



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:09 AM UTC

PDB ID : 2G3N / pdb_00002g3n
Title : Crystal structure of the Sulfolobus solfataricus alpha-glucosidase MalA in complex with beta-octyl-glucopyranoside
Authors : Ernst, H.A.; Lo Leggio, L.; Willemoes, M.; Leonard, G.; Blum, P.; Larsen, S.
Deposited on : 2006-02-20
Resolution : 2.55 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

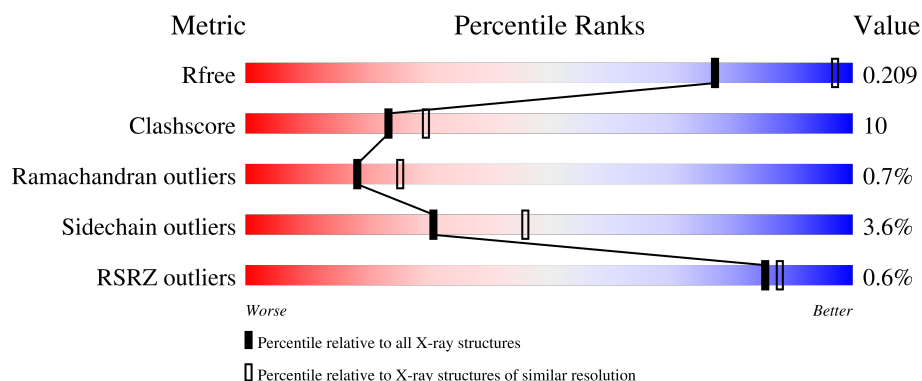
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	693	73% 24%
1	B	693	74% 23%
1	C	693	73% 24%
1	D	693	74% 23%
1	E	693	76% 22%

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Mol	Chain	Length	Quality of chain
1	F	693	% 75% 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34797 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 Alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	1	0
			5683	3703	919	1046	15			
1	B	691	Total	C	N	O	S	0	1	0
			5683	3703	919	1046	15			
1	C	691	Total	C	N	O	S	0	1	0
			5683	3703	919	1046	15			
1	D	691	Total	C	N	O	S	0	1	0
			5683	3703	919	1046	15			
1	E	691	Total	C	N	O	S	0	1	0
			5683	3703	919	1046	15			
1	F	691	Total	C	N	O	S	0	1	0
			5683	3703	919	1046	15			

There are 24 discrepancies between the modelled and reference sequences:

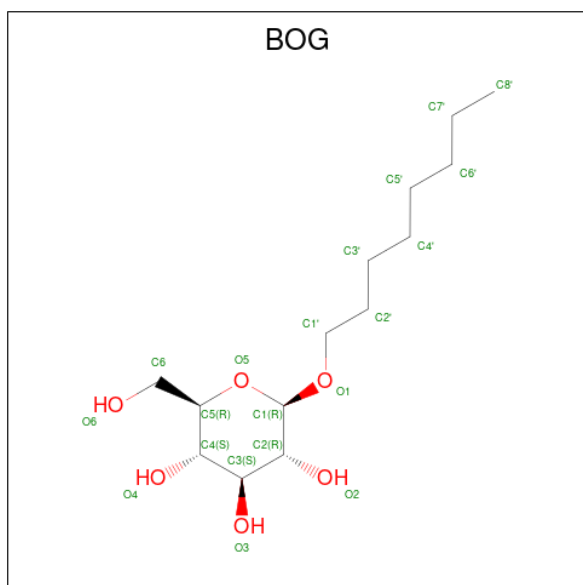
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP O59645
A	2	ARG	-	cloning artifact	UNP O59645
A	3	ILE	-	cloning artifact	UNP O59645
A	4	LEU	-	cloning artifact	UNP O59645
B	1	MET	-	cloning artifact	UNP O59645
B	2	ARG	-	cloning artifact	UNP O59645
B	3	ILE	-	cloning artifact	UNP O59645
B	4	LEU	-	cloning artifact	UNP O59645
C	1	MET	-	cloning artifact	UNP O59645
C	2	ARG	-	cloning artifact	UNP O59645
C	3	ILE	-	cloning artifact	UNP O59645
C	4	LEU	-	cloning artifact	UNP O59645
D	1	MET	-	cloning artifact	UNP O59645
D	2	ARG	-	cloning artifact	UNP O59645
D	3	ILE	-	cloning artifact	UNP O59645
D	4	LEU	-	cloning artifact	UNP O59645
E	1	MET	-	cloning artifact	UNP O59645

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	ARG	-	cloning artifact	UNP O59645
E	3	ILE	-	cloning artifact	UNP O59645
E	4	LEU	-	cloning artifact	UNP O59645
F	1	MET	-	cloning artifact	UNP O59645
F	2	ARG	-	cloning artifact	UNP O59645
F	3	ILE	-	cloning artifact	UNP O59645
F	4	LEU	-	cloning artifact	UNP O59645

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	8	6		
2	B	1	Total	C	O	0	0
			14	8	6		
2	C	1	Total	C	O	0	0
			14	8	6		
2	D	1	Total	C	O	0	0
			14	8	6		
2	E	1	Total	C	O	0	0
			14	8	6		
2	F	1	Total	C	O	0	0
			14	8	6		

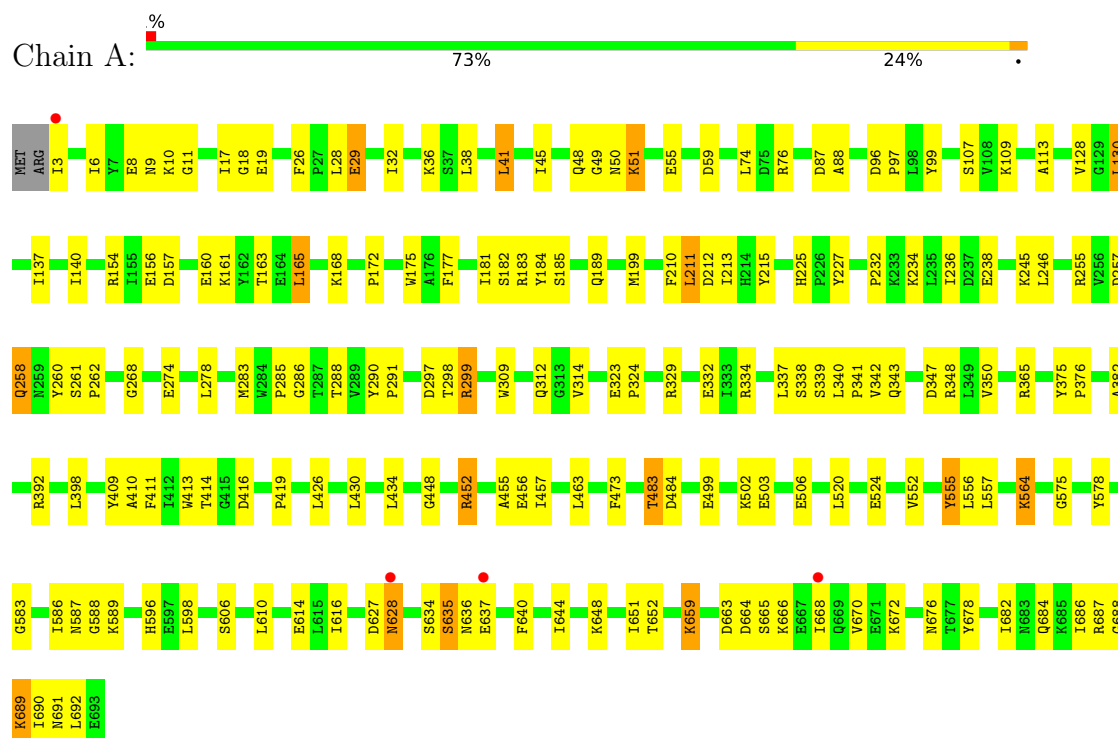
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total 83	O 83	0	0
3	B	74	Total 74	O 74	0	0
3	C	96	Total 96	O 96	0	0
3	D	103	Total 103	O 103	0	0
3	E	127	Total 127	O 127	0	0
3	F	132	Total 132	O 132	0	0

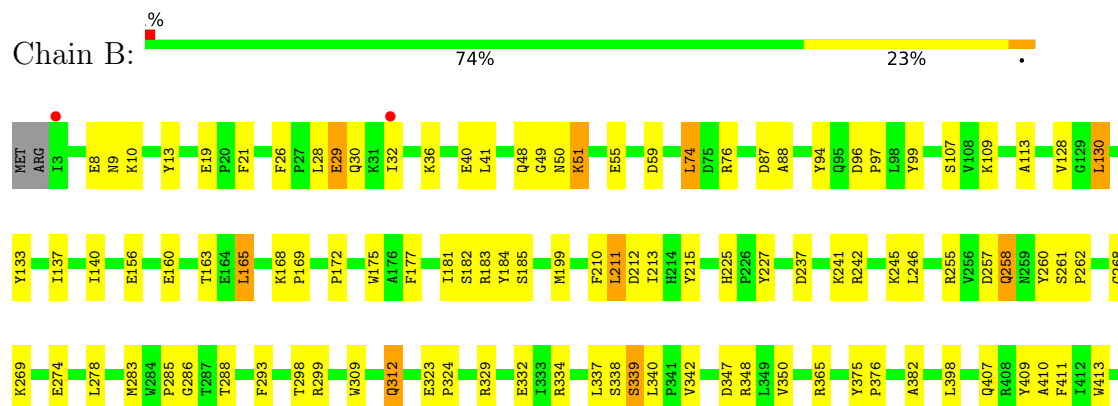
3 Residue-property plots [i](#)

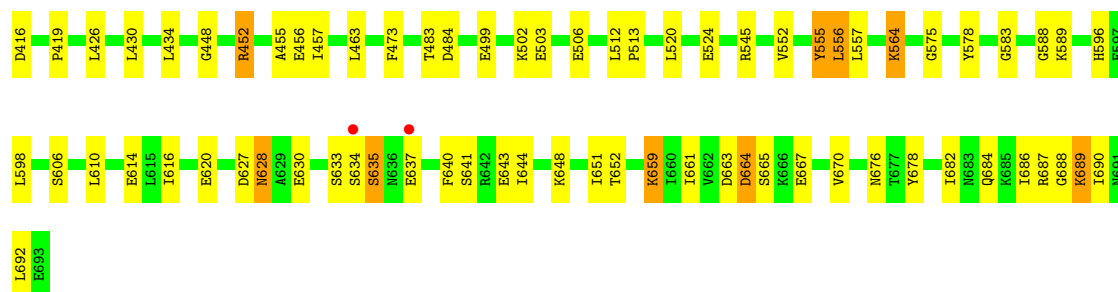
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Alpha-glucosidase

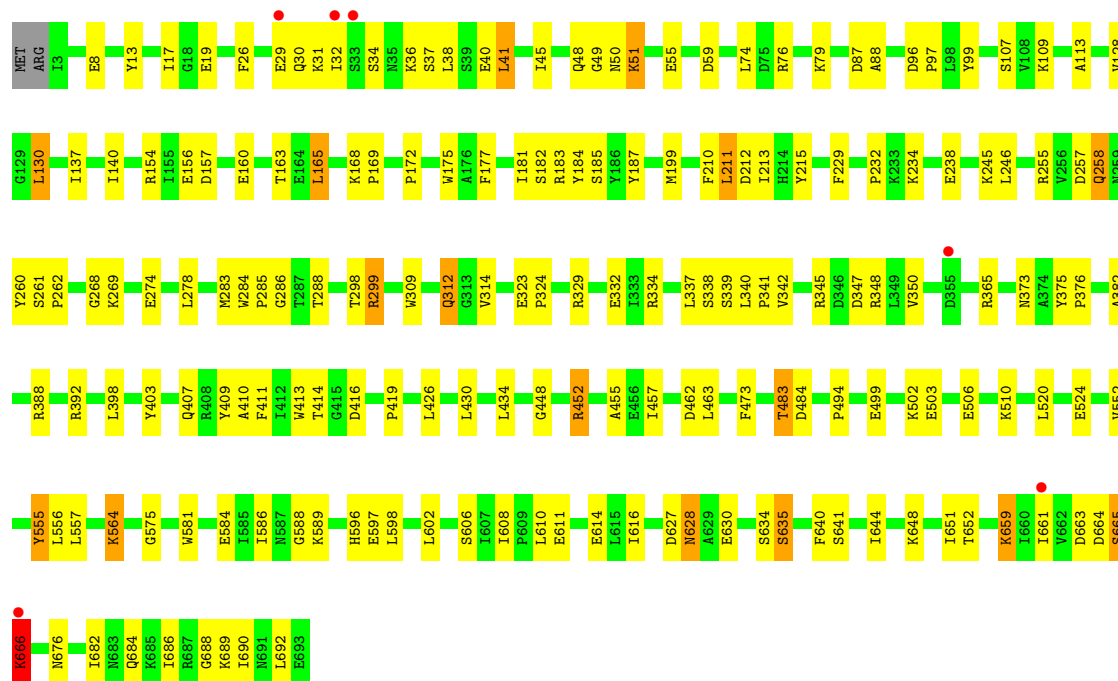
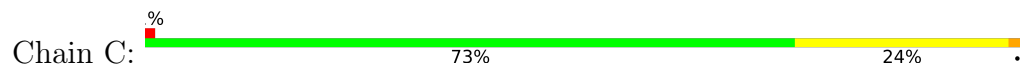


• Molecule 1: Alpha-glucosidase

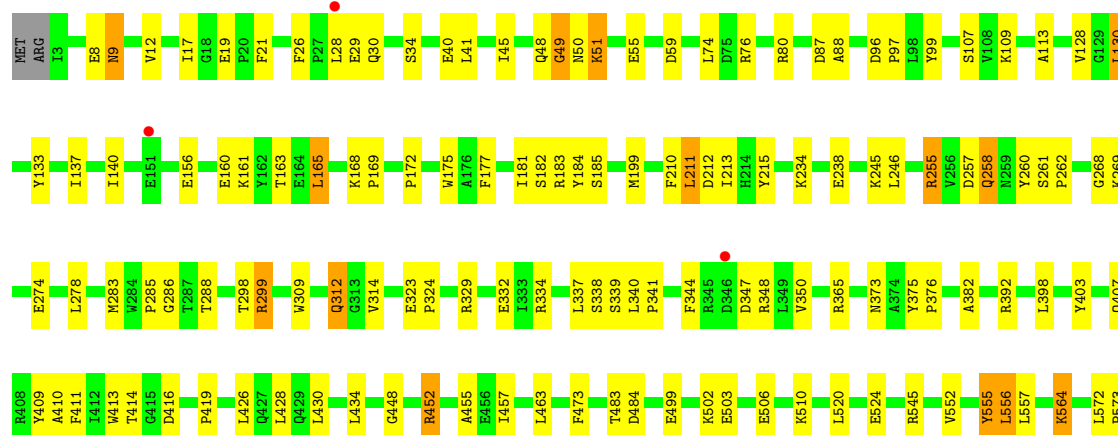
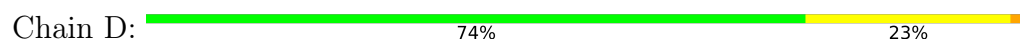


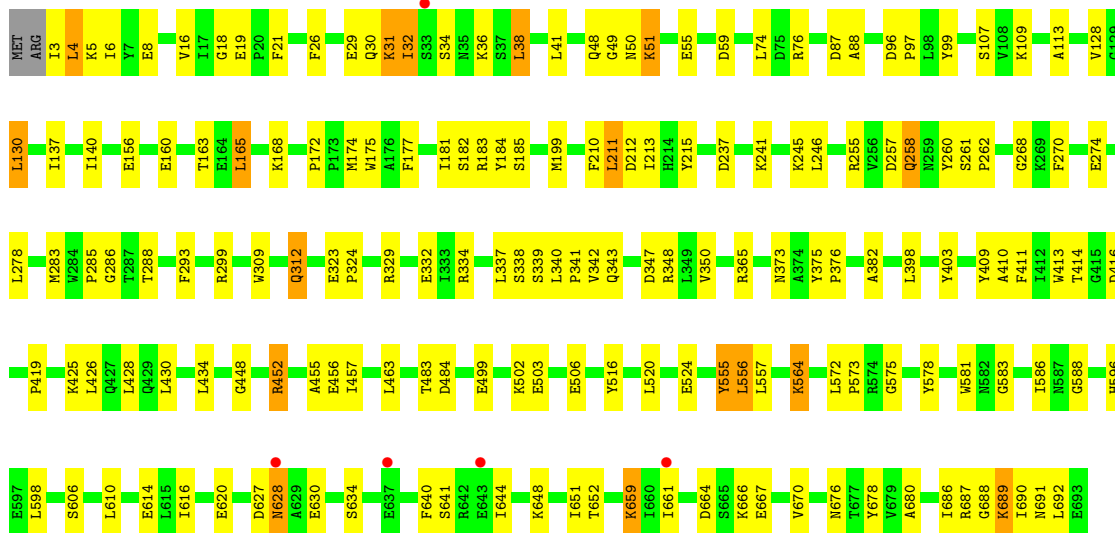


• Molecule 1: Alpha-glucosidase



• Molecule 1: Alpha-glucosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.09Å 174.43Å 144.03Å 90.00° 109.05° 90.00°	Depositor
Resolution (Å)	24.16 – 2.55 24.16 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.3 (24.16-2.55) 96.1 (24.16-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.213 0.184 , 0.209	Depositor DCC
R_{free} test set	7699 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34797	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: BOG

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	0.41	0/5837	0.91	18/7902 (0.2%)
1	B	0.42	0/5837	0.90	17/7902 (0.2%)
1	C	0.41	0/5837	0.89	17/7902 (0.2%)
1	D	0.42	0/5837	0.90	19/7902 (0.2%)
1	E	0.43	0/5837	0.89	16/7902 (0.2%)
1	F	0.46	0/5837	0.90	18/7902 (0.2%)
All	All	0.43	0/35022	0.90	105/47412 (0.2%)

There are no bond length outliers.

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	VAL	N-CA-C	8.64	115.45	106.21
1	D	455	ALA	N-CA-C	8.18	121.23	111.33
1	B	455	ALA	N-CA-C	8.07	121.09	111.33
1	F	455	ALA	N-CA-C	7.93	120.92	111.33
1	E	455	ALA	N-CA-C	7.86	120.84	111.33
1	B	410	ALA	N-CA-C	7.84	120.05	108.60
1	F	410	ALA	N-CA-C	7.84	120.04	108.60
1	A	455	ALA	N-CA-C	7.83	120.80	111.33
1	C	410	ALA	N-CA-C	7.78	119.97	108.60
1	A	410	ALA	N-CA-C	7.76	119.93	108.60
1	C	455	ALA	N-CA-C	7.60	120.52	111.33
1	D	410	ALA	N-CA-C	7.51	120.28	108.79
1	D	76	ARG	N-CA-C	7.38	122.13	113.20
1	F	21	PHE	CA-C-N	7.32	125.00	119.66
1	F	21	PHE	C-N-CA	7.32	125.00	119.66
1	A	76	ARG	N-CA-C	7.31	122.04	113.20
1	B	76	ARG	N-CA-C	7.25	121.97	113.20
1	A	555	TYR	N-CA-C	7.17	122.16	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	76	ARG	N-CA-C	7.17	121.87	113.20
1	E	410	ALA	N-CA-C	7.13	119.70	108.79
1	B	21	PHE	CA-C-N	7.11	124.85	119.66
1	B	21	PHE	C-N-CA	7.11	124.85	119.66
1	C	76	ARG	N-CA-C	7.07	121.75	113.20
1	E	76	ARG	N-CA-C	7.01	121.68	113.20
1	E	555	TYR	N-CA-C	6.87	121.79	113.41
1	D	21	PHE	CA-C-N	6.84	124.65	119.66
1	D	21	PHE	C-N-CA	6.84	124.65	119.66
1	B	555	TYR	N-CA-C	6.81	121.72	113.41
1	D	555	TYR	N-CA-C	6.79	121.69	113.41
1	C	555	TYR	N-CA-C	6.73	121.78	113.50
1	A	636	ASN	N-CA-C	-6.71	103.25	112.03
1	F	555	TYR	N-CA-C	6.59	121.45	113.41
1	C	416	ASP	N-CA-C	6.42	119.59	109.39
1	F	689	LYS	N-CA-C	6.40	118.58	108.79
1	A	414	THR	N-CA-C	6.37	120.53	113.21
1	A	689	LYS	N-CA-C	6.37	118.53	108.79
1	F	414	THR	N-CA-C	6.36	120.53	113.21
1	F	213	ILE	N-CA-C	6.34	122.53	109.34
1	B	416	ASP	N-CA-C	6.33	119.45	109.39
1	C	213	ILE	N-CA-C	6.32	122.49	109.34
1	D	414	THR	N-CA-C	6.32	120.48	113.21
1	E	213	ILE	N-CA-C	6.28	122.40	109.34
1	E	414	THR	N-CA-C	6.23	120.38	113.21
1	D	213	ILE	N-CA-C	6.22	122.28	109.34
1	B	213	ILE	N-CA-C	6.21	122.26	109.34
1	C	414	THR	N-CA-C	6.20	120.34	113.21
1	E	416	ASP	N-CA-C	6.19	119.23	109.39
1	A	213	ILE	N-CA-C	6.17	122.17	109.34
1	E	689	LYS	N-CA-C	6.16	117.90	108.42
1	A	99	TYR	N-CA-C	6.08	118.87	111.82
1	D	416	ASP	N-CA-C	6.03	118.97	109.39
1	C	581	TRP	N-CA-C	6.02	119.09	111.69
1	C	689	LYS	N-CA-C	6.01	117.98	108.79
1	F	416	ASP	N-CA-C	5.99	118.91	109.39
1	F	411	PHE	N-CA-C	-5.97	101.69	110.52
1	D	689	LYS	N-CA-C	5.93	117.86	108.79
1	B	689	LYS	N-CA-C	5.87	117.78	108.79
1	B	99	TYR	N-CA-C	5.87	118.62	111.82
1	A	416	ASP	N-CA-C	5.86	118.71	109.39
1	E	99	TYR	N-CA-C	5.82	118.57	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	99	TYR	N-CA-C	5.75	118.49	111.82
1	B	128	VAL	N-CA-C	5.72	114.85	106.55
1	C	411	PHE	N-CA-C	-5.71	102.07	110.52
1	E	128	VAL	N-CA-C	5.68	114.79	106.55
1	D	411	PHE	N-CA-C	-5.63	102.18	110.52
1	B	411	PHE	N-CA-C	-5.60	102.23	110.52
1	C	99	TYR	N-CA-C	5.57	118.29	111.82
1	B	339	SER	N-CA-C	5.54	117.32	111.28
1	D	128	VAL	N-CA-C	5.54	114.58	106.55
1	F	128	VAL	N-CA-C	5.53	114.57	106.55
1	D	409	TYR	N-CA-C	5.49	121.75	114.12
1	A	411	PHE	N-CA-C	-5.48	102.42	110.52
1	D	99	TYR	N-CA-C	5.47	118.16	111.82
1	C	128	VAL	N-CA-C	5.40	114.38	106.55
1	D	19	GLU	CA-C-N	5.40	125.34	119.78
1	D	19	GLU	C-N-CA	5.40	125.34	119.78
1	E	409	TYR	N-CA-C	5.40	121.62	114.12
1	E	411	PHE	N-CA-C	-5.39	102.54	110.52
1	B	409	TYR	N-CA-C	5.34	121.54	114.12
1	A	189	GLN	N-CA-C	5.31	117.76	111.33
1	B	19	GLU	CA-C-N	5.31	125.25	119.78
1	B	19	GLU	C-N-CA	5.31	125.25	119.78
1	F	409	TYR	N-CA-C	5.29	121.14	114.31
1	C	409	TYR	N-CA-C	5.28	121.46	114.12
1	F	556	LEU	N-CA-C	5.26	117.54	109.07
1	D	581	TRP	N-CA-C	5.25	119.75	112.45
1	B	556	LEU	N-CA-C	5.23	117.50	109.07
1	D	40	GLU	N-CA-C	-5.20	106.44	112.89
1	A	409	TYR	N-CA-C	5.16	121.30	114.12
1	F	581	TRP	N-CA-C	5.15	118.72	112.23
1	E	483	THR	N-CA-C	5.13	117.27	111.11
1	E	463	LEU	N-CA-C	-5.13	105.77	111.36
1	F	19	GLU	CA-C-N	5.12	125.06	119.78
1	F	19	GLU	C-N-CA	5.12	125.06	119.78
1	A	483	THR	N-CA-C	5.12	117.25	111.11
1	A	556	LEU	N-CA-C	5.11	117.30	109.07
1	C	483	THR	N-CA-C	5.11	117.24	111.11
1	C	556	LEU	N-CA-C	5.08	117.25	109.07
1	C	19	GLU	CA-C-N	5.07	125.01	119.78
1	C	19	GLU	C-N-CA	5.07	125.01	119.78
1	D	556	LEU	N-CA-C	5.07	117.24	109.07
1	A	19	GLU	CA-C-N	5.01	124.94	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	GLU	C-N-CA	5.01	124.94	119.78
1	E	19	GLU	CA-C-N	5.01	124.94	119.78
1	E	19	GLU	C-N-CA	5.01	124.94	119.78

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	5683	0	5651	124	0
1	B	5683	0	5651	129	0
1	C	5683	0	5651	131	0
1	D	5683	0	5653	124	0
1	E	5683	0	5651	113	0
1	F	5683	0	5651	126	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
3	A	83	0	0	0	0
3	B	74	0	0	0	0
3	C	96	0	0	3	0
3	D	103	0	0	0	0
3	E	127	0	0	1	0
3	F	132	0	0	1	0
All	All	34797	0	33986	693	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 10.

All (693) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:GLU:HG3	1:F:332:GLU:HG3	1.32	1.11
1:B:332:GLU:HG3	1:D:332:GLU:HG3	1.40	1.04
1:F:564:LYS:HE3	1:F:564:LYS:H	1.23	1.04
1:A:564:LYS:HE3	1:A:564:LYS:H	1.24	1.02
1:E:564:LYS:HE3	1:E:564:LYS:H	1.25	1.01
1:D:564:LYS:HE3	1:D:564:LYS:H	1.25	1.00
1:C:564:LYS:HE3	1:C:564:LYS:H	1.23	0.99
1:E:299:ARG:HG3	1:E:382:ALA:HB2	1.44	0.98
1:B:564:LYS:HE3	1:B:564:LYS:H	1.25	0.96
1:A:332:GLU:HG3	1:E:332:GLU:HG3	1.45	0.95
1:C:596:HIS:HD2	1:C:598:LEU:H	1.16	0.93
1:C:278:LEU:HD21	1:F:258:GLN:HG3	1.50	0.93
1:A:36:LYS:HG2	1:A:41:LEU:HD13	1.52	0.89
1:C:666:LYS:HA	1:C:666:LYS:HE3	1.54	0.88
1:C:299:ARG:HG3	1:C:382:ALA:HB2	1.53	0.87
1:D:299:ARG:HG3	1:D:382:ALA:HB2	1.54	0.87
1:F:31:LYS:HG3	1:F:32:ILE:H	1.37	0.87
1:B:258:GLN:HG3	1:D:278:LEU:HD21	1.55	0.86
1:A:596:HIS:HD2	1:A:598:LEU:H	1.24	0.85
1:A:163:THR:HG22	1:A:168:LYS:HD3	1.58	0.85
1:B:163:THR:HG22	1:B:168:LYS:HD3	1.58	0.85
1:C:163:THR:HG22	1:C:168:LYS:HD3	1.59	0.85
1:F:163:THR:HG22	1:F:168:LYS:HD3	1.56	0.85
1:F:4:LEU:HD23	1:F:4:LEU:H	1.42	0.85
1:A:258:GLN:HG3	1:E:278:LEU:HD21	1.56	0.85
1:E:163:THR:HG22	1:E:168:LYS:HD3	1.57	0.84
1:D:163:THR:HG22	1:D:168:LYS:HD3	1.57	0.84
1:C:258:GLN:HG3	1:F:278:LEU:HD21	1.62	0.81
1:B:278:LEU:HD21	1:D:258:GLN:HG3	1.62	0.80
1:B:337:LEU:HD21	1:D:337:LEU:HD21	1.63	0.80
1:A:299:ARG:HG3	1:A:382:ALA:HB2	1.62	0.79
1:E:334:ARG:O	1:E:338:SER:HB3	1.83	0.79
1:D:596:HIS:HD2	1:D:598:LEU:H	1.32	0.77
1:C:564:LYS:HE3	1:C:564:LYS:N	2.00	0.76
1:F:31:LYS:O	1:F:32:ILE:HG12	1.85	0.75
1:F:299:ARG:CG	1:F:382:ALA:HB2	2.17	0.75
1:F:687:ARG:HH11	1:F:687:ARG:HG3	1.50	0.75
1:F:564:LYS:HE3	1:F:564:LYS:N	1.99	0.75
1:B:564:LYS:HE3	1:B:564:LYS:N	2.01	0.74
1:A:278:LEU:HD21	1:E:258:GLN:HG3	1.70	0.74
1:C:258:GLN:HG2	1:F:268:GLY:H	1.52	0.74
1:B:268:GLY:H	1:D:258:GLN:HG2	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:O	1:A:338:SER:HB3	1.88	0.73
1:D:564:LYS:HE3	1:D:564:LYS:N	2.02	0.73
1:C:36:LYS:HA	1:C:40:GLU:OE1	1.89	0.72
1:A:564:LYS:HE3	1:A:564:LYS:N	2.00	0.72
1:B:258:GLN:CG	1:D:278:LEU:HD21	2.18	0.72
1:D:596:HIS:CD2	1:D:598:LEU:H	2.08	0.72
1:E:564:LYS:HE3	1:E:564:LYS:N	2.01	0.71
1:F:299:ARG:HG3	1:F:382:ALA:HB2	1.71	0.71
1:C:651:ILE:HD13	1:C:692:LEU:HD21	1.72	0.71
1:F:6:ILE:HD11	1:F:38:LEU:HD13	1.72	0.71
1:C:278:LEU:HD21	1:F:258:GLN:CG	2.21	0.71
1:D:651:ILE:HD13	1:D:692:LEU:HD21	1.72	0.71
1:F:614:GLU:HG2	1:F:648:LYS:HB3	1.73	0.70
1:B:299:ARG:HG3	1:B:382:ALA:HB2	1.74	0.70
1:A:596:HIS:CD2	1:A:598:LEU:H	2.10	0.69
1:A:686:ILE:HD13	1:A:690:ILE:HD11	1.75	0.69
1:F:4:LEU:HD23	1:F:4:LEU:N	2.06	0.69
1:C:299:ARG:CG	1:C:382:ALA:HB2	2.22	0.69
1:A:614:GLU:HG2	1:A:648:LYS:HB3	1.75	0.69
1:B:686:ILE:HD13	1:B:690:ILE:HD11	1.74	0.69
1:B:299:ARG:CG	1:B:382:ALA:HB2	2.24	0.68
1:E:596:HIS:HD2	1:E:598:LEU:H	1.42	0.68
1:E:8:GLU:O	1:E:9:ASN:HB2	1.93	0.68
1:F:163:THR:CG2	1:F:168:LYS:HD3	2.25	0.67
1:D:614:GLU:HG2	1:D:648:LYS:HB3	1.75	0.67
1:F:686:ILE:HD13	1:F:690:ILE:HD11	1.76	0.67
1:C:234:LYS:O	1:C:238:GLU:HG3	1.94	0.67
1:C:8:GLU:HB2	1:C:34:SER:HB3	1.77	0.67
1:E:285:PRO:HG2	1:E:288:THR:CG2	2.25	0.67
1:C:686:ILE:HD13	1:C:690:ILE:HD11	1.76	0.66
1:D:686:ILE:HD13	1:D:690:ILE:HD11	1.77	0.66
1:B:285:PRO:HG2	1:B:288:THR:CG2	2.26	0.66
1:A:9:ASN:HD21	1:A:29:GLU:HB2	1.61	0.66
1:C:285:PRO:HG2	1:C:288:THR:CG2	2.25	0.66
1:F:31:LYS:HG3	1:F:32:ILE:N	2.11	0.66
1:D:285:PRO:HG2	1:D:288:THR:CG2	2.26	0.65
1:F:87:ASP:O	1:F:348:ARG:HD3	1.96	0.65
1:A:163:THR:CG2	1:A:168:LYS:HD3	2.25	0.65
1:A:285:PRO:HG2	1:A:288:THR:CG2	2.26	0.65
1:B:185:SER:OG	1:B:212:ASP:HB3	1.96	0.65
1:E:686:ILE:HD13	1:E:690:ILE:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:614:GLU:HG2	1:C:648:LYS:HB3	1.79	0.65
1:A:185:SER:OG	1:A:212:ASP:HB3	1.97	0.65
1:A:258:GLN:CG	1:E:278:LEU:HD21	2.25	0.65
1:F:334:ARG:O	1:F:338:SER:HB3	1.96	0.65
1:D:87:ASP:O	1:D:348:ARG:HD3	1.94	0.65
1:E:651:ILE:HD13	1:E:692:LEU:HD21	1.79	0.65
1:E:87:ASP:O	1:E:348:ARG:HD3	1.97	0.65
1:C:87:ASP:O	1:C:348:ARG:HD3	1.96	0.64
1:D:163:THR:CG2	1:D:168:LYS:HD3	2.26	0.64
1:C:564:LYS:H	1:C:564:LYS:CE	2.07	0.64
1:D:564:LYS:H	1:D:564:LYS:CE	2.07	0.64
1:E:163:THR:CG2	1:E:168:LYS:HD3	2.26	0.64
1:E:614:GLU:HG2	1:E:648:LYS:HB3	1.78	0.64
1:A:651:ILE:HD13	1:A:692:LEU:HD21	1.80	0.64
1:F:596:HIS:HD2	1:F:598:LEU:H	1.45	0.64
1:F:651:ILE:HD13	1:F:692:LEU:HD21	1.78	0.64
1:A:564:LYS:H	1:A:564:LYS:CE	2.07	0.64
1:A:87:ASP:O	1:A:348:ARG:HD3	1.98	0.64
1:C:596:HIS:CD2	1:C:598:LEU:H	2.06	0.64
1:B:87:ASP:O	1:B:348:ARG:HD3	1.98	0.64
1:C:332:GLU:HG3	1:F:332:GLU:CG	2.21	0.64
1:D:334:ARG:O	1:D:338:SER:HB3	1.97	0.64
1:A:286:GLY:O	1:A:288:THR:HG23	1.98	0.63
1:D:666:LYS:HE3	1:D:666:LYS:HA	1.81	0.63
1:B:163:THR:CG2	1:B:168:LYS:HD3	2.27	0.63
1:D:452:ARG:HD3	1:D:484:ASP:O	1.98	0.63
1:B:286:GLY:O	1:B:288:THR:HG23	1.99	0.63
1:D:627:ASP:O	1:D:628:ASN:HB3	1.97	0.63
1:E:286:GLY:O	1:E:288:THR:HG23	1.99	0.63
1:B:610:LEU:HD11	1:B:616:ILE:HD11	1.80	0.63
1:E:564:LYS:H	1:E:564:LYS:CE	2.09	0.63
1:B:334:ARG:O	1:B:338:SER:HB3	1.99	0.63
1:D:299:ARG:CG	1:D:382:ALA:HB2	2.29	0.63
1:E:3:ILE:HB	1:E:18:GLY:HA2	1.80	0.63
1:E:4:LEU:HD23	1:E:17:ILE:HD13	1.80	0.63
1:F:285:PRO:HG2	1:F:288:THR:CG2	2.28	0.63
1:B:452:ARG:HD3	1:B:484:ASP:O	1.99	0.63
1:C:332:GLU:CG	1:F:332:GLU:HG3	2.20	0.63
1:D:9:ASN:OD1	1:D:30:GLN:HB2	1.98	0.62
1:B:13:TYR:CZ	1:B:36:LYS:HD2	2.34	0.62
1:C:575:GLY:O	1:C:588:GLY:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:GLY:O	1:F:288:THR:HG23	1.99	0.62
1:A:686:ILE:CD1	1:A:690:ILE:HD11	2.29	0.62
1:E:452:ARG:HD3	1:E:484:ASP:O	1.99	0.62
1:F:627:ASP:O	1:F:628:ASN:HB3	1.99	0.62
1:E:185:SER:OG	1:E:212:ASP:HB3	1.99	0.62
1:F:596:HIS:CD2	1:F:598:LEU:H	2.18	0.62
1:C:163:THR:CG2	1:C:168:LYS:HD3	2.28	0.62
1:C:258:GLN:HG2	1:F:268:GLY:N	2.14	0.62
1:C:286:GLY:O	1:C:288:THR:HG23	1.98	0.62
1:C:452:ARG:HD3	1:C:484:ASP:O	1.99	0.62
1:D:286:GLY:O	1:D:288:THR:HG23	1.99	0.61
1:A:452:ARG:HD3	1:A:484:ASP:O	1.99	0.61
1:E:299:ARG:CG	1:E:382:ALA:HB2	2.24	0.61
1:A:627:ASP:O	1:A:628:ASN:HB3	2.01	0.61
1:B:268:GLY:N	1:D:258:GLN:HG2	2.16	0.61
1:B:614:GLU:HG2	1:B:648:LYS:HB3	1.82	0.61
1:B:627:ASP:O	1:B:628:ASN:HB3	2.00	0.61
1:C:185:SER:OG	1:C:212:ASP:HB3	2.00	0.61
1:E:575:GLY:O	1:E:588:GLY:N	2.33	0.61
1:A:6:ILE:HD11	1:A:38:LEU:CD1	2.31	0.61
1:D:8:GLU:O	1:D:9:ASN:HB2	2.01	0.61
1:F:620:GLU:HG2	1:F:634:SER:HA	1.83	0.61
1:C:59:ASP:OD2	1:C:109:LYS:HD2	2.01	0.61
1:C:211:LEU:HD22	1:C:246:LEU:HD11	1.83	0.61
1:C:340:LEU:C	1:C:342:VAL:H	2.09	0.61
1:F:452:ARG:HD3	1:F:484:ASP:O	2.00	0.61
1:A:575:GLY:O	1:A:588:GLY:N	2.34	0.60
1:B:575:GLY:O	1:B:588:GLY:N	2.33	0.60
1:E:211:LEU:HD22	1:E:246:LEU:HD11	1.83	0.60
1:D:185:SER:OG	1:D:212:ASP:HB3	2.00	0.60
1:E:620:GLU:HG2	1:E:634:SER:HA	1.83	0.60
1:E:670:VAL:CG1	1:E:678:TYR:HB3	2.31	0.60
1:B:651:ILE:HD13	1:B:692:LEU:HD21	1.83	0.60
1:B:686:ILE:CD1	1:B:690:ILE:HD11	2.30	0.60
1:F:342:VAL:HG22	1:F:343:GLN:H	1.65	0.60
1:F:687:ARG:HG3	1:F:687:ARG:NH1	2.16	0.60
1:B:258:GLN:HG2	1:D:268:GLY:H	1.67	0.60
1:D:575:GLY:O	1:D:588:GLY:N	2.33	0.60
1:B:278:LEU:HD21	1:D:258:GLN:CG	2.30	0.60
1:F:6:ILE:HD11	1:F:38:LEU:CD1	2.32	0.60
1:A:339:SER:CB	1:F:339:SER:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:PHE:O	1:F:299:ARG:HD3	2.02	0.59
1:E:4:LEU:HD22	1:E:5:LYS:N	2.18	0.59
1:F:575:GLY:O	1:F:588:GLY:N	2.34	0.59
1:E:627:ASP:O	1:E:628:ASN:HB3	2.02	0.59
1:F:185:SER:OG	1:F:212:ASP:HB3	2.03	0.59
1:F:323:GLU:N	1:F:324:PRO:HA	2.18	0.59
1:A:211:LEU:HD22	1:A:246:LEU:HD11	1.85	0.59
1:D:269:LYS:HB3	1:D:298:THR:OG1	2.02	0.59
1:F:299:ARG:HG2	1:F:382:ALA:HB2	1.85	0.59
1:A:663:ASP:C	1:A:665:SER:H	2.11	0.59
1:B:59:ASP:OD2	1:B:109:LYS:HD2	2.03	0.59
1:B:323:GLU:N	1:B:324:PRO:HA	2.18	0.59
1:A:59:ASP:OD2	1:A:109:LYS:HD2	2.03	0.58
1:B:225:HIS:CE1	1:B:227:TYR:HB2	2.37	0.58
1:C:269:LYS:HB3	1:C:298:THR:OG1	2.03	0.58
1:C:337:LEU:HD21	1:F:337:LEU:HD21	1.85	0.58
1:E:610:LEU:HD11	1:E:616:ILE:HD11	1.85	0.58
1:C:627:ASP:O	1:C:628:ASN:HB3	2.03	0.58
1:F:340:LEU:HD12	1:F:341:PRO:HD2	1.86	0.58
1:A:9:ASN:HD21	1:A:10:LYS:HZ2	1.50	0.58
1:B:211:LEU:HD22	1:B:246:LEU:HD11	1.84	0.58
1:F:578:TYR:CE1	1:F:583:GLY:HA2	2.38	0.58
1:D:610:LEU:HD11	1:D:616:ILE:HD11	1.85	0.58
1:C:686:ILE:CD1	1:C:690:ILE:HD11	2.34	0.57
1:D:59:ASP:OD2	1:D:109:LYS:HD2	2.03	0.57
1:D:261:SER:HB3	1:D:262:PRO:HD3	1.86	0.57
1:E:634:SER:O	1:E:635:SER:C	2.46	0.57
1:E:323:GLU:N	1:E:324:PRO:HA	2.19	0.57
1:E:596:HIS:CD2	1:E:598:LEU:H	2.22	0.57
1:D:323:GLU:N	1:D:324:PRO:HA	2.19	0.57
1:B:36:LYS:HA	1:B:40:GLU:OE1	2.05	0.57
1:D:26:PHE:HB3	1:D:165:LEU:HD22	1.85	0.57
1:E:59:ASP:OD2	1:E:109:LYS:HD2	2.04	0.57
1:F:610:LEU:HD11	1:F:616:ILE:HD11	1.87	0.57
1:B:670:VAL:HG11	1:B:678:TYR:HB3	1.87	0.57
1:C:323:GLU:N	1:C:324:PRO:HA	2.19	0.56
1:F:59:ASP:OD2	1:F:109:LYS:HD2	2.04	0.56
1:B:26:PHE:HB3	1:B:165:LEU:HD22	1.87	0.56
1:B:564:LYS:H	1:B:564:LYS:CE	2.09	0.56
1:F:564:LYS:N	1:F:564:LYS:CE	2.68	0.56
1:A:261:SER:HB3	1:A:262:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:GLU:HG2	1:C:137:ILE:HG12	1.88	0.56
1:D:130:LEU:HD22	1:E:483:THR:HG22	1.88	0.56
1:D:666:LYS:CE	1:D:667:GLU:H	2.18	0.56
1:F:564:LYS:H	1:F:564:LYS:CE	2.07	0.56
1:B:661:ILE:HG12	1:B:667:GLU:HG3	1.86	0.56
1:C:26:PHE:HB3	1:C:165:LEU:HD22	1.86	0.56
1:C:258:GLN:CG	1:F:278:LEU:HD21	2.34	0.56
1:F:3:ILE:HG23	1:F:18:GLY:HA2	1.86	0.56
1:F:26:PHE:HB3	1:F:165:LEU:HD22	1.88	0.56
1:D:564:LYS:N	1:D:564:LYS:CE	2.68	0.56
1:C:334:ARG:O	1:C:338:SER:HB3	2.05	0.56
1:C:499:GLU:O	1:C:503:GLU:HG3	2.05	0.56
1:C:610:LEU:HD11	1:C:616:ILE:HD11	1.88	0.56
1:E:670:VAL:HG11	1:E:678:TYR:HB3	1.88	0.56
1:C:557:LEU:C	1:C:557:LEU:HD23	2.30	0.56
1:E:261:SER:HB3	1:E:262:PRO:HD3	1.87	0.56
1:D:211:LEU:HD22	1:D:246:LEU:HD11	1.87	0.56
1:F:686:ILE:CD1	1:F:690:ILE:HD11	2.35	0.56
1:A:323:GLU:N	1:A:324:PRO:HA	2.20	0.56
1:A:299:ARG:CG	1:A:382:ALA:HB2	2.35	0.56
1:C:634:SER:O	1:C:635:SER:C	2.49	0.56
1:E:9:ASN:ND2	1:E:10:LYS:HD3	2.21	0.55
1:F:261:SER:HB3	1:F:262:PRO:HD3	1.87	0.55
1:A:557:LEU:HD23	1:A:557:LEU:C	2.32	0.55
1:B:640:PHE:CE2	1:B:644:ILE:HD11	2.41	0.55
1:B:499:GLU:O	1:B:503:GLU:HG3	2.06	0.55
1:D:669:GLN:HE21	1:D:669:GLN:CA	2.18	0.55
1:C:261:SER:HB3	1:C:262:PRO:HD3	1.89	0.55
1:E:26:PHE:HB3	1:E:165:LEU:HD22	1.87	0.55
1:A:55:GLU:HG2	1:A:137:ILE:HG12	1.89	0.55
1:A:268:GLY:H	1:E:258:GLN:HG2	1.71	0.55
1:A:285:PRO:HG2	1:A:288:THR:HG21	1.89	0.55
1:A:564:LYS:N	1:A:564:LYS:CE	2.68	0.55
1:B:664:ASP:OD2	1:B:689:LYS:HE2	2.06	0.55
1:F:55:GLU:HG2	1:F:137:ILE:HG12	1.88	0.55
1:F:640:PHE:CE2	1:F:644:ILE:HD11	2.42	0.55
1:B:670:VAL:CG1	1:B:678:TYR:HB3	2.37	0.55
1:E:487:ASP:OD1	3:E:2054:HOH:O	2.18	0.55
1:E:564:LYS:N	1:E:564:LYS:CE	2.69	0.55
1:F:211:LEU:HD22	1:F:246:LEU:HD11	1.87	0.55
1:F:557:LEU:HD23	1:F:557:LEU:C	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:HB	1:A:18:GLY:HA2	1.88	0.55
1:B:261:SER:HB3	1:B:262:PRO:HD3	1.89	0.55
1:B:557:LEU:C	1:B:557:LEU:HD23	2.31	0.55
1:C:285:PRO:HG2	1:C:288:THR:HG21	1.88	0.55
1:D:257:ASP:HB3	1:D:260:TYR:CB	2.37	0.54
1:D:686:ILE:CD1	1:D:690:ILE:HD11	2.36	0.54
1:E:686:ILE:CD1	1:E:690:ILE:HD11	2.37	0.54
1:B:596:HIS:CD2	1:B:598:LEU:H	2.25	0.54
1:D:499:GLU:O	1:D:503:GLU:HG3	2.07	0.54
1:E:557:LEU:C	1:E:557:LEU:HD23	2.33	0.54
1:E:635:SER:OG	1:E:636:ASN:N	2.41	0.54
1:A:26:PHE:HB3	1:A:165:LEU:HD22	1.89	0.54
1:A:181:ILE:HG21	1:A:199:MET:HE2	1.90	0.54
1:C:664:ASP:O	1:C:665:SER:HB3	2.06	0.54
1:E:237:ASP:O	1:E:241:LYS:HG3	2.08	0.54
1:B:13:TYR:OH	1:B:36:LYS:HD2	2.08	0.54
1:D:182:SER:HB2	1:D:210:PHE:HB2	1.90	0.54
1:C:564:LYS:N	1:C:564:LYS:CE	2.68	0.54
1:E:234:LYS:O	1:E:238:GLU:HG3	2.07	0.54
1:A:340:LEU:C	1:A:342:VAL:H	2.15	0.54
1:A:499:GLU:O	1:A:503:GLU:HG3	2.08	0.54
1:B:285:PRO:HG2	1:B:288:THR:HG21	1.90	0.54
1:E:55:GLU:HG2	1:E:137:ILE:HG12	1.90	0.54
1:E:285:PRO:HG2	1:E:288:THR:HG21	1.89	0.54
1:A:278:LEU:HD21	1:E:258:GLN:CG	2.38	0.53
1:D:586:ILE:N	1:D:586:ILE:HD12	2.23	0.53
1:A:9:ASN:ND2	1:A:29:GLU:HB2	2.23	0.53
1:E:687:ARG:HG2	1:E:687:ARG:HH11	1.73	0.53
1:F:257:ASP:HB3	1:F:260:TYR:CB	2.39	0.53
1:A:640:PHE:CE2	1:A:644:ILE:HD11	2.43	0.53
1:D:285:PRO:HG2	1:D:288:THR:HG21	1.88	0.53
1:B:578:TYR:CE1	1:B:583:GLY:HA2	2.43	0.53
1:D:557:LEU:HD23	1:D:557:LEU:C	2.33	0.53
1:A:225:HIS:CE1	1:A:227:TYR:HB2	2.44	0.53
1:A:337:LEU:HD21	1:E:337:LEU:HD21	1.90	0.53
1:A:483:THR:HG22	1:C:130:LEU:HD22	1.90	0.53
1:A:578:TYR:CE1	1:A:583:GLY:HA2	2.43	0.53
1:C:640:PHE:CE2	1:C:644:ILE:HD11	2.43	0.53
1:D:29:GLU:O	1:D:30:GLN:HG2	2.09	0.53
1:F:285:PRO:HG2	1:F:288:THR:HG21	1.90	0.53
1:B:55:GLU:HG2	1:B:137:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:ARG:HA	1:A:687:ARG:HH11	1.73	0.53
1:C:257:ASP:HB3	1:C:260:TYR:CB	2.39	0.53
1:E:499:GLU:O	1:E:503:GLU:HG3	2.09	0.53
1:C:339:SER:O	1:C:340:LEU:HD22	2.09	0.53
1:F:31:LYS:C	1:F:32:ILE:HG23	2.32	0.53
1:F:499:GLU:O	1:F:503:GLU:HG3	2.09	0.53
1:A:664:ASP:OD1	1:A:689:LYS:HE2	2.09	0.53
1:E:257:ASP:HB3	1:E:260:TYR:CB	2.39	0.53
1:D:8:GLU:HB2	1:D:34:SER:HB2	1.92	0.52
1:B:564:LYS:N	1:B:564:LYS:CE	2.69	0.52
1:D:234:LYS:O	1:D:238:GLU:HG3	2.09	0.52
1:A:634:SER:O	1:A:635:SER:C	2.52	0.52
1:B:257:ASP:HB3	1:B:260:TYR:CB	2.39	0.52
1:C:175:TRP:CE3	1:C:245:LYS:HG3	2.45	0.52
1:F:419:PRO:HG3	1:F:448:GLY:HA3	1.91	0.52
1:B:258:GLN:CD	1:D:278:LEU:HD21	2.35	0.52
1:A:257:ASP:HB3	1:A:260:TYR:CB	2.40	0.52
1:D:652:THR:HA	1:D:676:ASN:O	2.09	0.52
1:A:610:LEU:HD11	1:A:616:ILE:HD11	1.91	0.51
1:E:4:LEU:HD22	1:E:5:LYS:H	1.75	0.51
1:D:55:GLU:HG2	1:D:137:ILE:HG12	1.92	0.51
1:A:9:ASN:ND2	1:A:10:LYS:HZ2	2.09	0.51
1:E:175:TRP:CE3	1:E:245:LYS:HG3	2.46	0.51
1:A:130:LEU:HD22	1:B:483:THR:HG22	1.93	0.50
1:A:502:LYS:O	1:A:506:GLU:HG3	2.11	0.50
1:C:182:SER:HB2	1:C:210:PHE:HB2	1.93	0.50
1:A:154:ARG:HB2	1:A:157:ASP:OD2	2.10	0.50
1:B:181:ILE:HG21	1:B:199:MET:HE2	1.94	0.50
1:F:182:SER:HB2	1:F:210:PHE:HB2	1.93	0.50
1:D:634:SER:O	1:D:635:SER:C	2.54	0.50
1:E:181:ILE:HG21	1:E:199:MET:HE2	1.92	0.50
1:A:182:SER:HB2	1:A:210:PHE:HB2	1.92	0.50
1:A:268:GLY:N	1:E:258:GLN:HG2	2.27	0.50
1:A:666:LYS:HD3	1:A:668:ILE:HD11	1.94	0.50
1:B:8:GLU:O	1:B:32:ILE:HB	2.11	0.50
1:E:578:TYR:CE1	1:E:583:GLY:HA2	2.46	0.50
1:F:664:ASP:OD2	1:F:689:LYS:HE2	2.12	0.50
1:C:510:LYS:HA	1:C:611:GLU:CB	2.41	0.50
1:F:237:ASP:O	1:F:241:LYS:HG3	2.12	0.50
1:B:502:LYS:O	1:B:506:GLU:HG3	2.12	0.50
1:D:640:PHE:CE2	1:D:644:ILE:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:PRO:HG3	1:B:448:GLY:HA3	1.93	0.50
1:E:555:TYR:HB3	1:E:606:SER:OG	2.12	0.50
1:A:659:LYS:HA	1:A:670:VAL:HG23	1.94	0.50
1:D:340:LEU:HD12	1:D:341:PRO:HD2	1.94	0.50
1:F:175:TRP:CE3	1:F:245:LYS:HG3	2.46	0.50
1:C:181:ILE:HG21	1:C:199:MET:HE2	1.93	0.49
1:D:175:TRP:CE3	1:D:245:LYS:HG3	2.48	0.49
1:D:257:ASP:HB3	1:D:260:TYR:HB2	1.94	0.49
1:F:342:VAL:HG22	1:F:343:GLN:N	2.27	0.49
1:A:11:GLY:HA3	1:A:161:LYS:HE2	1.94	0.49
1:E:182:SER:HB2	1:E:210:PHE:HB2	1.92	0.49
1:A:419:PRO:HG3	1:A:448:GLY:HA3	1.95	0.49
1:A:652:THR:HA	1:A:676:ASN:O	2.13	0.49
1:D:666:LYS:HE3	1:D:667:GLU:H	1.75	0.49
1:D:181:ILE:HG21	1:D:199:MET:HE2	1.93	0.49
1:E:652:THR:HA	1:E:676:ASN:O	2.13	0.49
1:C:13:TYR:CZ	1:C:36:LYS:HD2	2.48	0.49
1:F:181:ILE:HG21	1:F:199:MET:HE2	1.94	0.49
1:B:225:HIS:HE1	1:B:227:TYR:HB2	1.77	0.49
1:F:670:VAL:HG22	1:F:680:ALA:HB2	1.95	0.49
1:F:425:LYS:HG3	3:F:2093:HOH:O	2.13	0.49
1:A:9:ASN:OD1	1:A:10:LYS:HG3	2.13	0.48
1:A:175:TRP:CE3	1:A:245:LYS:HG3	2.47	0.48
1:A:225:HIS:HE1	1:A:227:TYR:HB2	1.76	0.48
1:A:9:ASN:ND2	1:A:10:LYS:NZ	2.62	0.48
1:B:182:SER:HB2	1:B:210:PHE:HB2	1.95	0.48
1:C:462:ASP:HB2	3:C:2091:HOH:O	2.13	0.48
1:D:555:TYR:HB3	1:D:606:SER:OG	2.13	0.48
1:F:257:ASP:HB3	1:F:260:TYR:HB2	1.94	0.48
1:C:154:ARG:HB2	1:C:157:ASP:OD2	2.13	0.48
1:C:665:SER:O	1:C:666:LYS:C	2.56	0.48
1:D:183:ARG:O	1:D:185:SER:HA	2.13	0.48
1:F:31:LYS:O	1:F:32:ILE:HG23	2.13	0.48
1:F:555:TYR:HB3	1:F:606:SER:OG	2.13	0.48
1:B:51:LYS:HB2	1:B:51:LYS:NZ	2.28	0.48
1:B:285:PRO:HG2	1:B:288:THR:HG22	1.96	0.48
1:F:31:LYS:CG	1:F:32:ILE:H	2.08	0.48
1:A:672:LYS:HD2	1:A:678:TYR:CE1	2.48	0.48
1:A:51:LYS:HB2	1:A:51:LYS:NZ	2.28	0.48
1:B:652:THR:HA	1:B:676:ASN:O	2.14	0.48
1:E:659:LYS:NZ	1:E:659:LYS:HB3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:TRP:CE3	1:B:245:LYS:HG3	2.49	0.48
1:C:140:ILE:HD12	1:C:140:ILE:N	2.29	0.48
1:C:156:GLU:O	1:C:160:GLU:HG3	2.13	0.48
1:C:215:TYR:CD1	1:C:215:TYR:C	2.92	0.48
1:E:285:PRO:HG2	1:E:288:THR:HG22	1.94	0.48
1:D:133:TYR:HB3	1:E:187:TYR:O	2.13	0.48
1:E:183:ARG:O	1:E:185:SER:HA	2.14	0.48
1:E:502:LYS:O	1:E:506:GLU:HG3	2.14	0.48
1:B:183:ARG:HG2	1:B:184:TYR:N	2.29	0.47
1:B:257:ASP:HB3	1:B:260:TYR:HB2	1.95	0.47
1:C:285:PRO:HG2	1:C:288:THR:HG22	1.96	0.47
1:E:347:ASP:O	1:E:350:VAL:HG12	2.14	0.47
1:A:258:GLN:CD	1:E:278:LEU:HD21	2.39	0.47
1:C:555:TYR:HB3	1:C:606:SER:OG	2.14	0.47
1:F:4:LEU:N	1:F:4:LEU:CD2	2.76	0.47
1:A:183:ARG:HG2	1:A:184:TYR:N	2.30	0.47
1:C:257:ASP:HB3	1:C:260:TYR:HB2	1.96	0.47
1:C:510:LYS:HA	1:C:611:GLU:HB3	1.97	0.47
1:C:666:LYS:HA	1:C:666:LYS:CE	2.36	0.47
1:B:215:TYR:CD1	1:B:215:TYR:C	2.92	0.47
1:B:347:ASP:O	1:B:350:VAL:HG12	2.15	0.47
1:F:51:LYS:HB2	1:F:51:LYS:NZ	2.30	0.47
1:A:340:LEU:HD13	1:A:341:PRO:HD2	1.95	0.47
1:B:663:ASP:C	1:B:665:SER:H	2.22	0.47
1:C:36:LYS:HD3	1:C:41:LEU:HD13	1.97	0.47
1:C:258:GLN:OE1	1:F:270:PHE:N	2.32	0.47
1:C:661:ILE:CG2	1:C:665:SER:H	2.28	0.47
1:D:502:LYS:O	1:D:506:GLU:HG3	2.14	0.47
1:E:257:ASP:HB3	1:E:260:TYR:HB2	1.96	0.47
1:F:3:ILE:O	1:F:3:ILE:HG12	2.15	0.47
1:B:9:ASN:C	1:B:10:LYS:HG2	2.40	0.47
1:B:183:ARG:O	1:B:185:SER:HA	2.15	0.47
1:C:652:THR:HA	1:C:676:ASN:O	2.14	0.47
1:D:215:TYR:CD1	1:D:215:TYR:C	2.92	0.47
1:D:682:ILE:HG22	1:D:684:GLN:HG2	1.96	0.47
1:F:419:PRO:HD2	1:F:457:ILE:HG23	1.96	0.47
1:D:545:ARG:HB2	1:E:494:PRO:HG3	1.97	0.47
1:E:215:TYR:CD1	1:E:215:TYR:C	2.92	0.47
1:A:297:ASP:OD1	1:A:298:THR:N	2.47	0.47
1:C:340:LEU:O	1:C:342:VAL:N	2.47	0.47
1:C:584:GLU:CD	1:C:586:ILE:HD11	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:LYS:NZ	1:D:51:LYS:HB2	2.29	0.47
1:A:257:ASP:HB3	1:A:260:TYR:HB2	1.97	0.47
1:B:242:ARG:HH11	1:B:242:ARG:HG3	1.80	0.47
1:C:51:LYS:HB2	1:C:51:LYS:NZ	2.30	0.47
1:C:419:PRO:HD2	1:C:457:ILE:HG23	1.97	0.47
1:C:665:SER:OG	1:C:666:LYS:N	2.45	0.47
1:C:96:ASP:OD1	1:C:97:PRO:HA	2.15	0.46
1:F:347:ASP:O	1:F:350:VAL:HG12	2.15	0.46
1:D:347:ASP:O	1:D:350:VAL:HG12	2.15	0.46
1:E:156:GLU:O	1:E:160:GLU:HG3	2.15	0.46
1:A:285:PRO:HG2	1:A:288:THR:HG22	1.97	0.46
1:B:156:GLU:O	1:B:160:GLU:HG3	2.15	0.46
1:D:669:GLN:HA	1:D:669:GLN:NE2	2.29	0.46
1:E:51:LYS:HB2	1:E:51:LYS:NZ	2.28	0.46
1:C:392:ARG:HD3	3:C:2094:HOH:O	2.15	0.46
1:B:94:TYR:CZ	1:C:452:ARG:HG2	2.51	0.46
1:D:419:PRO:HD2	1:D:457:ILE:HG23	1.97	0.46
1:E:215:TYR:HA	1:E:229:PHE:CE1	2.51	0.46
1:F:502:LYS:O	1:F:506:GLU:HG3	2.16	0.46
1:A:589:LYS:HD2	1:A:589:LYS:HA	1.79	0.46
1:C:502:LYS:O	1:C:506:GLU:HG3	2.14	0.46
1:A:332:GLU:HG3	1:E:332:GLU:CG	2.32	0.46
1:C:419:PRO:HG3	1:C:448:GLY:HA3	1.98	0.46
1:B:596:HIS:HD2	1:B:598:LEU:H	1.63	0.46
1:C:183:ARG:HG2	1:C:184:TYR:N	2.31	0.46
1:D:285:PRO:HG2	1:D:288:THR:HG22	1.96	0.46
1:F:652:THR:HA	1:F:676:ASN:O	2.16	0.46
1:A:347:ASP:O	1:A:350:VAL:HG12	2.16	0.46
1:C:278:LEU:HD21	1:F:258:GLN:CD	2.41	0.46
1:F:183:ARG:HG2	1:F:184:TYR:N	2.31	0.46
1:A:342:VAL:CG1	1:A:343:GLN:N	2.79	0.46
1:B:26:PHE:HB3	1:B:165:LEU:CD2	2.46	0.46
1:D:659:LYS:NZ	1:D:659:LYS:HB3	2.31	0.46
1:F:586:ILE:HD12	1:F:586:ILE:N	2.30	0.46
1:A:255:ARG:HG2	1:A:257:ASP:HB2	1.97	0.45
1:D:8:GLU:HG2	1:D:9:ASN:N	2.31	0.45
1:E:96:ASP:OD1	1:E:97:PRO:HA	2.16	0.45
1:F:4:LEU:HD12	1:F:38:LEU:HD21	1.98	0.45
1:F:5:LYS:HB2	1:F:5:LYS:NZ	2.30	0.45
1:B:237:ASP:O	1:B:241:LYS:HB2	2.17	0.45
1:C:347:ASP:O	1:C:350:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:ILE:HD13	1:C:692:LEU:CD2	2.44	0.45
1:C:682:ILE:HG22	1:C:684:GLN:HG2	1.98	0.45
1:D:96:ASP:OD1	1:D:97:PRO:HA	2.16	0.45
1:D:602:LEU:HD22	1:D:608:ILE:CD1	2.46	0.45
1:B:51:LYS:HB2	1:B:51:LYS:HZ2	1.81	0.45
1:D:156:GLU:O	1:D:160:GLU:HG3	2.17	0.45
1:F:555:TYR:HB3	1:F:606:SER:CB	2.46	0.45
1:B:293:PHE:O	1:B:299:ARG:HD3	2.16	0.45
1:D:669:GLN:HE21	1:D:669:GLN:HA	1.80	0.45
1:E:183:ARG:HG2	1:E:184:TYR:N	2.32	0.45
1:E:419:PRO:HG3	1:E:448:GLY:HA3	1.97	0.45
1:A:375:TYR:N	1:A:376:PRO:HD2	2.32	0.45
1:A:156:GLU:O	1:A:160:GLU:HG3	2.16	0.45
1:A:215:TYR:CD1	1:A:215:TYR:C	2.93	0.45
1:F:285:PRO:HG2	1:F:288:THR:HG22	1.98	0.45
1:C:31:LYS:C	1:C:32:ILE:HG13	2.42	0.45
1:D:183:ARG:HG2	1:D:184:TYR:N	2.31	0.45
1:A:88:ALA:O	1:A:348:ARG:HD2	2.17	0.45
1:C:602:LEU:HD22	1:C:608:ILE:CD1	2.47	0.45
1:D:140:ILE:N	1:D:140:ILE:HD12	2.32	0.45
1:D:419:PRO:HG3	1:D:448:GLY:HA3	1.98	0.45
1:F:215:TYR:CD1	1:F:215:TYR:C	2.94	0.45
1:B:258:GLN:HG2	1:D:268:GLY:N	2.30	0.45
1:C:510:LYS:HE2	1:C:610:LEU:HD13	1.99	0.45
1:C:183:ARG:O	1:C:185:SER:HA	2.16	0.44
1:D:51:LYS:HB2	1:D:51:LYS:HZ2	1.82	0.44
1:A:48:GLN:O	1:A:50:ASN:N	2.50	0.44
1:B:48:GLN:O	1:B:50:ASN:N	2.50	0.44
1:E:4:LEU:HD23	1:E:17:ILE:CD1	2.47	0.44
1:E:80[A]:ARG:NH1	1:E:127:ASP:OD2	2.47	0.44
1:F:172:PRO:HG2	1:F:177:PHE:CE1	2.52	0.44
1:F:255:ARG:HG2	1:F:257:ASP:HB2	1.99	0.44
1:A:183:ARG:O	1:A:185:SER:HA	2.17	0.44
1:B:419:PRO:HD2	1:B:457:ILE:HG23	1.99	0.44
1:F:48:GLN:O	1:F:50:ASN:N	2.50	0.44
1:B:13:TYR:CE2	1:B:36:LYS:HD2	2.52	0.44
1:C:596:HIS:CD2	1:C:597:GLU:N	2.85	0.44
1:D:26:PHE:HB3	1:D:165:LEU:CD2	2.47	0.44
1:E:257:ASP:HB3	1:E:260:TYR:HB3	2.00	0.44
1:F:140:ILE:N	1:F:140:ILE:HD12	2.33	0.44
1:B:28:LEU:O	1:B:29:GLU:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLN:HE21	1:B:30:GLN:HA	1.82	0.44
1:B:630:GLU:HB2	1:B:641:SER:HB3	1.99	0.44
1:C:48:GLN:O	1:C:50:ASN:N	2.51	0.44
1:E:419:PRO:HD2	1:E:457:ILE:HG23	1.98	0.44
1:E:640:PHE:CE2	1:E:644:ILE:HD11	2.52	0.44
1:F:156:GLU:O	1:F:160:GLU:HG3	2.16	0.44
1:A:309:TRP:O	1:A:312:GLN:HG3	2.17	0.44
1:D:659:LYS:HA	1:D:670:VAL:HG23	2.00	0.44
1:A:586:ILE:HG22	1:A:587:ASN:N	2.33	0.44
1:A:659:LYS:NZ	1:A:659:LYS:HB3	2.33	0.44
1:B:545:ARG:HB2	1:C:494:PRO:HG3	1.98	0.44
1:C:589:LYS:HD2	1:C:589:LYS:HA	1.79	0.44
1:D:48:GLN:O	1:D:50:ASN:N	2.51	0.44
1:E:172:PRO:HG2	1:E:177:PHE:CE1	2.53	0.44
1:F:309:TRP:O	1:F:312:GLN:HG3	2.17	0.44
1:F:659:LYS:NZ	1:F:659:LYS:HB3	2.32	0.44
1:A:96:ASP:OD1	1:A:97:PRO:HA	2.18	0.44
1:B:172:PRO:HG2	1:B:177:PHE:CE1	2.53	0.44
1:B:183:ARG:C	1:B:185:SER:HA	2.43	0.44
1:B:255:ARG:HG2	1:B:257:ASP:HB2	2.00	0.44
1:F:34:SER:OG	1:F:36:LYS:HB2	2.17	0.44
1:A:172:PRO:HG2	1:A:177:PHE:CE1	2.53	0.44
1:A:419:PRO:HD2	1:A:457:ILE:HG23	2.00	0.44
1:B:555:TYR:HB3	1:B:606:SER:OG	2.17	0.44
1:C:183:ARG:C	1:C:185:SER:HA	2.43	0.44
1:D:257:ASP:HB3	1:D:260:TYR:HB3	1.98	0.44
1:E:375:TYR:N	1:E:376:PRO:HD2	2.33	0.44
1:A:687:ARG:NH1	1:A:687:ARG:HB3	2.33	0.43
1:C:257:ASP:HB3	1:C:260:TYR:HB3	1.99	0.43
1:C:309:TRP:O	1:C:312:GLN:HG3	2.17	0.43
1:B:133:TYR:HB3	1:C:187:TYR:O	2.17	0.43
1:C:172:PRO:HG2	1:C:177:PHE:CE1	2.53	0.43
1:A:689:LYS:HE3	1:A:691:ASN:OD1	2.17	0.43
1:B:96:ASP:OD1	1:B:97:PRO:HA	2.19	0.43
1:B:375:TYR:N	1:B:376:PRO:HD2	2.32	0.43
1:B:659:LYS:HD3	1:B:667:GLU:CD	2.43	0.43
1:B:589:LYS:HD2	1:B:589:LYS:HA	1.79	0.43
1:B:610:LEU:HD11	1:B:616:ILE:CD1	2.48	0.43
1:D:172:PRO:HG2	1:D:177:PHE:CE1	2.53	0.43
1:B:339:SER:OG	1:E:339:SER:OG	2.32	0.43
1:D:107:SER:O	1:D:113:ALA:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:577:TRP:O	1:D:585:ILE:HA	2.19	0.43
1:E:48:GLN:O	1:E:50:ASN:N	2.51	0.43
1:B:682:ILE:HG22	1:B:684:GLN:HG2	2.00	0.43
1:E:38:LEU:HD11	1:E:45:ILE:HD12	2.00	0.43
1:E:309:TRP:O	1:E:312:GLN:HG3	2.19	0.43
1:A:26:PHE:HB3	1:A:165:LEU:CD2	2.49	0.43
1:B:269:LYS:HB3	1:B:298:THR:OG1	2.19	0.43
1:B:473:PHE:CG	1:B:552:VAL:HG21	2.53	0.43
1:D:130:LEU:CD2	1:E:483:THR:HG22	2.49	0.43
1:D:183:ARG:C	1:D:185:SER:HA	2.43	0.43
1:D:314:VAL:O	1:D:392:ARG:NH2	2.52	0.43
1:C:107:SER:O	1:C:113:ALA:HA	2.18	0.43
1:C:314:VAL:O	1:C:392:ARG:NH2	2.52	0.43
1:D:373:ASN:O	1:D:403:TYR:HB2	2.18	0.43
1:E:107:SER:O	1:E:113:ALA:HA	2.19	0.43
1:F:183:ARG:O	1:F:185:SER:HA	2.19	0.43
1:F:373:ASN:O	1:F:403:TYR:HB2	2.18	0.43
1:A:258:GLN:HG2	1:E:268:GLY:H	1.84	0.43
1:B:140:ILE:HD12	1:B:140:ILE:N	2.33	0.43
1:C:37:SER:OG	1:C:40:GLU:HG3	2.19	0.43
1:F:4:LEU:HA	1:F:16:VAL:O	2.19	0.43
1:C:659:LYS:NZ	1:C:659:LYS:HB3	2.34	0.42
1:E:183:ARG:C	1:E:185:SER:HA	2.44	0.42
1:F:375:TYR:N	1:F:376:PRO:HD2	2.33	0.42
1:A:257:ASP:HB3	1:A:260:TYR:HB3	2.01	0.42
1:B:520:LEU:O	1:B:524:GLU:HG3	2.18	0.42
1:C:375:TYR:N	1:C:376:PRO:HD2	2.34	0.42
1:E:130:LEU:HD22	1:F:483:THR:HG22	2.00	0.42
1:F:107:SER:O	1:F:113:ALA:HA	2.18	0.42
1:F:661:ILE:HA	1:F:666:LYS:O	2.19	0.42
1:F:670:VAL:CG1	1:F:678:TYR:HB3	2.49	0.42
1:B:9:ASN:OD1	1:B:29:GLU:HB2	2.17	0.42
1:C:169:PRO:HA	1:C:407:GLN:O	2.19	0.42
1:A:107:SER:O	1:A:113:ALA:HA	2.19	0.42
1:C:88:ALA:C	1:C:348:ARG:HD2	2.43	0.42
1:D:630:GLU:HB2	1:D:641:SER:HB3	2.00	0.42
1:D:651:ILE:HD13	1:D:692:LEU:CD2	2.45	0.42
1:E:26:PHE:HB3	1:E:165:LEU:CD2	2.49	0.42
1:E:428:LEU:HD12	1:E:428:LEU:HA	1.88	0.42
1:A:140:ILE:N	1:A:140:ILE:HD12	2.34	0.42
1:B:659:LYS:NZ	1:B:659:LYS:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ALA:O	1:C:348:ARG:HD2	2.19	0.42
1:D:375:TYR:N	1:D:376:PRO:HD2	2.33	0.42
1:D:666:LYS:HE2	1:D:667:GLU:H	1.84	0.42
1:D:669:GLN:CA	1:D:669:GLN:NE2	2.82	0.42
1:E:628:ASN:O	1:E:628:ASN:CG	2.62	0.42
1:F:257:ASP:HB3	1:F:260:TYR:HB3	2.01	0.42
1:F:428:LEU:HD12	1:F:428:LEU:HA	1.88	0.42
1:B:88:ALA:C	1:B:348:ARG:HD2	2.45	0.42
1:B:643:GLU:OE1	1:B:687:ARG:CZ	2.67	0.42
1:C:26:PHE:HB3	1:C:165:LEU:CD2	2.48	0.42
1:D:309:TRP:O	1:D:312:GLN:HG3	2.19	0.42
1:C:339:SER:HB2	1:D:339:SER:CB	2.49	0.42
1:D:324:PRO:HB3	1:D:375:TYR:CE2	2.55	0.42
1:A:88:ALA:C	1:A:348:ARG:HD2	2.45	0.42
1:C:373:ASN:O	1:C:403:TYR:HB2	2.20	0.42
1:D:169:PRO:HA	1:D:407:GLN:O	2.20	0.42
1:D:483:THR:HG22	1:F:130:LEU:HD22	2.02	0.42
1:A:341:PRO:O	1:C:345:ARG:HG2	2.20	0.42
1:C:255:ARG:HG2	1:C:257:ASP:HB2	2.02	0.42
1:D:12:VAL:HG23	1:D:161:LYS:HD3	2.01	0.42
1:E:456:GLU:CD	1:E:456:GLU:N	2.78	0.42
1:F:456:GLU:N	1:F:456:GLU:CD	2.78	0.42
1:F:659:LYS:HD3	1:F:667:GLU:OE1	2.20	0.42
1:A:28:LEU:O	1:A:29:GLU:C	2.61	0.42
1:A:555:TYR:HB3	1:A:606:SER:OG	2.20	0.42
1:B:169:PRO:HA	1:B:407:GLN:O	2.19	0.42
1:B:74:LEU:HD12	1:B:74:LEU:HA	1.89	0.41
1:B:340:LEU:C	1:B:342:VAL:H	2.27	0.41
1:C:340:LEU:C	1:C:342:VAL:N	2.76	0.41
1:D:473:PHE:CG	1:D:552:VAL:HG21	2.56	0.41
1:E:473:PHE:CG	1:E:552:VAL:HG21	2.55	0.41
1:E:602:LEU:HD22	1:E:608:ILE:CD1	2.49	0.41
1:F:26:PHE:HB3	1:F:165:LEU:CD2	2.49	0.41
1:A:183:ARG:C	1:A:185:SER:HA	2.45	0.41
1:C:630:GLU:HB2	1:C:641:SER:HB3	2.02	0.41
1:D:344:PHE:HA	1:E:342:VAL:HA	2.03	0.41
1:E:274:GLU:O	1:E:365:ARG:NH2	2.54	0.41
1:B:107:SER:O	1:B:113:ALA:HA	2.20	0.41
1:C:229:PHE:O	1:C:232:PRO:HD3	2.19	0.41
1:E:37:SER:OG	1:E:40:GLU:HG3	2.21	0.41
1:F:340:LEU:HD12	1:F:340:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:520:LEU:O	1:F:524:GLU:HG3	2.19	0.41
1:A:17:ILE:HD11	1:A:45:ILE:HD13	2.02	0.41
1:C:388:ARG:HD3	3:C:2072:HOH:O	2.20	0.41
1:D:255:ARG:HG2	1:D:257:ASP:HB2	2.02	0.41
1:F:88:ALA:C	1:F:348:ARG:HD2	2.45	0.41
1:B:640:PHE:HE2	1:B:644:ILE:HD11	1.83	0.41
1:C:17:ILE:HD11	1:C:45:ILE:HD13	2.03	0.41
1:C:520:LEU:O	1:C:524:GLU:HG3	2.20	0.41
1:E:140:ILE:HD12	1:E:140:ILE:N	2.35	0.41
1:E:174:MET:HE3	1:E:516:TYR:CB	2.51	0.41
1:E:663:ASP:O	1:E:664:ASP:HB2	2.21	0.41
1:A:651:ILE:HD13	1:A:692:LEU:CD2	2.49	0.41
1:A:682:ILE:HG22	1:A:684:GLN:HG2	2.03	0.41
1:B:620:GLU:HA	1:B:633:SER:OG	2.20	0.41
1:B:637:GLU:OE2	1:B:689:LYS:HD2	2.21	0.41
1:D:88:ALA:C	1:D:348:ARG:HD2	2.46	0.41
1:D:510:LYS:HA	1:D:611:GLU:CB	2.50	0.41
1:D:556:LEU:C	1:D:556:LEU:HD23	2.46	0.41
1:D:572:LEU:HA	1:D:573:PRO:HD3	1.95	0.41
1:E:255:ARG:HG2	1:E:257:ASP:HB2	2.02	0.41
1:A:51:LYS:NZ	1:A:51:LYS:CB	2.84	0.41
1:A:314:VAL:O	1:A:392:ARG:NH2	2.54	0.41
1:B:172:PRO:HG2	1:B:177:PHE:HE1	1.86	0.41
1:B:257:ASP:HB3	1:B:260:TYR:HB3	2.01	0.41
1:B:274:GLU:O	1:B:365:ARG:NH2	2.54	0.41
1:B:324:PRO:HB3	1:B:375:TYR:CE2	2.56	0.41
1:C:510:LYS:HA	1:C:611:GLU:HB2	2.03	0.41
1:D:8:GLU:O	1:D:9:ASN:CB	2.68	0.41
1:F:556:LEU:C	1:F:556:LEU:HD23	2.46	0.41
1:A:8:GLU:O	1:A:32:ILE:HB	2.21	0.41
1:A:234:LYS:O	1:A:238:GLU:HG3	2.20	0.41
1:A:274:GLU:O	1:A:365:ARG:NH2	2.54	0.41
1:B:634:SER:O	1:B:635:SER:C	2.64	0.41
1:B:643:GLU:HA	1:B:686:ILE:O	2.21	0.41
1:D:589:LYS:HD2	1:D:589:LYS:HA	1.78	0.41
1:F:96:ASP:OD1	1:F:97:PRO:HA	2.20	0.41
1:F:183:ARG:C	1:F:185:SER:HA	2.46	0.41
1:A:342:VAL:CG1	1:B:342:VAL:HG13	2.51	0.41
1:B:299:ARG:HG2	1:B:382:ALA:HB2	1.98	0.41
1:C:79:LYS:HD2	1:C:79:LYS:HA	1.94	0.41
1:C:268:GLY:H	1:F:258:GLN:HG2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:PHE:CG	1:C:552:VAL:HG21	2.55	0.41
1:E:41:LEU:HD12	1:E:41:LEU:HA	1.91	0.41
1:E:51:LYS:NZ	1:E:51:LYS:CB	2.84	0.41
1:F:274:GLU:O	1:F:365:ARG:NH2	2.54	0.41
1:F:689:LYS:HE3	1:F:691:ASN:OD1	2.21	0.41
1:B:556:LEU:HD23	1:B:556:LEU:C	2.45	0.40
1:D:17:ILE:HD11	1:D:45:ILE:HD13	2.03	0.40
1:E:651:ILE:HD13	1:E:692:LEU:CD2	2.49	0.40
1:A:290:TYR:HA	1:A:291:PRO:HD3	1.92	0.40
1:A:456:GLU:N	1:A:456:GLU:CD	2.79	0.40
1:B:10:LYS:HE2	1:B:10:LYS:HB3	1.90	0.40
1:B:51:LYS:NZ	1:B:51:LYS:CB	2.83	0.40
1:B:309:TRP:O	1:B:312:GLN:HG3	2.19	0.40
1:B:512:LEU:HB3	1:B:513:PRO:HD3	2.02	0.40
1:D:274:GLU:O	1:D:365:ARG:NH2	2.54	0.40
1:A:520:LEU:O	1:A:524:GLU:HG3	2.21	0.40
1:B:456:GLU:N	1:B:456:GLU:CD	2.78	0.40
1:C:284:TRP:HA	1:C:284:TRP:HE3	1.86	0.40
1:D:659:LYS:HA	1:D:670:VAL:CG2	2.51	0.40
1:E:512:LEU:HB3	1:E:513:PRO:HD3	2.04	0.40
1:F:630:GLU:HB2	1:F:641:SER:HB3	2.03	0.40
1:A:637:GLU:OE2	1:A:689:LYS:HD2	2.22	0.40
1:B:88:ALA:O	1:B:348:ARG:HD2	2.20	0.40
1:C:258:GLN:CG	1:F:268:GLY:H	2.27	0.40
1:C:274:GLU:O	1:C:365:ARG:NH2	2.55	0.40
1:C:324:PRO:HB3	1:C:375:TYR:CE2	2.56	0.40
1:C:663:ASP:O	1:C:664:ASP:HB2	2.20	0.40
1:F:572:LEU:HA	1:F:573:PRO:HD3	1.94	0.40
1:A:232:PRO:O	1:A:236:ILE:HG13	2.21	0.40
1:A:473:PHE:CG	1:A:552:VAL:HG21	2.56	0.40
1:B:130:LEU:HD22	1:C:483:THR:HG22	2.04	0.40
1:D:48:GLN:HB3	1:D:49:GLY:H	1.70	0.40
1:D:428:LEU:HD12	1:D:428:LEU:HA	1.88	0.40
1:D:520:LEU:O	1:D:524:GLU:HG3	2.22	0.40
1:F:174:MET:HE3	1:F:516:TYR:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	690/693 (100%)	648 (94%)	38 (6%)	4 (1%)	21	29
1	B	690/693 (100%)	645 (94%)	40 (6%)	5 (1%)	18	25
1	C	690/693 (100%)	647 (94%)	36 (5%)	7 (1%)	12	17
1	D	690/693 (100%)	653 (95%)	33 (5%)	4 (1%)	21	29
1	E	690/693 (100%)	654 (95%)	31 (4%)	5 (1%)	18	25
1	F	690/693 (100%)	652 (94%)	32 (5%)	6 (1%)	14	20
All	All	4140/4158 (100%)	3899 (94%)	210 (5%)	31 (1%)	18	25

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	635	SER
1	C	29	GLU
1	C	635	SER
1	C	665	SER
1	D	9	ASN
1	D	635	SER
1	E	9	ASN
1	F	29	GLU
1	F	31	LYS
1	A	49	GLY
1	B	49	GLY
1	C	49	GLY
1	D	49	GLY
1	E	49	GLY
1	E	635	SER
1	F	32	ILE
1	F	49	GLY
1	C	666	LYS
1	C	688	GLY

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Mol	Chain	Res	Type
1	E	29	GLU
1	E	688	GLY
1	F	30	GLN
1	B	688	GLY
1	F	688	GLY
1	A	688	GLY
1	B	29	GLU
1	B	635	SER
1	B	664	ASP
1	C	341	PRO
1	D	688	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	623/624 (100%)	603 (97%)	20 (3%)	34	51
1	B	623/624 (100%)	603 (97%)	20 (3%)	34	51
1	C	623/624 (100%)	599 (96%)	24 (4%)	28	43
1	D	623/624 (100%)	598 (96%)	25 (4%)	28	42
1	E	623/624 (100%)	600 (96%)	23 (4%)	30	45
1	F	623/624 (100%)	600 (96%)	23 (4%)	30	45
All	All	3738/3744 (100%)	3603 (96%)	135 (4%)	31	46

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	51	LYS
1	A	74	LEU
1	A	130	LEU
1	A	165	LEU
1	A	211	LEU
1	A	258	GLN

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Mol	Chain	Res	Type
1	A	283	MET
1	A	299	ARG
1	A	329	ARG
1	A	398	LEU
1	A	413	TRP
1	A	426	LEU
1	A	430	LEU
1	A	434	LEU
1	A	452	ARG
1	A	463	LEU
1	A	564	LYS
1	A	628	ASN
1	A	659	LYS
1	B	41	LEU
1	B	51	LYS
1	B	74	LEU
1	B	130	LEU
1	B	165	LEU
1	B	211	LEU
1	B	258	GLN
1	B	283	MET
1	B	312	GLN
1	B	329	ARG
1	B	398	LEU
1	B	413	TRP
1	B	426	LEU
1	B	430	LEU
1	B	434	LEU
1	B	452	ARG
1	B	463	LEU
1	B	564	LYS
1	B	628	ASN
1	B	659	LYS
1	C	30	GLN
1	C	38	LEU
1	C	41	LEU
1	C	51	LYS
1	C	74	LEU
1	C	130	LEU
1	C	165	LEU
1	C	211	LEU
1	C	258	GLN

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Mol	Chain	Res	Type
1	C	283	MET
1	C	299	ARG
1	C	312	GLN
1	C	329	ARG
1	C	398	LEU
1	C	413	TRP
1	C	426	LEU
1	C	430	LEU
1	C	434	LEU
1	C	452	ARG
1	C	463	LEU
1	C	564	LYS
1	C	628	ASN
1	C	659	LYS
1	C	666	LYS
1	D	28	LEU
1	D	41	LEU
1	D	51	LYS
1	D	74	LEU
1	D	130	LEU
1	D	165	LEU
1	D	211	LEU
1	D	255	ARG
1	D	258	GLN
1	D	283	MET
1	D	299	ARG
1	D	312	GLN
1	D	329	ARG
1	D	398	LEU
1	D	413	TRP
1	D	426	LEU
1	D	430	LEU
1	D	434	LEU
1	D	452	ARG
1	D	463	LEU
1	D	564	LYS
1	D	628	ASN
1	D	659	LYS
1	D	666	LYS
1	D	669	GLN
1	E	4	LEU
1	E	41	LEU

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Mol	Chain	Res	Type
1	E	51	LYS
1	E	74	LEU
1	E	130	LEU
1	E	165	LEU
1	E	211	LEU
1	E	258	GLN
1	E	283	MET
1	E	299	ARG
1	E	312	GLN
1	E	329	ARG
1	E	398	LEU
1	E	413	TRP
1	E	426	LEU
1	E	430	LEU
1	E	434	LEU
1	E	452	ARG
1	E	463	LEU
1	E	564	LYS
1	E	628	ASN
1	E	659	LYS
1	E	666	LYS
1	F	4	LEU
1	F	8	GLU
1	F	38	LEU
1	F	41	LEU
1	F	51	LYS
1	F	74	LEU
1	F	130	LEU
1	F	165	LEU
1	F	211	LEU
1	F	258	GLN
1	F	283	MET
1	F	312	GLN
1	F	329	ARG
1	F	398	LEU
1	F	413	TRP
1	F	426	LEU
1	F	430	LEU
1	F	434	LEU
1	F	452	ARG
1	F	463	LEU
1	F	564	LYS

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Mol	Chain	Res	Type
1	F	628	ASN
1	F	659	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	48	GLN
1	A	50	ASN
1	A	243	ASN
1	A	429	GLN
1	A	459	ASN
1	A	587	ASN
1	A	596	HIS
1	A	683	ASN
1	B	30	GLN
1	B	48	GLN
1	B	50	ASN
1	B	243	ASN
1	B	343	GLN
1	B	429	GLN
1	B	459	ASN
1	B	587	ASN
1	B	596	HIS
1	B	683	ASN
1	C	9	ASN
1	C	48	GLN
1	C	50	ASN
1	C	243	ASN
1	C	429	GLN
1	C	459	ASN
1	C	587	ASN
1	C	596	HIS
1	C	683	ASN
1	D	48	GLN
1	D	429	GLN
1	D	459	ASN
1	D	587	ASN
1	D	596	HIS
1	D	669	GLN
1	D	683	ASN
1	E	9	ASN

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Mol	Chain	Res	Type
1	E	30	GLN
1	E	48	GLN
1	E	50	ASN
1	E	429	GLN
1	E	459	ASN
1	E	587	ASN
1	E	596	HIS
1	E	636	ASN
1	E	684	GLN
1	F	9	ASN
1	F	30	GLN
1	F	48	GLN
1	F	50	ASN
1	F	429	GLN
1	F	459	ASN
1	F	587	ASN
1	F	596	HIS
1	F	636	ASN
1	F	683	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BOG	B	2000	-	14,14,20	1.48	3 (21%)	19,19,25	0.67	0
2	BOG	D	2000	-	14,14,20	1.40	3 (21%)	19,19,25	0.68	0
2	BOG	F	2000	-	14,14,20	1.44	3 (21%)	19,19,25	0.66	0
2	BOG	C	2000	-	14,14,20	1.35	3 (21%)	19,19,25	0.68	0
2	BOG	E	2000	-	14,14,20	1.47	3 (21%)	19,19,25	0.69	0
2	BOG	A	2000	-	14,14,20	1.36	2 (14%)	19,19,25	0.67	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
2	BOG	B	2000	-	-	2/5/25/31	0/1/1/1
2	BOG	D	2000	-	-	3/5/25/31	0/1/1/1
2	BOG	F	2000	-	-	2/5/25/31	0/1/1/1
2	BOG	C	2000	-	-	3/5/25/31	0/1/1/1
2	BOG	E	2000	-	-	2/5/25/31	0/1/1/1
2	BOG	A	2000	-	-	3/5/25/31	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	BOG	O5-C1	3.03	1.49	1.41
2	E	2000	BOG	O5-C1	2.93	1.49	1.41
2	F	2000	BOG	O5-C1	2.86	1.49	1.41
2	D	2000	BOG	O5-C1	2.79	1.49	1.41
2	A	2000	BOG	O5-C1	2.76	1.48	1.41
2	C	2000	BOG	O5-C1	2.76	1.48	1.41
2	E	2000	BOG	C4-C5	2.64	1.58	1.53
2	F	2000	BOG	C4-C5	2.61	1.58	1.53
2	B	2000	BOG	C4-C5	2.61	1.58	1.53
2	D	2000	BOG	C4-C5	2.45	1.58	1.53
2	E	2000	BOG	O1-C1	2.33	1.44	1.40
2	A	2000	BOG	C4-C5	2.26	1.57	1.53
2	F	2000	BOG	O1-C1	2.23	1.43	1.40
2	C	2000	BOG	C4-C5	2.21	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	BOG	O1-C1	2.18	1.43	1.40
2	C	2000	BOG	O1-C1	2.12	1.43	1.40
2	D	2000	BOG	O1-C1	2.05	1.43	1.40

There are no bond angle outliers.

There are no chirality outliers.

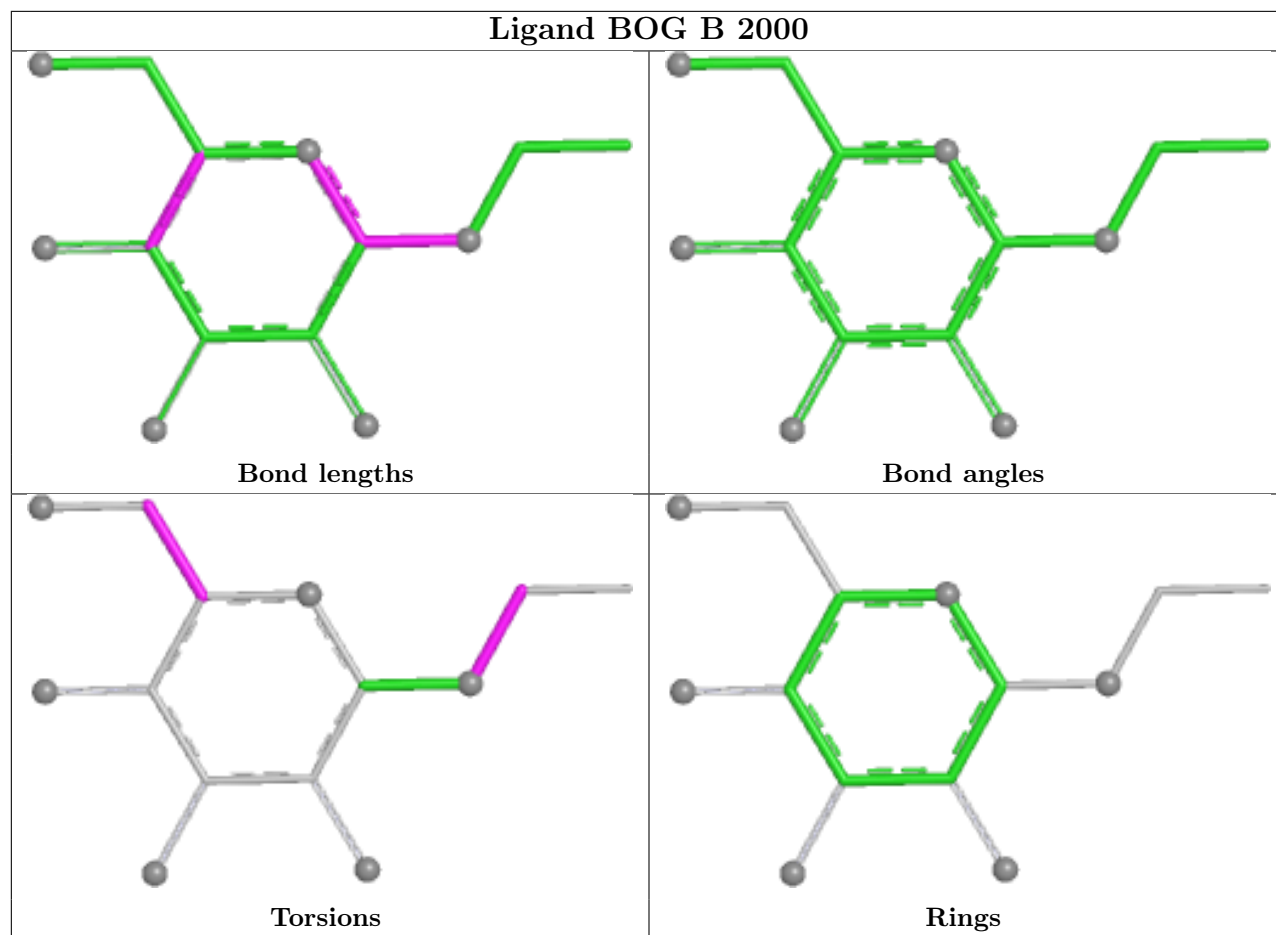
All (15) torsion outliers are listed below:

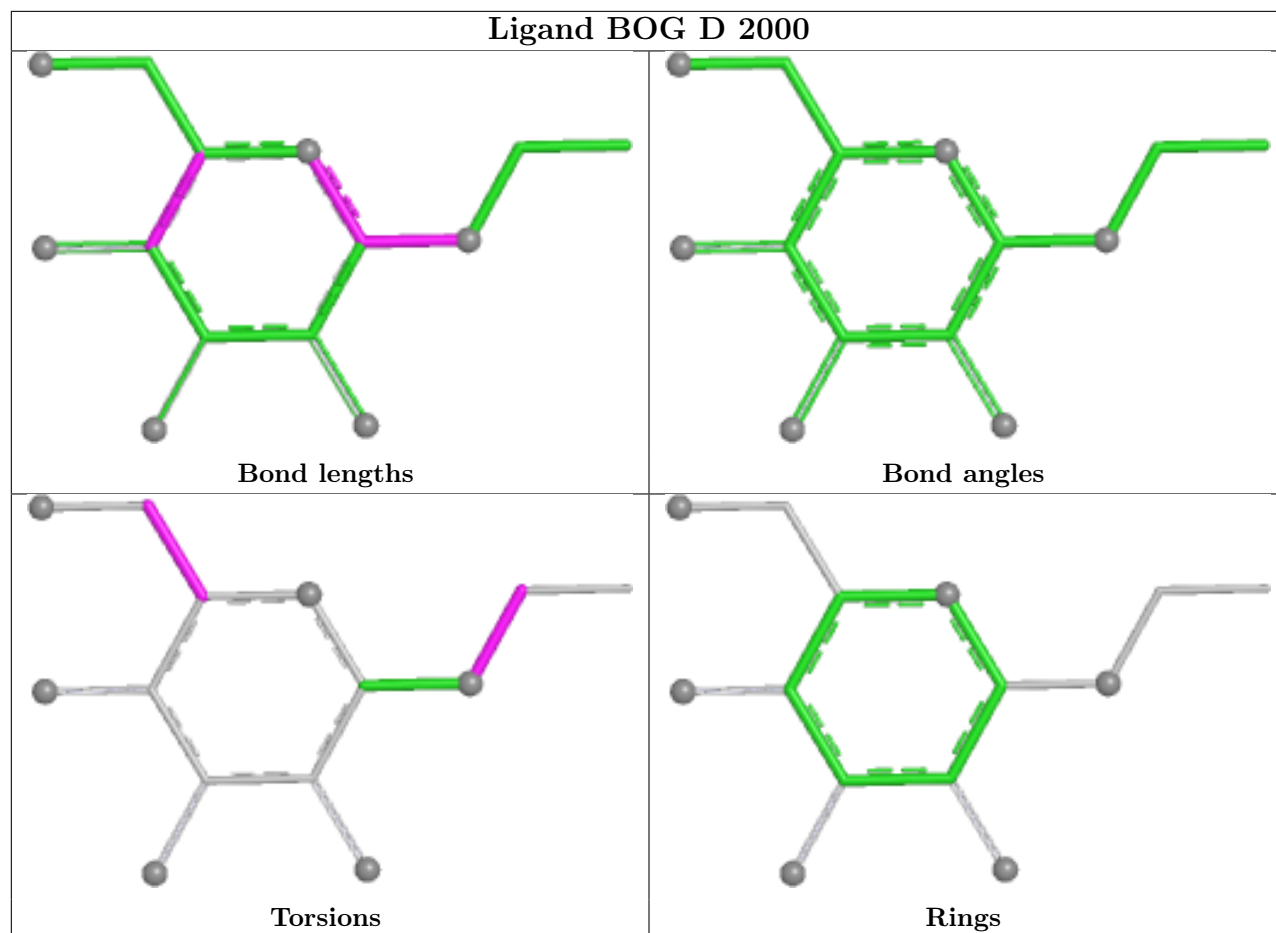
Mol	Chain	Res	Type	Atoms
2	D	2000	BOG	O5-C5-C6-O6
2	A	2000	BOG	O5-C5-C6-O6
2	C	2000	BOG	O5-C5-C6-O6
2	B	2000	BOG	O5-C5-C6-O6
2	F	2000	BOG	O5-C5-C6-O6
2	E	2000	BOG	O5-C5-C6-O6
2	D	2000	BOG	C4-C5-C6-O6
2	A	2000	BOG	C2'-C1'-O1-C1
2	B	2000	BOG	C2'-C1'-O1-C1
2	C	2000	BOG	C2'-C1'-O1-C1
2	D	2000	BOG	C2'-C1'-O1-C1
2	E	2000	BOG	C2'-C1'-O1-C1
2	F	2000	BOG	C2'-C1'-O1-C1
2	A	2000	BOG	C4-C5-C6-O6
2	C	2000	BOG	C4-C5-C6-O6

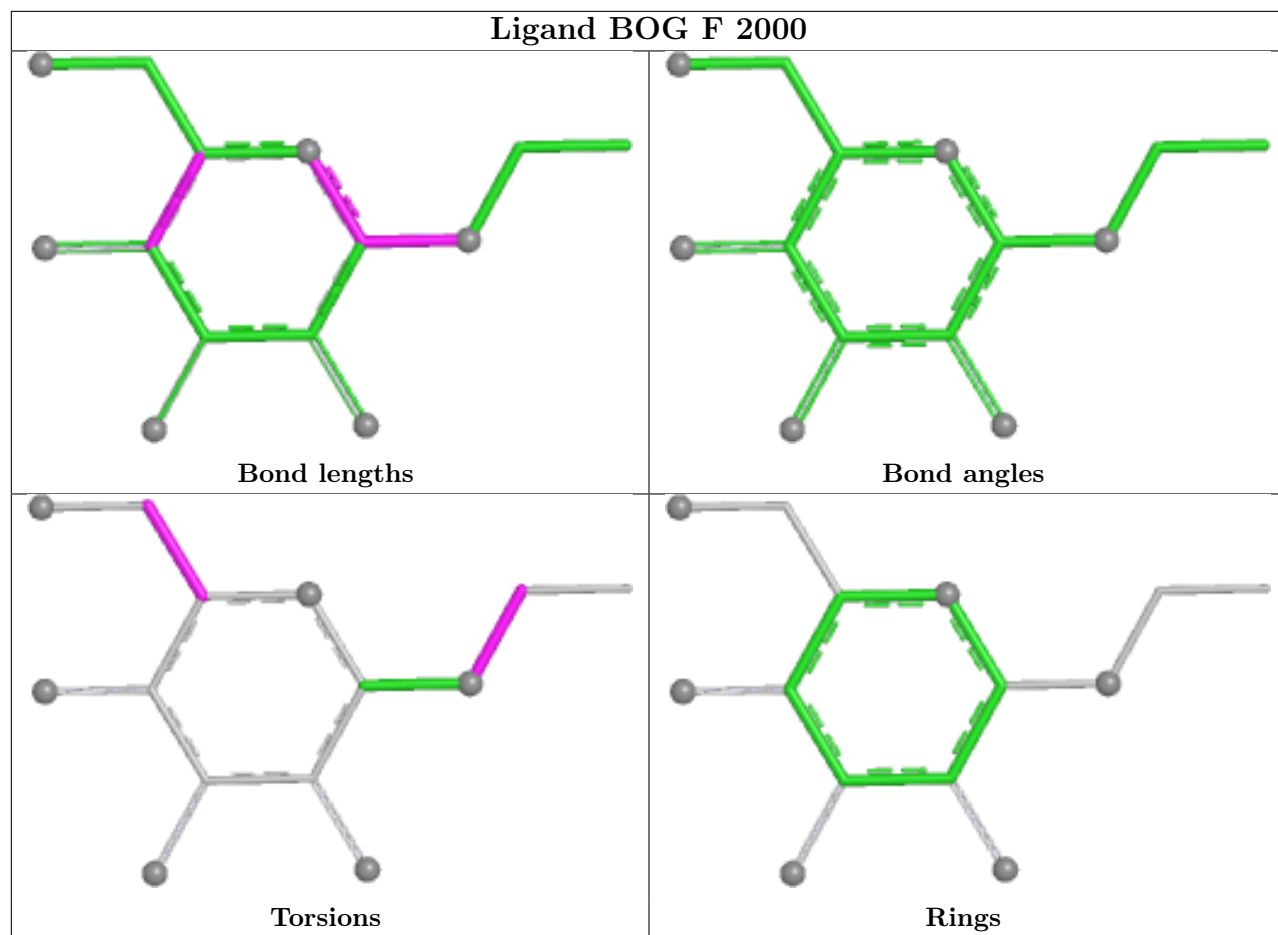
There are no ring outliers.

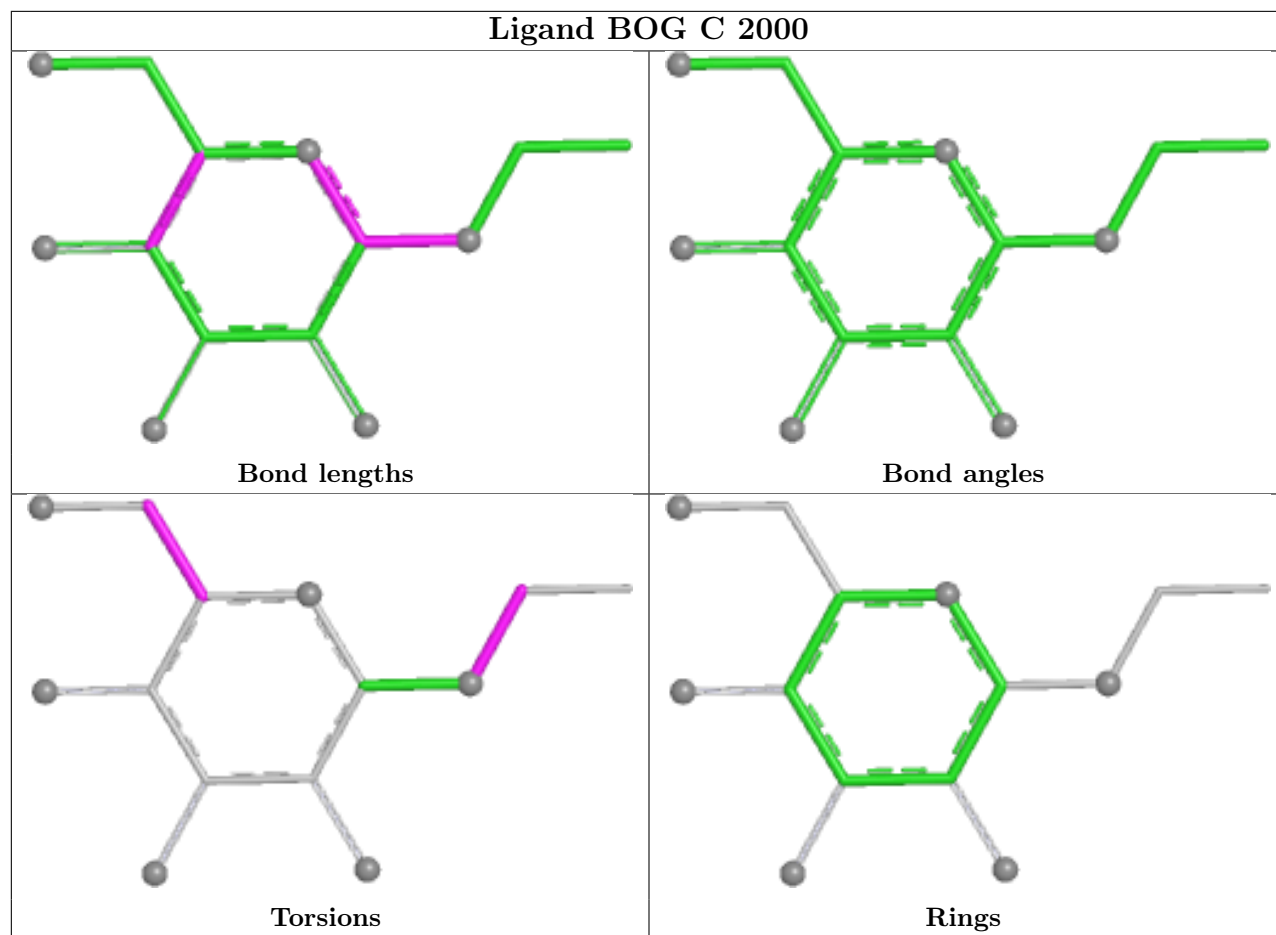
No monomer is involved in short contacts.

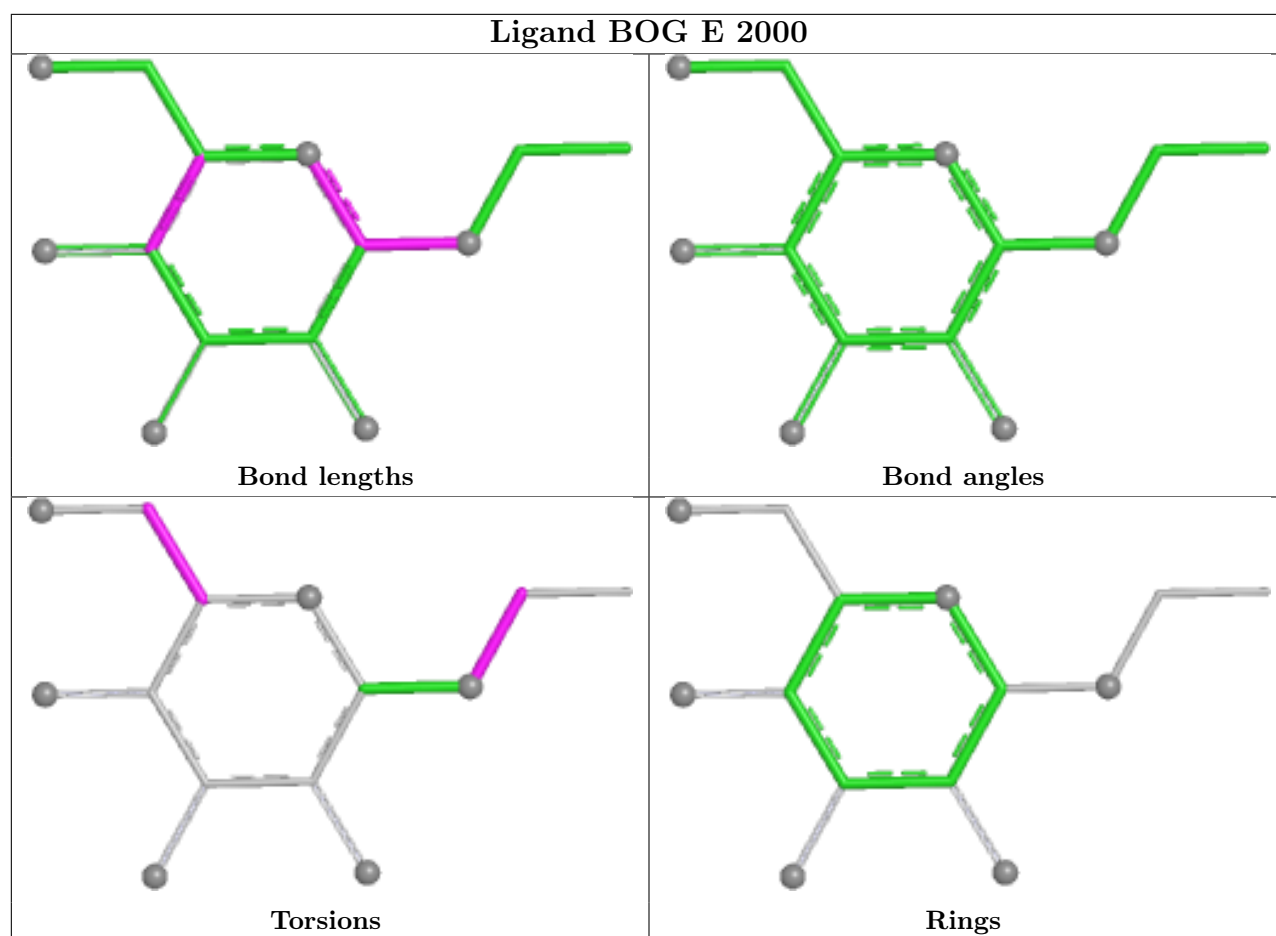
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

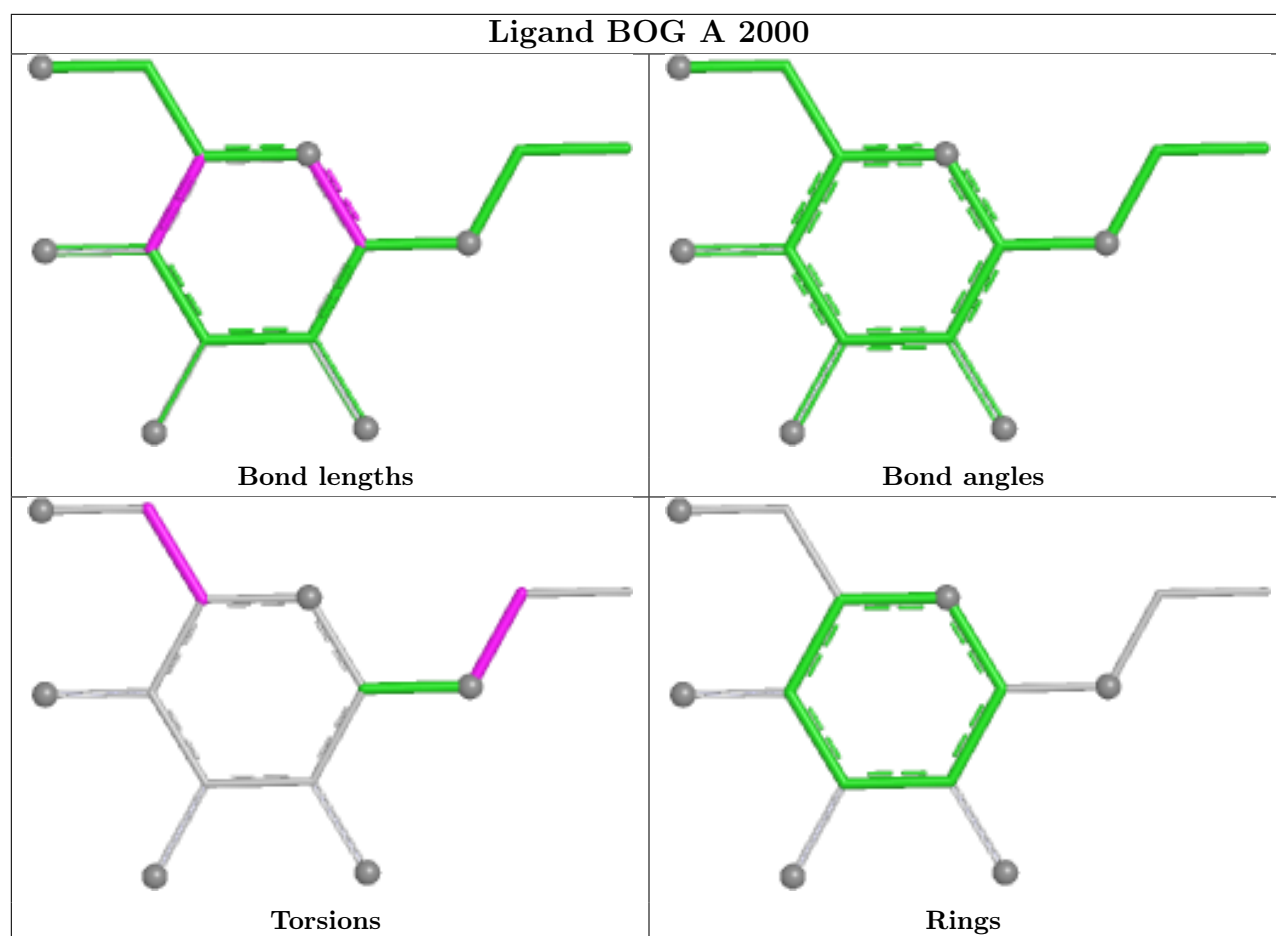












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	691/693 (99%)	-0.14	4 (0%)	85 88	20, 42, 68, 87	1 (0%)
1	B	691/693 (99%)	-0.07	4 (0%)	85 88	19, 42, 69, 89	1 (0%)
1	C	691/693 (99%)	-0.18	6 (0%)	81 83	21, 41, 67, 85	1 (0%)
1	D	691/693 (99%)	-0.20	3 (0%)	88 90	18, 40, 67, 81	1 (0%)
1	E	691/693 (99%)	-0.18	3 (0%)	88 90	18, 39, 64, 84	1 (0%)
1	F	691/693 (99%)	-0.13	5 (0%)	84 86	17, 38, 62, 84	1 (0%)
All	All	4146/4158 (99%)	-0.15	25 (0%)	85 88	17, 40, 66, 89	6 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	637	GLU	3.2
1	E	49	GLY	3.1
1	C	29	GLU	2.8
1	C	666	LYS	2.7
1	C	32	ILE	2.6
1	F	628	ASN	2.5
1	B	32	ILE	2.5
1	B	634	SER	2.4
1	F	661	ILE	2.4
1	F	637	GLU	2.3
1	D	28	LEU	2.2
1	D	346	ASP	2.2
1	D	151	GLU	2.2
1	C	33	SER	2.2
1	B	3	ILE	2.1
1	E	237	ASP	2.1
1	A	668	ILE	2.1
1	C	661	ILE	2.1
1	A	628	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	637	GLU	2.1
1	E	637	GLU	2.1
1	A	3	ILE	2.1
1	F	643	GLU	2.0
1	C	355	ASP	2.0
1	F	33	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

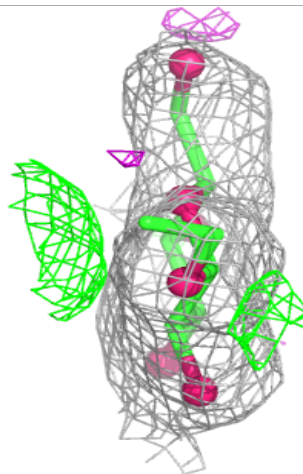
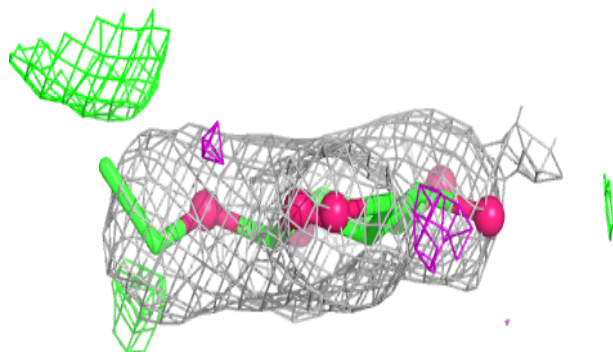
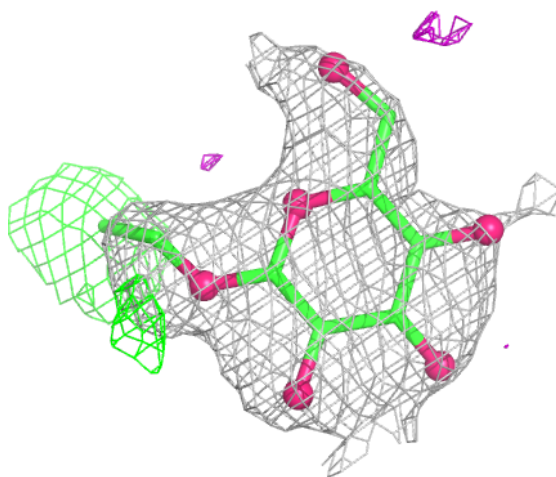
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BOG	E	2000	14/20	0.82	0.13	62,64,65,66	0
2	BOG	D	2000	14/20	0.85	0.11	62,64,64,65	0
2	BOG	A	2000	14/20	0.85	0.12	60,64,65,66	0
2	BOG	F	2000	14/20	0.86	0.11	62,64,65,65	0
2	BOG	C	2000	14/20	0.87	0.10	63,64,65,65	0
2	BOG	B	2000	14/20	0.89	0.09	64,65,66,66	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.

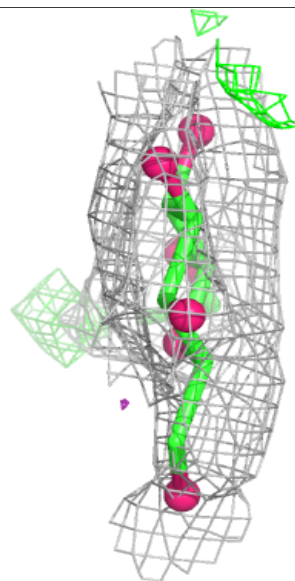
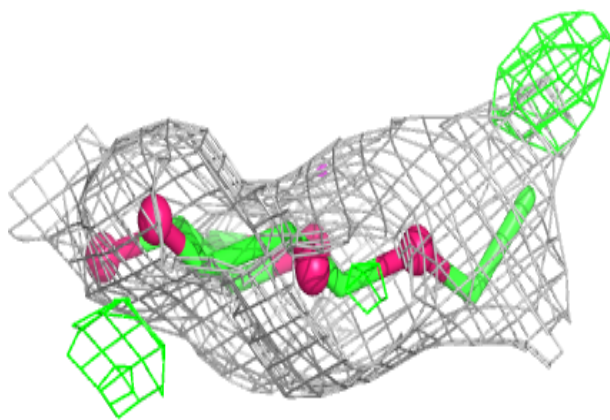
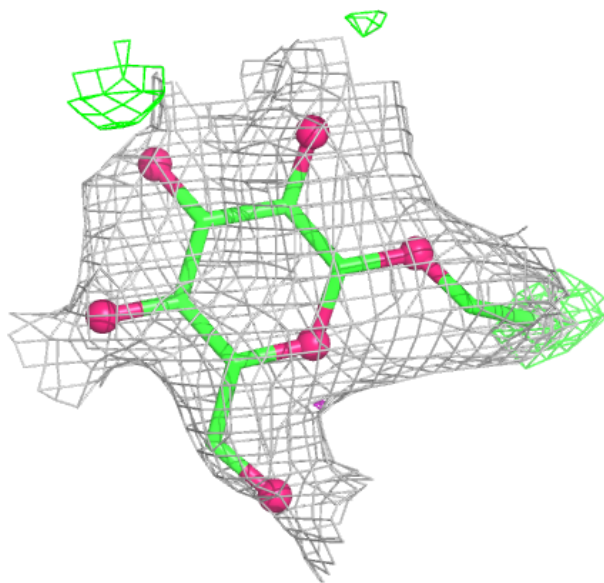
Electron density around BOG E 2000:

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



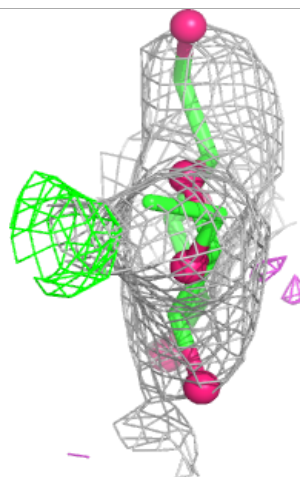
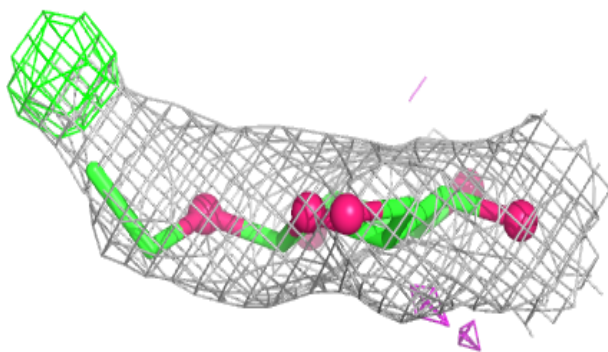
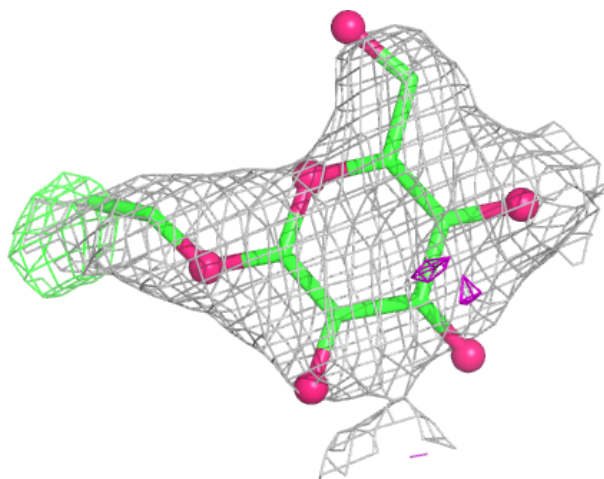
Electron density around BOG D 2000:

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



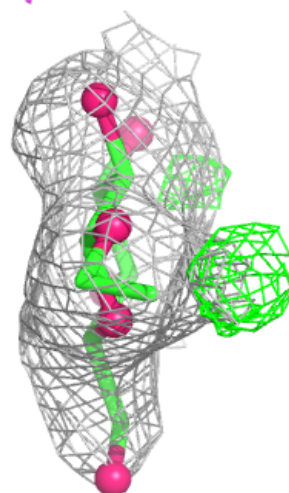
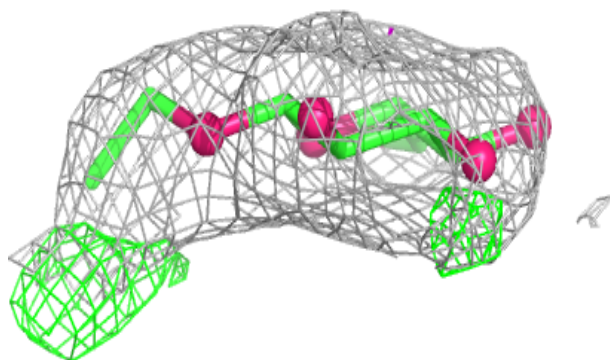
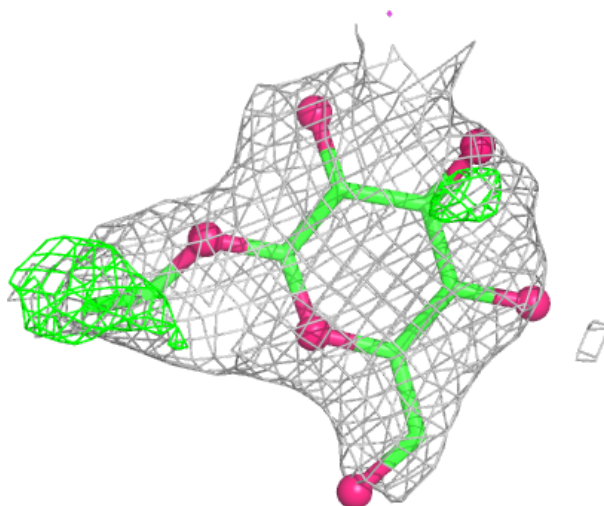
Electron density around BOG A 2000:

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



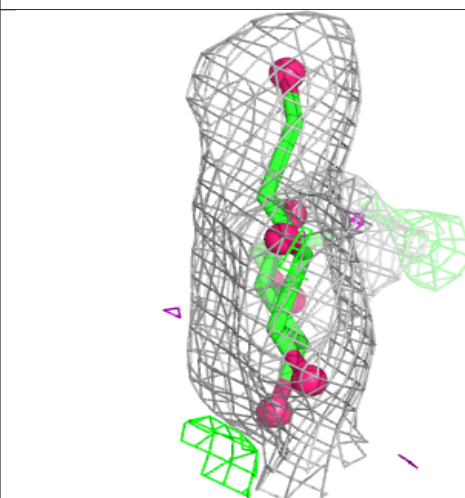
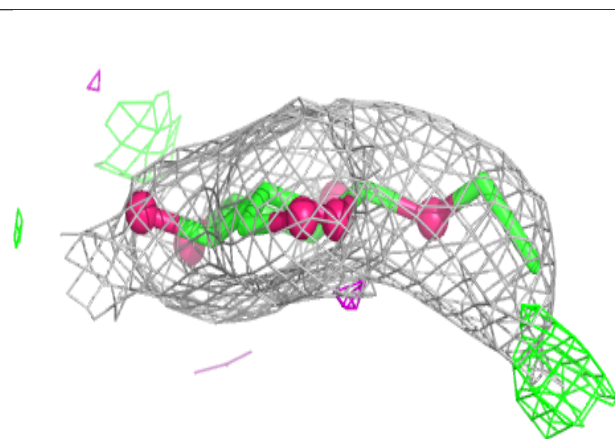
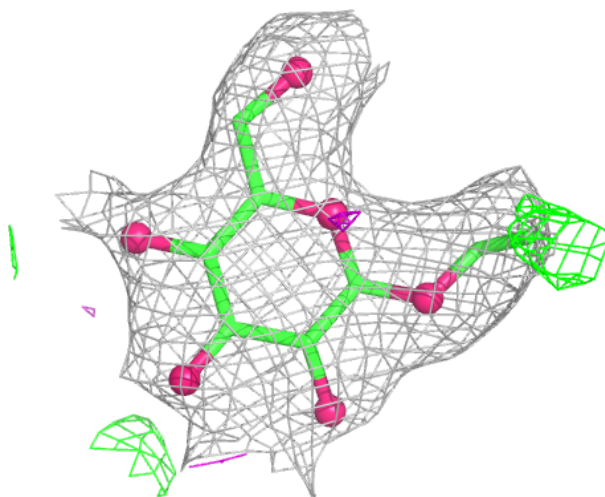
Electron density around BOG F 2000:

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



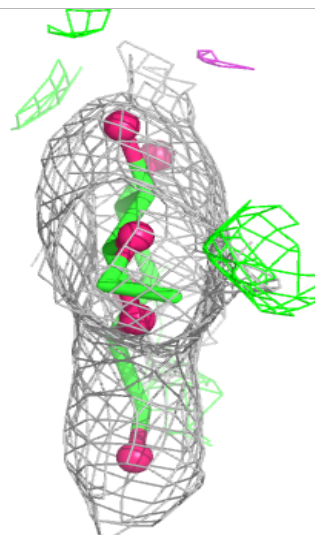
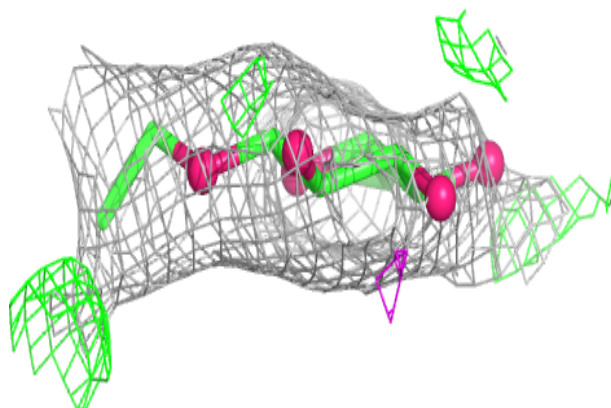
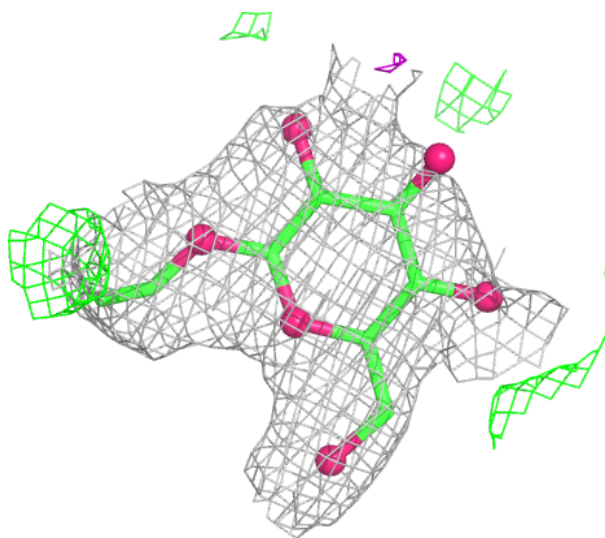
Electron density around BOG C 2000:

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



Electron density around BOG B 2000:

$2mF_o-DF_c$ (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.