:LEU:HD12	2.01	0.41
1:C:863:PHE:CD1	1:C:873:PRO:HB3	2.56	0.41
1:C:975:PRO:HG3	3:E:27:ARG:NH2	2.35	0.41
2:D:21:LYS:HG2	2:D:22:LYS:N	2.36	0.41
1:A:496:HIS:HE1	1:A:560:GLU:HA	1.85	0.41
1:A:508:LEU:HD11	1:A:528:LYS:HE2	2.02	0.41
1:A:936:SER:HB3	1:A:939:GLN:HG3	2.02	0.41
1:C:288:ILE:HD13	1:C:288:ILE:HA	1.85	0.41
1:C:340:THR:O	1:C:344:MET:HG2	2.21	0.41
1:C:496:HIS:HE1	1:C:560:GLU:HA	1.85	0.41
1:A:710:ASP:CG	1:A:711:GLY:N	2.79	0.41
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.82	0.41
2:B:179:LYS:HD2	2:B:256:GLN:NE2	2.36	0.41
2:B:238:PHE:HA	2:B:239:PRO:HD3	1.90	0.41
1:C:295:LEU:HD12	1:C:324:ASN:ND2	2.35	0.41
1:C:417:ILE:CD1	1:C:579:VAL:HG21	2.51	0.41
1:C:944:ASN:O	1:C:948:ILE:HG12	2.21	0.41
1:A:121:ASP:CG	6:A:2001:BUF:H11	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:PRO:O	1:A:232:THR:HG22	2.20	0.41
1:A:270:LEU:HB2	1:A:719:LYS:HG2	2.03	0.41
1:A:661:SER:OG	1:A:685:ARG:NH1	2.54	0.41
1:A:858:GLY:HA3	1:A:915:PHE:CZ	2.54	0.41
2:B:21:LYS:HG2	2:B:22:LYS:N	2.36	0.41
2:B:112:TYR:CE1	2:B:255:LEU:HB3	2.56	0.41
1:C:229:PRO:O	1:C:232:THR:HG22	2.21	0.41
1:C:488:ASN:HB2	1:C:495:ARG:O	2.20	0.41
1:C:555:ASP:OD1	1:C:555:ASP:N	2.52	0.41
1:C:626:ILE:O	1:C:680:GLU:HB3	2.21	0.41
2:D:140:ASN:O	2:D:146:ARG:NH2	2.53	0.41
2:D:179:LYS:HD2	2:D:256:GLN:NE2	2.36	0.41
1:A:814:SER:HB2	1:A:946:ILE:C	2.46	0.41
1:A:998:ARG:O	1:A:1002:ILE:HG13	2.21	0.41
1:C:103:LEU:HB3	1:C:318:ILE:HG23	2.03	0.41
1:C:549:CYS:HB3	1:C:578:PHE:HA	2.02	0.41
1:C:901:TYR:CZ	1:C:905:LYS:HE3	2.56	0.41
1:C:915:PHE:O	1:C:918:THR:HB	2.21	0.41
1:A:205:LYS:HG3	1:A:475:PHE:HZ	1.86	0.40
1:A:488:ASN:HA	1:A:489:PRO:HD2	1.94	0.40
1:C:194:ALA:HB1	1:C:253:TYR:O	2.20	0.40
1:C:512:SER:OG	1:C:513:SER:N	2.54	0.40
1:C:748:PHE:O	1:C:751:ILE:HB	2.21	0.40
2:D:169:TYR:O	2:D:170:LYS:HB3	2.21	0.40
1:A:821:GLU:OE1	1:A:933:ARG:HB2	2.21	0.40
1:A:901:TYR:CZ	1:A:905:LYS:HE3	2.57	0.40
1:C:710:ASP:CG	1:C:711:GLY:H	2.29	0.40
1:C:866:LEU:HB3	1:C:876:LEU:HD11	2.02	0.40
1:A:181:GLY:HA2	1:A:250:ILE:HG23	2.03	0.40
1:C:467:TYR:HB3	1:C:486:HIS:CB	2.52	0.40
1:C:821:GLU:OE2	1:C:933:ARG:N	2.55	0.40
1:C:1008:GLY:O	1:C:1012:LYS:HG2	2.21	0.40
2:D:21:LYS:HG2	2:D:22:LYS:H	1.85	0.40
2:D:178:ILE:HG22	2:D:238:PHE:HZ	1.87	0.40
2:D:217:ARG:NH1	2:D:218:ASP:OD2	2.54	0.40
1:A:295:LEU:O	1:A:299:PHE:HB2	2.21	0.40
1:A:488:ASN:HB2	1:A:495:ARG:O	2.21	0.40
1:A:743:LEU:HD11	1:A:751:ILE:HD13	2.03	0.40
1:C:713:ASN:OD1	1:C:713:ASN:N	2.51	0.40
1:C:803:ILE:HG12	1:C:916:PHE:HD1	1.86	0.40
1:C:858:GLY:HA2	1:C:918:THR:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:CYS:HB3	1:A:578:PHE:HA	2.02	0.40
2:B:165:GLU:HB3	2:B:166:THR:CA	2.39	0.40
1:C:48:TYR:OH	1:C:252:VAL:HG13	2.21	0.40
1:C:799:THR:O	1:C:802:CYS:HB2	2.21	0.40
2:D:125:ASP:OD1	2:D:152:ARG:NH1	2.51	0.40
3:E:17:ASP:N	3:E:17:ASP:OD1	2.55	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	993/1021 (97%)	939 (95%)	53 (5%)	1 (0%)	48	78
1	C	993/1021 (97%)	937 (94%)	55 (6%)	1 (0%)	48	78
2	B	286/303 (94%)	265 (93%)	18 (6%)	3 (1%)	12	40
2	D	283/303 (93%)	263 (93%)	17 (6%)	3 (1%)	11	38
3	E	30/65 (46%)	30 (100%)	0	0	100	100
3	G	30/65 (46%)	30 (100%)	0	0	100	100
All	All	2615/2778 (94%)	2464 (94%)	143 (6%)	8 (0%)	36	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	170	LYS
2	B	217	ARG
2	D	170	LYS
2	D	217	ARG
1	A	78	THR
1	C	78	THR

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Mol	Chain	Res	Type
2	B	161	GLY
2	D	161	GLY

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	846/864 (98%)	817 (97%)	29 (3%)	32	57
1	C	846/864 (98%)	815 (96%)	31 (4%)	30	55
2	B	258/269 (96%)	240 (93%)	18 (7%)	14	40
2	D	255/269 (95%)	238 (93%)	17 (7%)	15	41
3	E	26/52 (50%)	24 (92%)	2 (8%)	12	37
3	G	26/52 (50%)	24 (92%)	2 (8%)	12	37
All	All	2257/2370 (95%)	2158 (96%)	99 (4%)	25	51

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	121	ASP
1	A	136	THR
1	A	243	VAL
1	A	285	ILE
1	A	307	GLU
1	A	314	VAL
1	A	332	THR
1	A	333	VAL
1	A	351	VAL
1	A	360	LEU
1	A	388	ASN
1	A	479	ASN
1	A	531	PHE
1	A	564	PHE
1	A	569	VAL

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Mol	Chain	Res	Type
1	A	635	GLU
1	A	712	VAL
1	A	735	SER
1	A	746	ASP
1	A	751	ILE
1	A	800	ILE
1	A	865	ILE
1	A	876	LEU
1	A	917	VAL
1	A	935	ASN
1	A	942	MET
1	A	947	LEU
1	A	995	ASP
2	B	32	TRP
2	B	36	LEU
2	B	40	VAL
2	B	54	ILE
2	B	77	LEU
2	B	80	ILE
2	B	105	ILE
2	B	111	LYS
2	B	117	GLN
2	B	159	CYS
2	B	169	TYR
2	B	204	TYR
2	B	232	LEU
2	B	256	GLN
2	B	267	THR
2	B	272	ILE
2	B	274	ILE
2	B	299	ILE
3	G	32	ILE
3	G	45	ILE
1	C	35	ASP
1	C	121	ASP
1	C	136	THR
1	C	243	VAL
1	C	285	ILE
1	C	288	ILE
1	C	307	GLU
1	C	314	VAL
1	C	332	THR

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Mol	Chain	Res	Type
1	C	333	VAL
1	C	351	VAL
1	C	360	LEU
1	C	388	ASN
1	C	479	ASN
1	C	531	PHE
1	C	564	PHE
1	C	569	VAL
1	C	635	GLU
1	C	712	VAL
1	C	735	SER
1	C	751	ILE
1	C	800	ILE
1	C	865	ILE
1	C	876	LEU
1	C	911	CYS
1	C	917	VAL
1	C	935	ASN
1	C	942	MET
1	C	947	LEU
1	C	971	LEU
1	C	995	ASP
2	D	32	TRP
2	D	36	LEU
2	D	40	VAL
2	D	54	ILE
2	D	77	LEU
2	D	80	ILE
2	D	105	ILE
2	D	117	GLN
2	D	159	CYS
2	D	169	TYR
2	D	204	TYR
2	D	232	LEU
2	D	256	GLN
2	D	267	THR
2	D	272	ILE
2	D	274	ILE
2	D	299	ILE
3	E	32	ILE
3	E	45	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	399	GLN
1	A	488	ASN
1	A	841	GLN
1	A	889	ASN
1	A	898	GLN
2	B	79	GLN
2	B	262	GLN
1	C	161	GLN
1	C	377	ASN
1	C	399	GLN
1	C	488	ASN
1	C	889	ASN
1	C	898	GLN
2	D	79	GLN
2	D	262	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PHD	C	369	1,9	9,11,12	1.42	1 (11%)	9,15,17	1.57	2 (22%)
1	PHD	A	369	1,9	9,11,12	1.42	1 (11%)	9,15,17	1.55	2 (22%)

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
1	PHD	C	369	1,9	-	1/8/11/13	-
1	PHD	A	369	1,9	-	1/8/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	369	PHD	CB-CA	-2.51	1.48	1.53
1	A	369	PHD	CB-CA	-2.41	1.48	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	PHD	OD2-CG-CB	-3.03	117.62	124.65
1	A	369	PHD	OD2-CG-CB	-3.01	117.66	124.65
1	A	369	PHD	OD1-CG-CB	2.74	117.39	110.95
1	C	369	PHD	OD1-CG-CB	2.66	117.19	110.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	369	PHD	CA-CB-CG-OD2
1	C	369	PHD	CA-CB-CG-OD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	369	PHD	1	0

5.5 Carbohydrates

6 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
4	NAG	F	1	2,4	14,14,15	0.54	0	17,19,21	0.63	0
4	NAG	F	2	4	14,14,15	0.34	0	17,19,21	0.41	0
5	GLC	H	1	5	11,11,12	0.53	0	15,15,17	1.85	2 (13%)
5	FRU	H	2	5	11,12,12	0.71	1 (9%)	10,18,18	0.84	0
5	GLC	I	1	5	11,11,12	0.53	0	15,15,17	1.23	1 (6%)
5	FRU	I	2	5	11,12,12	0.64	0	10,18,18	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
5	GLC	H	1	5	-	0/2/19/22	0/1/1/1
5	FRU	H	2	5	-	2/5/24/24	0/1/1/1
5	GLC	I	1	5	-	1/2/19/22	0/1/1/1
5	FRU	I	2	5	-	2/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	2	FRU	O2-C2	2.05	1.44	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	GLC	C1-O5-C5	5.29	119.28	112.19
5	I	1	GLC	C1-O5-C5	3.42	116.77	112.19
5	H	1	GLC	C1-C2-C3	2.53	113.33	109.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	2	FRU	C4-C5-C6-O6
5	I	2	FRU	C4-C5-C6-O6

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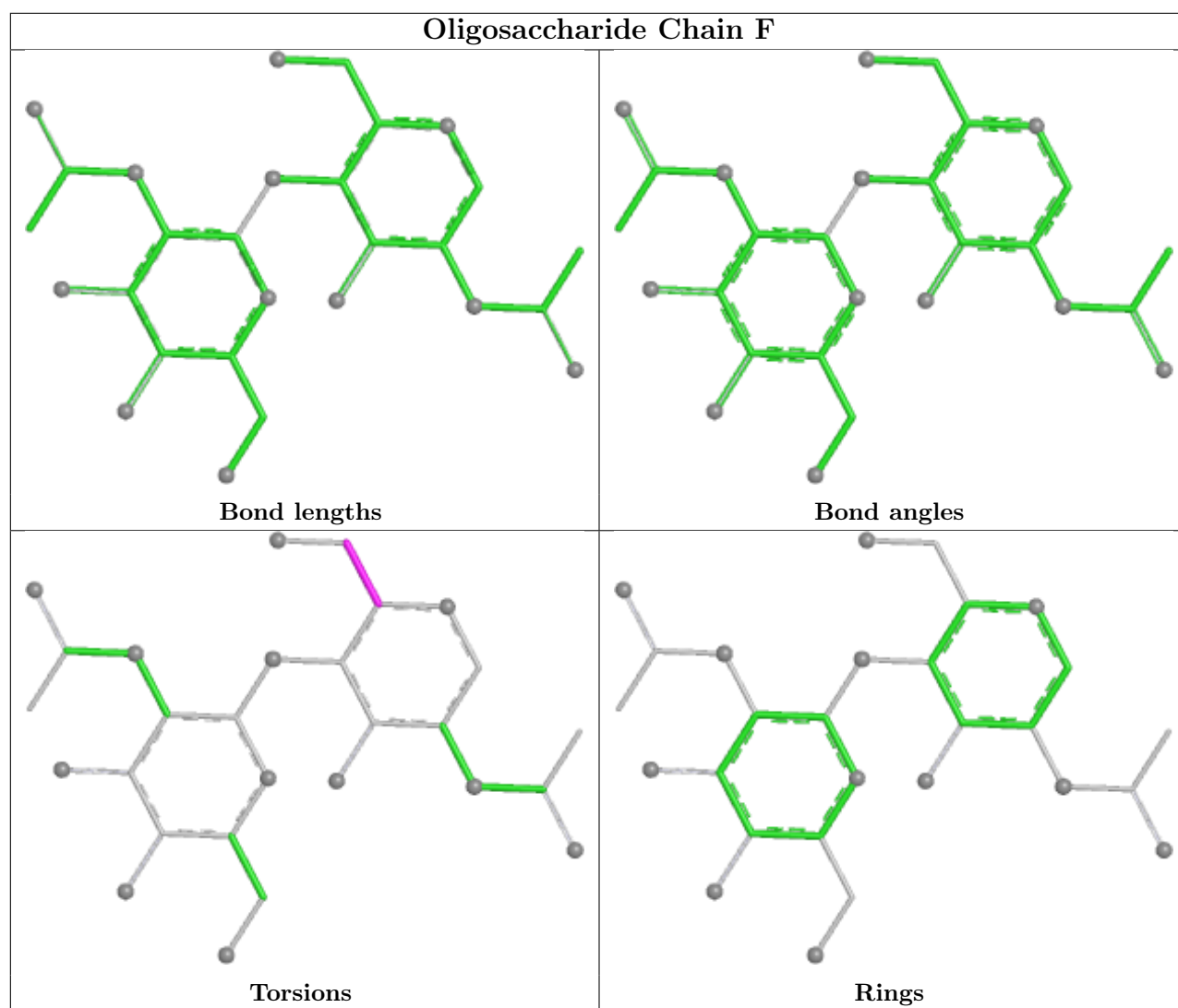
Mol	Chain	Res	Type	Atoms
5	H	2	FRU	O5-C5-C6-O6
5	I	2	FRU	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
5	I	1	GLC	O5-C5-C6-O6

There are no ring outliers.

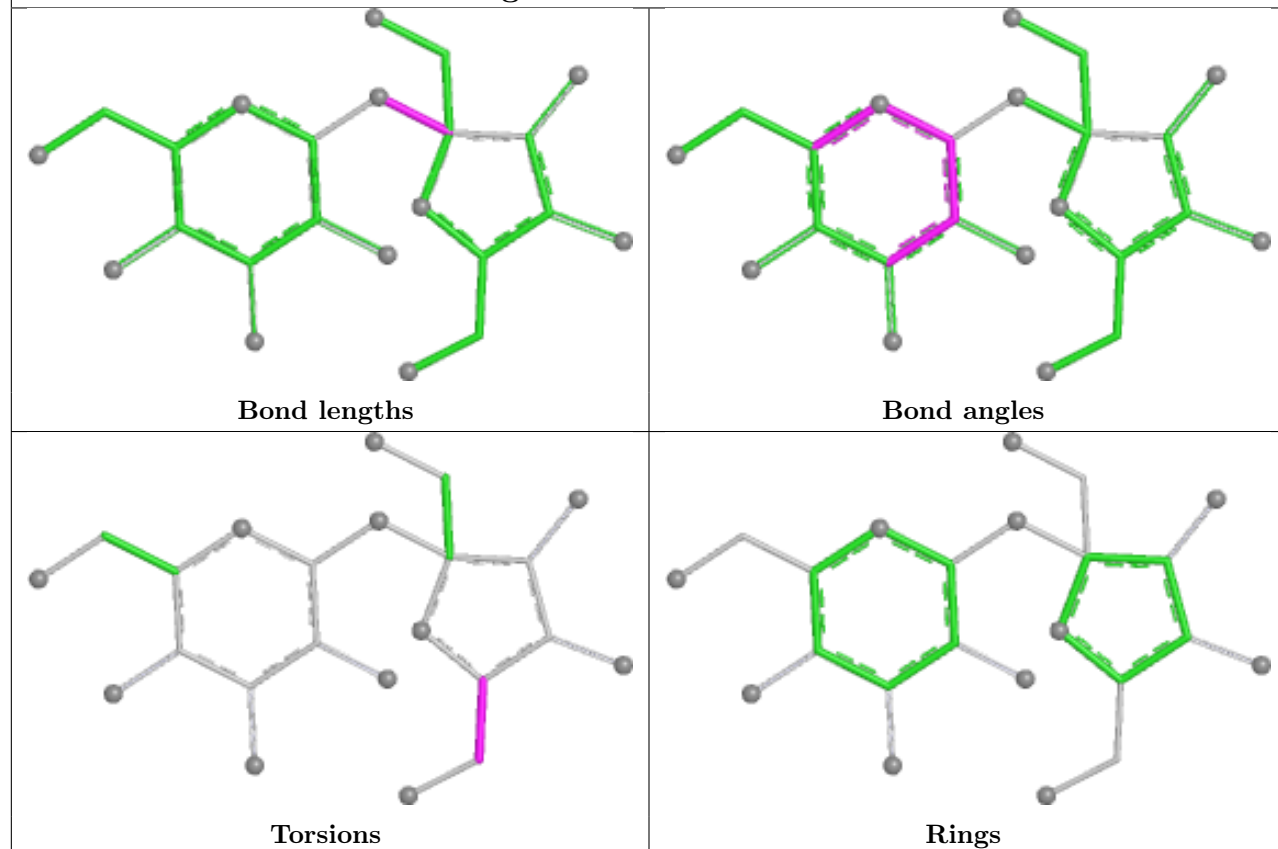
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	1	0
5	I	2	FRU	2	0
5	H	2	FRU	3	0

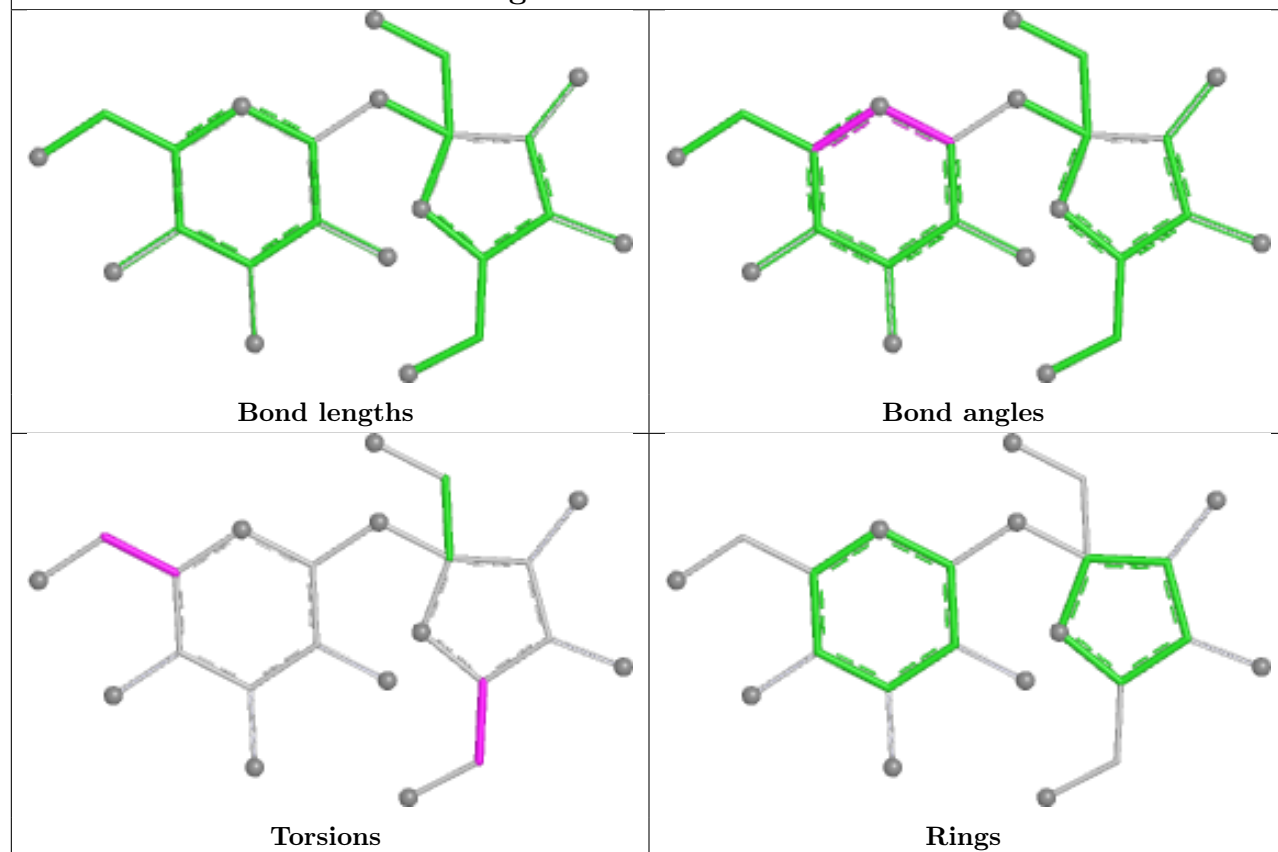
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain H



Oligosaccharide Chain I



5.6 Ligand geometry

Of 14 ligands modelled in this entry, 8 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
10	NAG	B	1001	2	14,14,15	0.43	0	17,19,21	0.56	0
11	17F	G	1001	-	17,18,53	1.79	4 (23%)	18,24,60	1.98	2 (11%)
7	CLR	A	2002	-	31,31,31	2.63	13 (41%)	48,48,48	2.95	21 (43%)
6	BUF	A	2001	8	32,32,32	0.92	2 (6%)	52,52,52	1.41	9 (17%)
7	CLR	E	101	-	31,31,31	2.60	10 (32%)	48,48,48	2.97	20 (41%)
6	BUF	C	1102	8	32,32,32	0.99	3 (9%)	52,52,52	1.49	8 (15%)

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
10	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
11	17F	G	1001	-	-	16/21/21/59	-
7	CLR	A	2002	-	-	3/10/68/68	0/4/4/4
6	BUF	A	2001	8	-	0/4/68/68	0/5/5/5
7	CLR	E	101	-	-	3/10/68/68	0/4/4/4
6	BUF	C	1102	8	-	0/4/68/68	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2002	CLR	C6-C5	9.73	1.53	1.33
7	E	101	CLR	C6-C5	9.69	1.53	1.33
7	A	2002	CLR	C11-C9	4.82	1.61	1.53
7	E	101	CLR	C11-C9	4.74	1.61	1.53
11	G	1001	17F	P1-O6	4.63	1.77	1.59
7	A	2002	CLR	C8-C14	4.03	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	101	CLR	C8-C14	3.76	1.60	1.53
7	E	101	CLR	C12-C13	3.70	1.60	1.54
7	A	2002	CLR	C13-C17	-3.66	1.48	1.55
7	E	101	CLR	C13-C17	-3.45	1.48	1.55
7	E	101	CLR	C20-C17	-3.34	1.48	1.54
7	A	2002	CLR	C20-C17	-3.34	1.48	1.54
7	A	2002	CLR	C12-C13	3.19	1.59	1.54
7	E	101	CLR	C15-C14	-2.98	1.48	1.54
11	G	1001	17F	C1-C2	2.76	1.59	1.52
7	A	2002	CLR	C15-C14	-2.72	1.48	1.54
6	C	1102	BUF	C14-C8	2.72	1.58	1.54
11	G	1001	17F	P1-O3	2.53	1.69	1.59
6	A	2001	BUF	C14-C8	2.47	1.57	1.54
7	E	101	CLR	C13-C14	-2.42	1.50	1.55
6	C	1102	BUF	O14-C14	-2.26	1.40	1.43
7	A	2002	CLR	C13-C14	-2.26	1.50	1.55
7	A	2002	CLR	C16-C17	2.23	1.58	1.54
6	C	1102	BUF	C4-C3	2.20	1.55	1.52
7	E	101	CLR	O1-C3	-2.16	1.37	1.43
7	A	2002	CLR	C19-C10	-2.15	1.51	1.54
7	A	2002	CLR	O1-C3	-2.09	1.37	1.43
7	A	2002	CLR	C4-C3	-2.05	1.48	1.52
7	A	2002	CLR	C1-C10	-2.03	1.50	1.54
7	E	101	CLR	C19-C10	-2.02	1.51	1.54
11	G	1001	17F	C4-C5	2.00	1.57	1.51
6	A	2001	BUF	O14-C14	-2.00	1.40	1.43

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2002	CLR	C4-C5-C6	-8.04	109.67	120.57
7	E	101	CLR	C4-C5-C6	-7.89	109.87	120.57
7	E	101	CLR	C7-C6-C5	-7.78	111.89	125.02
7	A	2002	CLR	C7-C6-C5	-7.42	112.48	125.02
11	G	1001	17F	O3-C1-C2	7.08	114.23	108.06
7	E	101	CLR	C10-C5-C6	-6.11	114.00	122.93
7	A	2002	CLR	C10-C5-C6	-5.80	114.46	122.93
7	A	2002	CLR	C12-C13-C17	-5.78	108.08	116.60
7	E	101	CLR	C1-C10-C9	5.75	116.35	108.74
7	E	101	CLR	C12-C13-C17	-5.72	108.17	116.60
7	A	2002	CLR	C1-C10-C9	5.44	115.94	108.74
7	A	2002	CLR	C7-C8-C9	5.41	115.98	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	101	CLR	C21-C20-C17	5.15	120.62	112.88
7	A	2002	CLR	C21-C20-C17	4.94	120.30	112.88
7	E	101	CLR	C7-C8-C9	4.84	115.32	109.72
7	E	101	CLR	C19-C10-C1	-4.03	103.30	109.43
7	A	2002	CLR	C19-C10-C9	-4.01	107.16	111.66
7	E	101	CLR	C19-C10-C9	-3.86	107.33	111.66
6	C	1102	BUF	C16-C17-C20	3.73	117.35	113.48
7	A	2002	CLR	C11-C9-C10	3.66	117.60	113.08
7	E	101	CLR	C16-C17-C13	-3.65	99.54	103.84
7	A	2002	CLR	C19-C10-C1	-3.54	104.05	109.43
7	E	101	CLR	C15-C14-C13	-3.53	99.68	103.84
7	A	2002	CLR	C16-C17-C13	-3.45	99.78	103.84
7	E	101	CLR	C11-C9-C10	3.42	117.30	113.08
7	A	2002	CLR	C3-C4-C5	-3.35	106.72	112.05
7	A	2002	CLR	C7-C8-C14	3.32	115.64	110.93
6	A	2001	BUF	C16-C17-C20	3.32	116.92	113.48
7	E	101	CLR	C3-C4-C5	-3.29	106.82	112.05
6	A	2001	BUF	C12-C13-C14	3.27	112.79	108.94
6	C	1102	BUF	C18-C13-C12	3.24	114.12	109.69
7	A	2002	CLR	C11-C12-C13	-3.04	107.60	112.74
6	C	1102	BUF	C14-C13-C17	2.99	106.84	103.61
6	A	2001	BUF	C18-C13-C12	2.94	113.71	109.69
7	E	101	CLR	C7-C8-C14	2.94	115.10	110.93
11	G	1001	17F	O2-P1-O1	2.93	126.10	112.44
7	A	2002	CLR	C15-C14-C13	-2.87	100.46	103.84
6	C	1102	BUF	C9-C10-C5	2.87	112.50	108.51
6	C	1102	BUF	C12-C13-C14	2.71	112.14	108.94
7	E	101	CLR	C11-C12-C13	-2.71	108.17	112.74
7	E	101	CLR	C11-C9-C8	2.68	115.52	111.78
7	A	2002	CLR	C16-C17-C20	-2.59	108.26	112.18
7	A	2002	CLR	C11-C9-C8	2.52	115.29	111.78
7	E	101	CLR	C17-C13-C14	2.49	102.96	100.10
7	A	2002	CLR	C21-C20-C22	-2.47	106.52	110.34
7	E	101	CLR	C21-C20-C22	-2.43	106.58	110.34
6	A	2001	BUF	C14-C13-C17	2.42	106.22	103.61
6	A	2001	BUF	C9-C10-C5	2.36	111.80	108.51
7	A	2002	CLR	C19-C10-C5	2.33	111.94	108.38
7	A	2002	CLR	C9-C10-C5	-2.25	106.36	109.65
6	C	1102	BUF	C15-C16-C17	2.22	108.78	104.22
7	E	101	CLR	C16-C17-C20	-2.22	108.82	112.18
6	A	2001	BUF	C15-C16-C17	2.19	108.70	104.22
6	A	2001	BUF	C7-C6-C5	2.13	115.97	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	101	CLR	C19-C10-C5	2.12	111.62	108.38
6	A	2001	BUF	C1-C2-C3	-2.09	107.71	110.48
6	A	2001	BUF	C18-C13-C14	-2.08	108.30	112.28
6	C	1102	BUF	C7-C6-C5	2.07	115.83	111.84
6	C	1102	BUF	C1-C2-C3	-2.06	107.75	110.48
7	A	2002	CLR	C17-C13-C14	2.06	102.46	100.10

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	G	1001	17F	C1-O3-P1-O6
11	G	1001	17F	C4-O6-P1-O1
11	G	1001	17F	C4-O6-P1-O2
11	G	1001	17F	C4-O6-P1-O3
11	G	1001	17F	C1-C2-C3-O4
11	G	1001	17F	C1-C2-C3-O5
11	G	1001	17F	N1-C2-C3-O4
11	G	1001	17F	O6-C4-C5-C6
11	G	1001	17F	C4-C5-C6-O7
10	B	1001	NAG	O5-C5-C6-O6
11	G	1001	17F	O9-C5-C6-O7
10	B	1001	NAG	C4-C5-C6-O6
11	G	1001	17F	N1-C2-C3-O5
11	G	1001	17F	O6-C4-C5-O9
7	A	2002	CLR	C22-C23-C24-C25
7	E	101	CLR	C22-C23-C24-C25
11	G	1001	17F	C8-C7-O7-C6
7	E	101	CLR	C20-C22-C23-C24
7	A	2002	CLR	C20-C22-C23-C24
7	A	2002	CLR	C23-C24-C25-C26
11	G	1001	17F	O8-C7-O7-C6
7	E	101	CLR	C23-C24-C25-C26
11	G	1001	17F	C2-C1-O3-P1
11	G	1001	17F	C1-O3-P1-O1

There are no ring outliers.

5 monomers are involved in 17 short contacts:

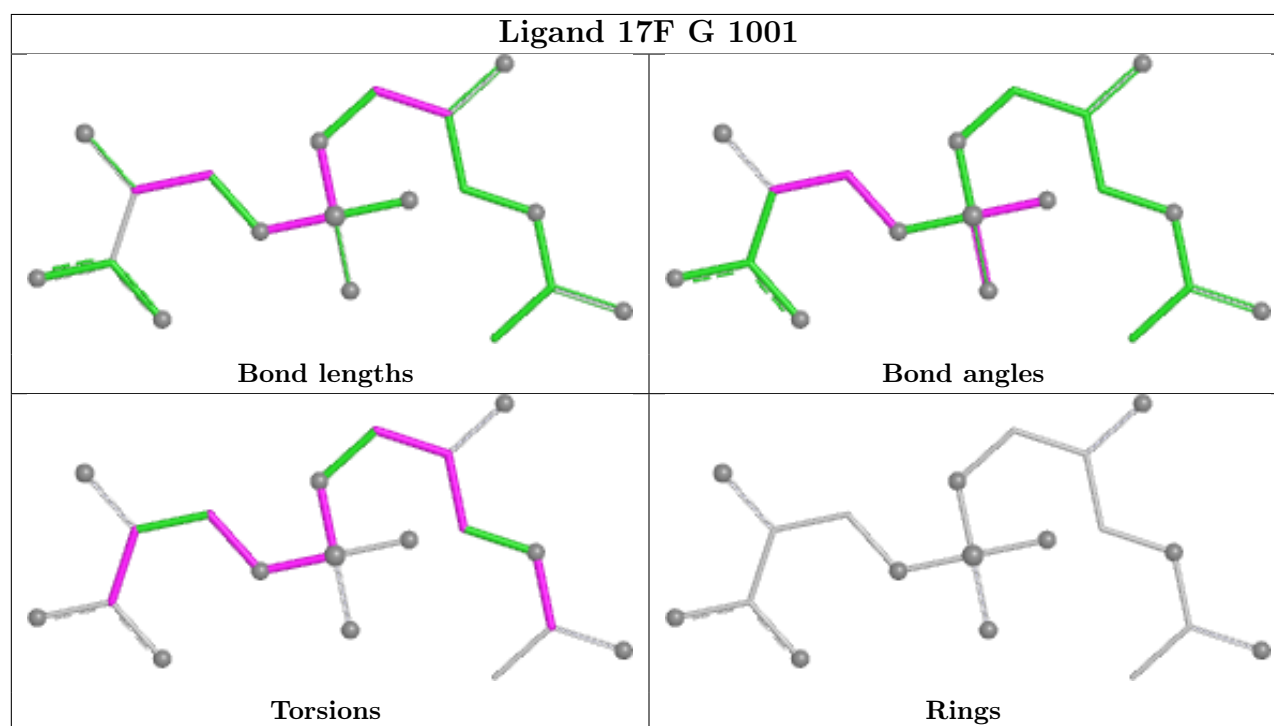
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1001	NAG	1	0

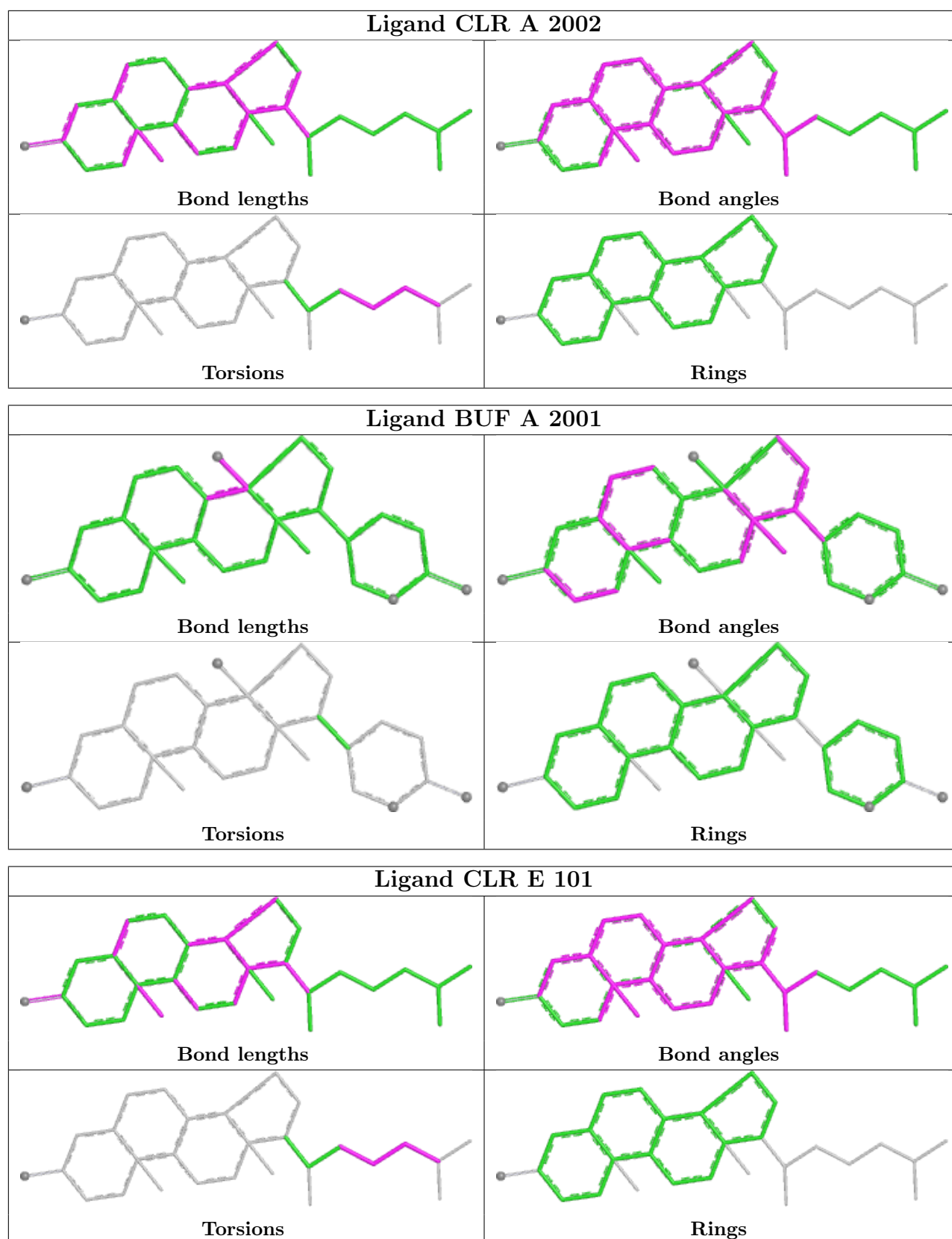
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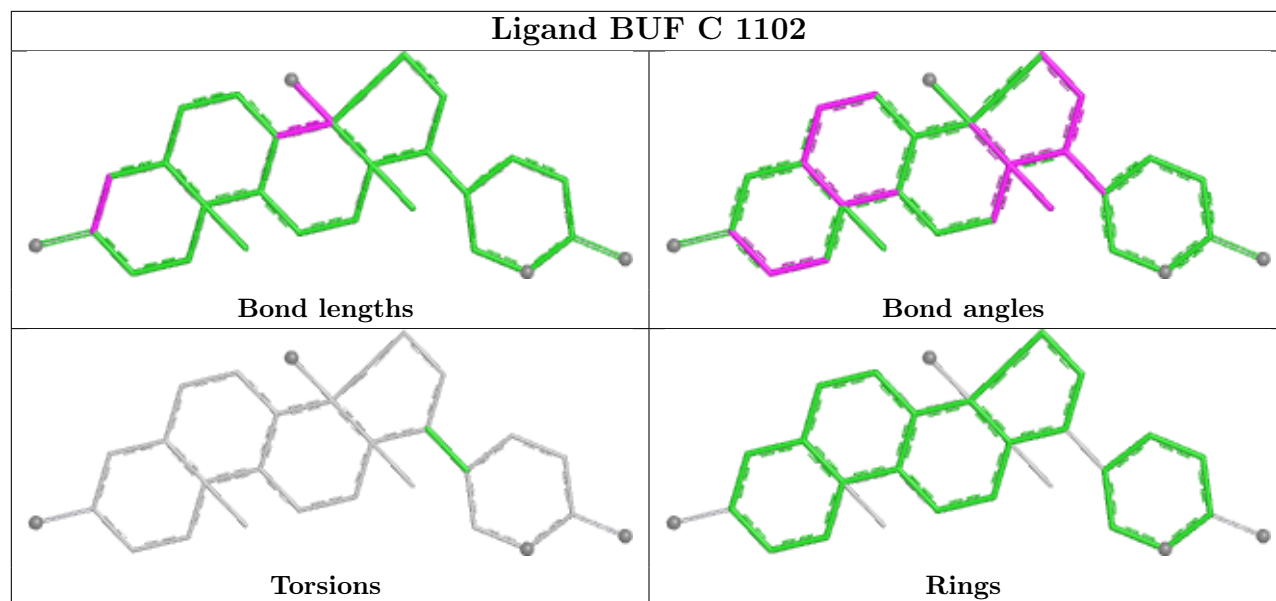
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2002	CLR	4	0
6	A	2001	BUF	3	0
7	E	101	CLR	4	0
6	C	1102	BUF	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	995/1021 (97%)	-0.97	0 100 100	40, 119, 201, 295	0
1	C	995/1021 (97%)	-0.95	1 (0%) 92 91	41, 124, 212, 292	0
2	B	288/303 (95%)	-0.95	0 100 100	53, 124, 205, 248	0
2	D	285/303 (94%)	-1.00	0 100 100	56, 120, 199, 326	0
3	E	32/65 (49%)	-1.36	0 100 100	51, 80, 158, 178	0
3	G	32/65 (49%)	-1.34	0 100 100	56, 86, 144, 172	0
All	All	2627/2778 (94%)	-0.97	1 (0%) 100 100	40, 121, 206, 326	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	40	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PHD	C	369	12/13	0.98	0.05	102,103,105,105	0
1	PHD	A	369	12/13	0.99	0.05	116,118,121,121	0

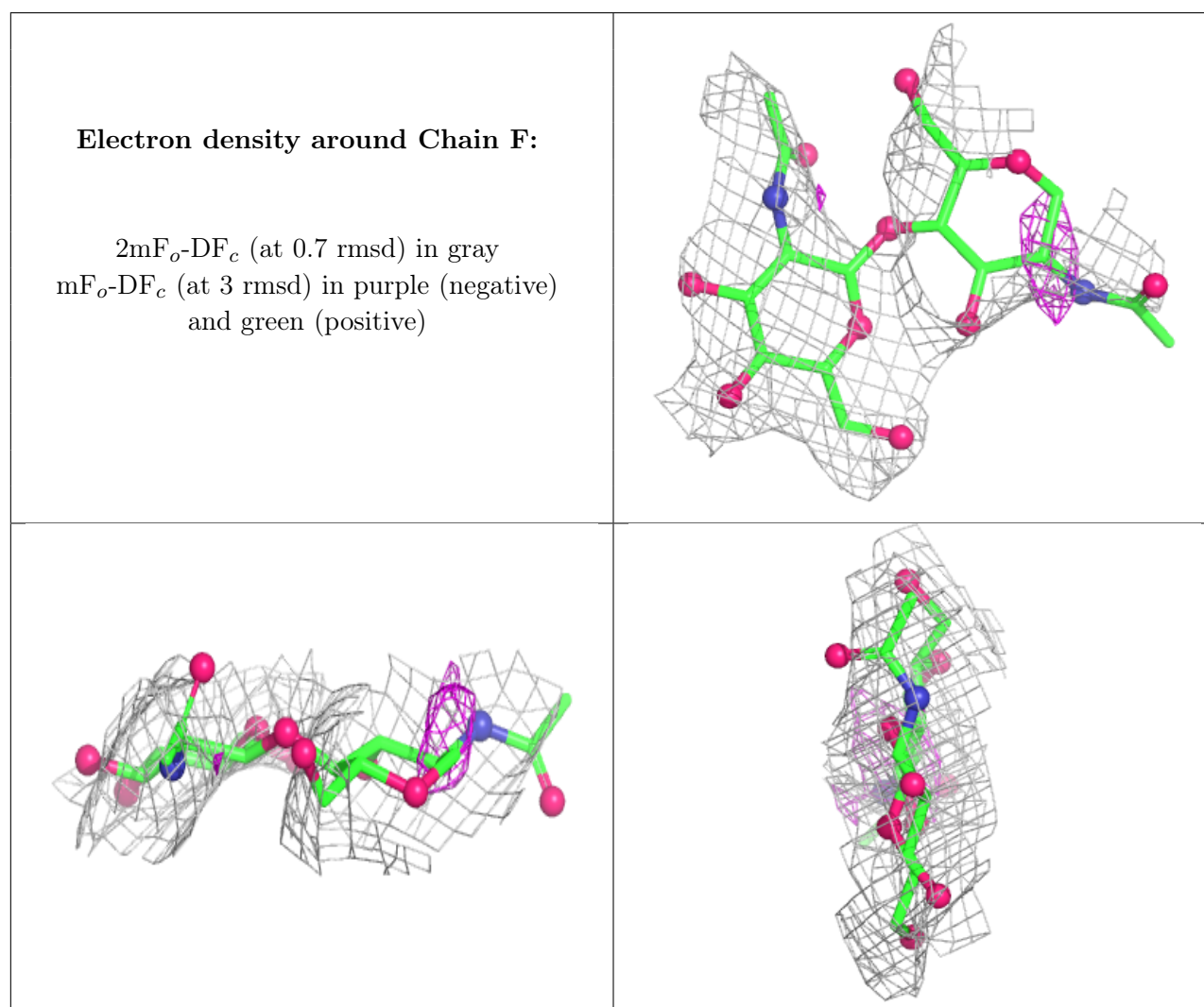
6.3 Carbohydrates [i](#)

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.

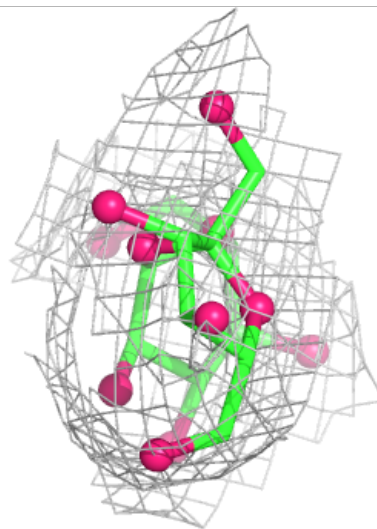
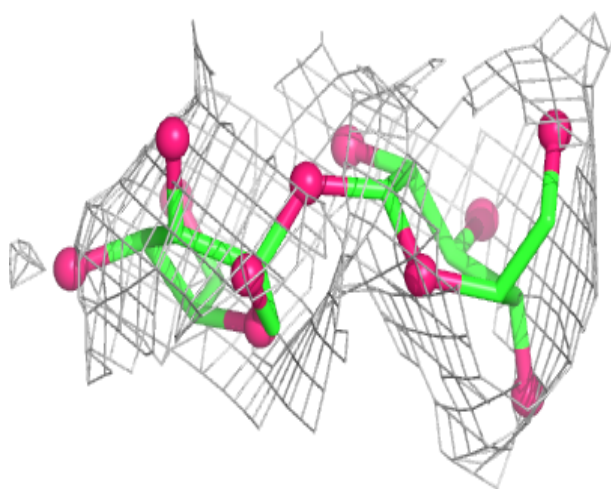
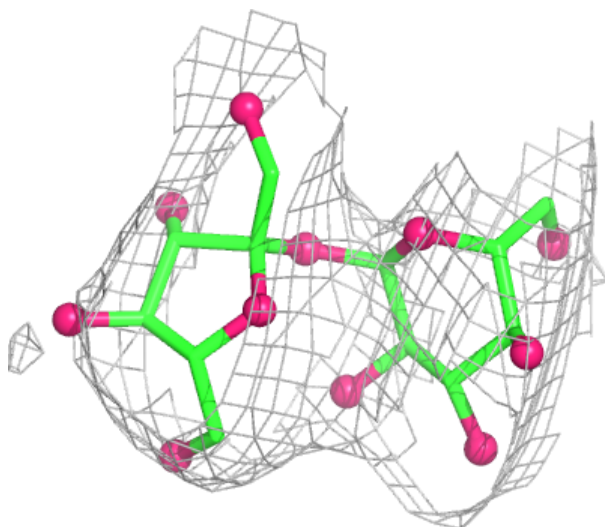
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	F	1	14/15	-	-	157,166,174,177	0
4	NAG	F	2	14/15	-	-	168,173,183,184	0
5	GLC	H	1	11/12	0.99	0.04	113,115,118,120	0
5	FRU	H	2	12/12	0.99	0.03	110,113,115,116	0
5	GLC	I	1	11/12	0.99	0.03	104,105,108,109	0
5	FRU	I	2	12/12	0.99	0.03	101,104,105,106	0

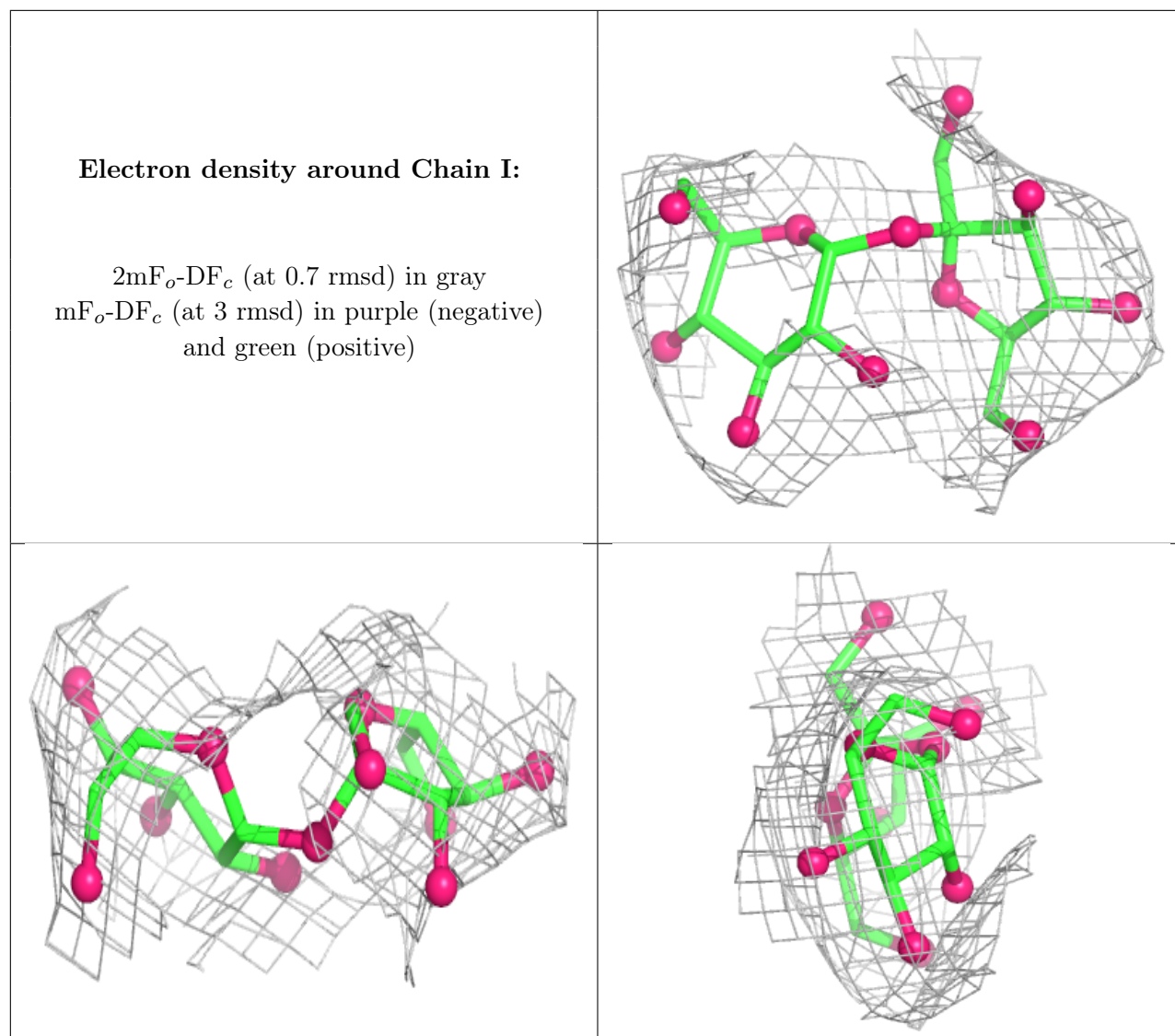
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain H:

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





6.4 Ligands [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.

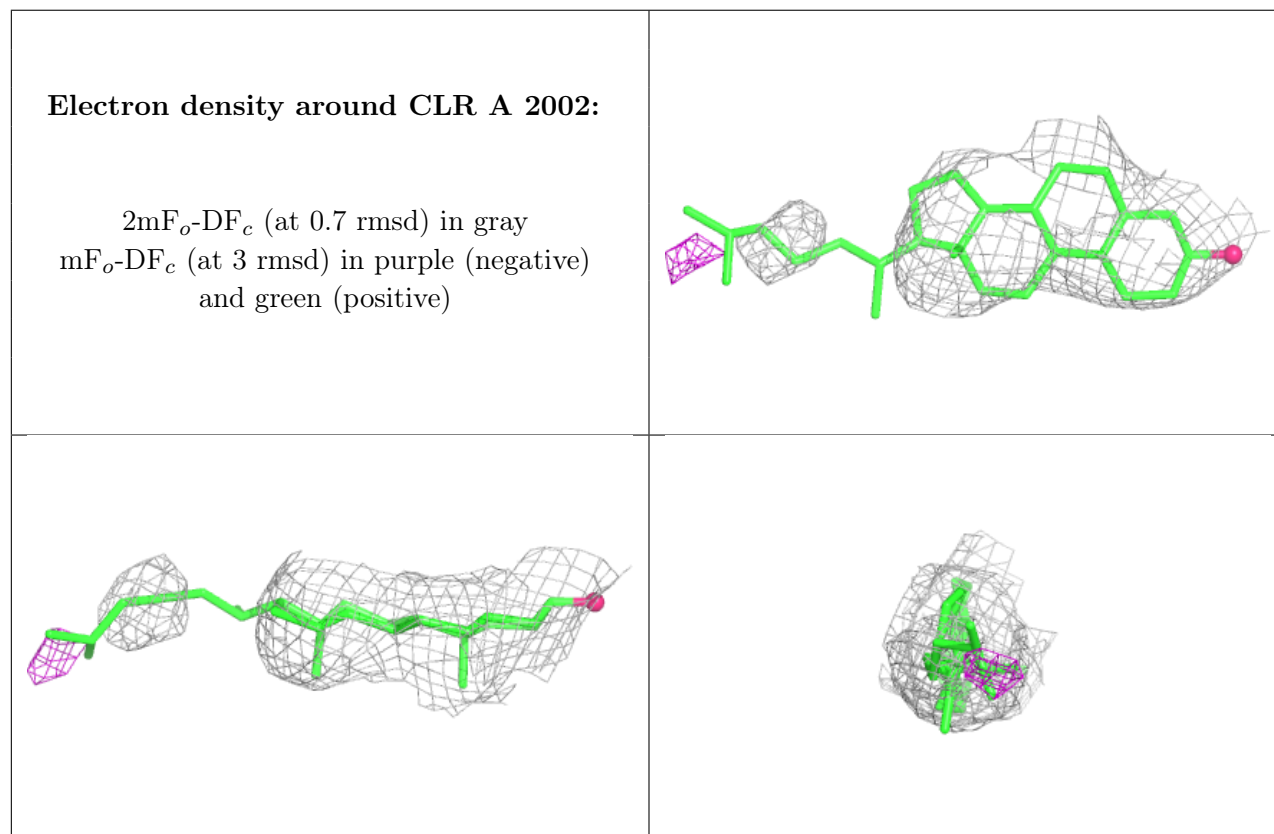
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	K	A	2005	1/1	0.95	0.07	121,121,121,121	0
10	NAG	B	1001	14/15	0.97	0.06	138,146,152,154	0
7	CLR	A	2002	28/28	0.99	0.06	40,44,51,53	0
7	CLR	E	101	28/28	0.99	0.05	56,60,65,67	0
8	K	A	2003	1/1	0.99	0.05	121,121,121,121	0
6	BUF	A	2001	28/28	0.99	0.05	93,97,101,102	0
8	K	C	1105	1/1	0.99	0.03	60,60,60,60	0

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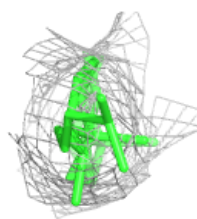
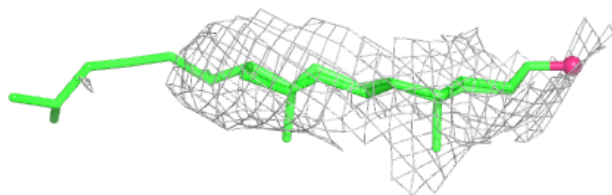
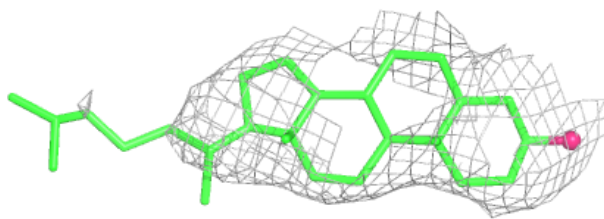
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BUF	C	1102	28/28	0.99	0.04	90,94,99,100	0
11	17F	G	1001	19/54	0.99	0.07	136,142,150,152	0
8	K	C	1106	1/1	1.00	0.01	69,69,69,69	0
9	MG	A	2006	1/1	1.00	0.05	71,71,71,71	0
9	MG	C	1107	1/1	1.00	0.05	106,106,106,106	0
8	K	C	1104	1/1	1.00	0.04	92,92,92,92	0
8	K	A	2004	1/1	1.00	0.02	54,54,54,54	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.

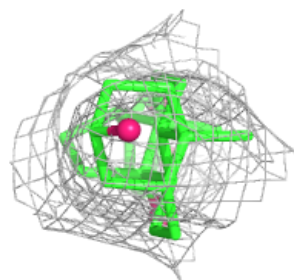
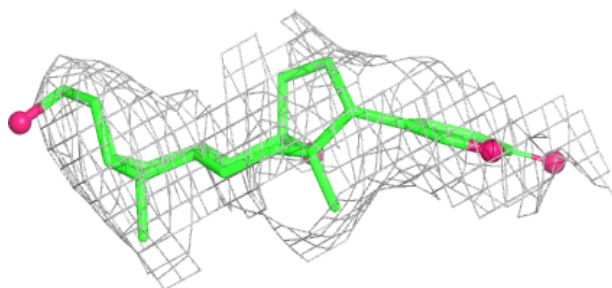
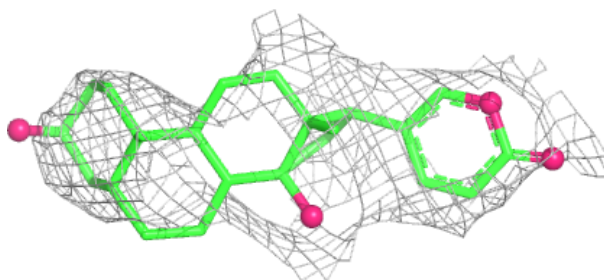


Electron density around CLR E 101:

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

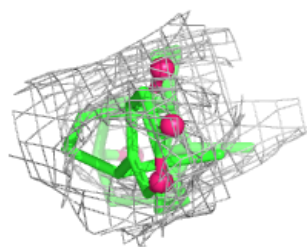
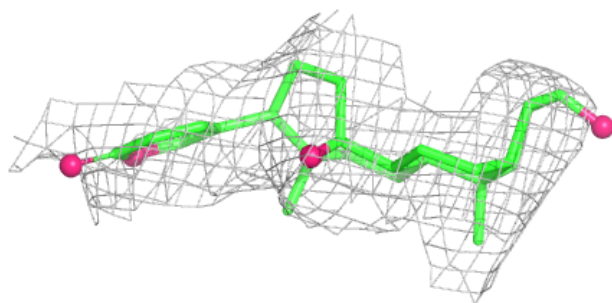
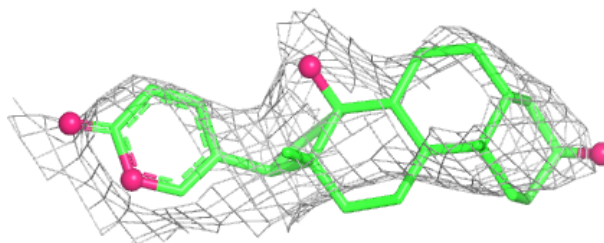
**Electron density around BUF A 2001:**

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

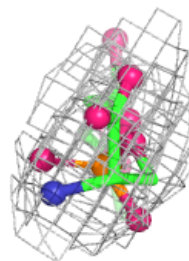
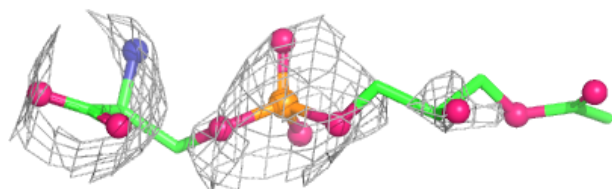
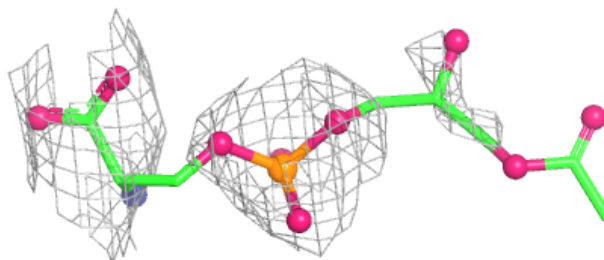


Electron density around BUF C 1102:

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

**Electron density around 17F G 1001:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.