



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:34 PM BST

PDB ID : 4D3S  
Title : Imine reductase from Nocardiosis halophila  
Authors : Man, H.; Hart, S.; Turkenburg, J.P.; Grogan, G.  
Deposited on : 2014-10-23  
Resolution : 2.24 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](mailto: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.

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

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

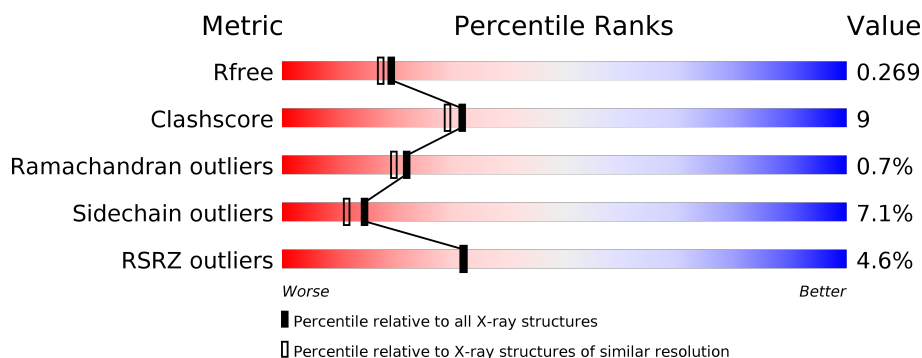
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	293	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 99%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>81%</span> <span>14%</span> <span>• •</span> </div> </div>
1	B	293	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 99%, yellow 1%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>82%</span> <span>12%</span> <span>• •</span> </div> </div>
1	C	293	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 99%, yellow 1%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>81%</span> <span>13%</span> <span>• •</span> </div> </div>
1	D	293	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 99%, yellow 1%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>83%</span> <span>11%</span> <span>• •</span> </div> </div>
1	E	293	<div> <div style="display: flex; justify-content: space-between; margin-bottom: 5px;"> <span>10%</span> <span>77%</span> <span>12%</span> <span>9%</span> </div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, green 87%, yellow 3%, grey 2%);"></div> </div>
1	F	293	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 99%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>78%</span> <span>14%</span> <span>• • •</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	293	<div><div></div><div>19%</div><div></div><div>72%</div><div></div><div>15%</div><div></div><div>•</div><div>8%</div></div>
1	H	293	<div><div></div><div>4%</div><div></div><div>76%</div><div></div><div>15%</div><div></div><div>•</div><div>5%</div></div>

## 2 Entry composition

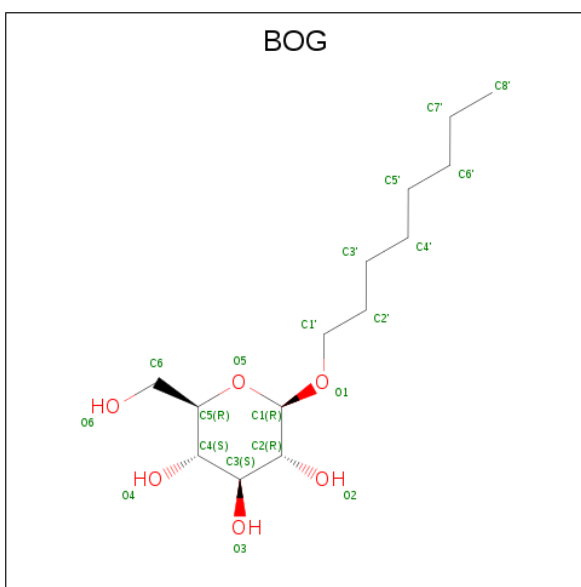
There are 3 unique types of molecules in this entry. The entry contains 16385 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 IMINE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2067	1303	352	402	10			
1	B	282	Total	C	N	O	S	0	0	0
			2013	1275	340	390	8			
1	C	283	Total	C	N	O	S	0	0	0
			2056	1296	346	404	10			
1	D	285	Total	C	N	O	S	0	0	0
			2047	1295	345	397	10			
1	E	267	Total	C	N	O	S	0	0	0
			1869	1188	310	361	10			
1	F	283	Total	C	N	O	S	0	0	0
			2036	1286	340	400	10			
1	G	269	Total	C	N	O	S	0	0	0
			1784	1119	312	343	10			
1	H	278	Total	C	N	O	S	0	0	0
			1966	1244	334	378	10			

- Molecule 2 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			20	14	6		
2	H	1	Total	C	O	0	0
			20	14	6		

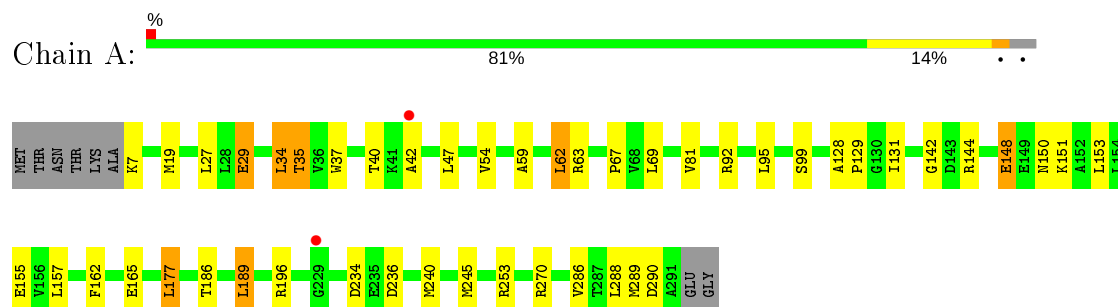
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total	O	0	0
			91	91		
3	B	73	Total	O	0	0
			73	73		
3	C	83	Total	O	0	0
			83	83		
3	D	97	Total	O	0	0
			97	97		
3	E	25	Total	O	0	0
			25	25		
3	F	69	Total	O	0	0
			69	69		
3	G	36	Total	O	0	0
			36	36		
3	H	33	Total	O	0	0
			33	33		

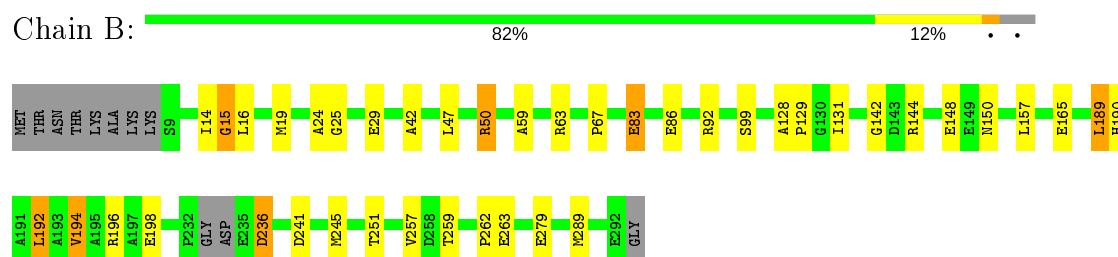
### 3 Residue-property plots [i](#)

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.

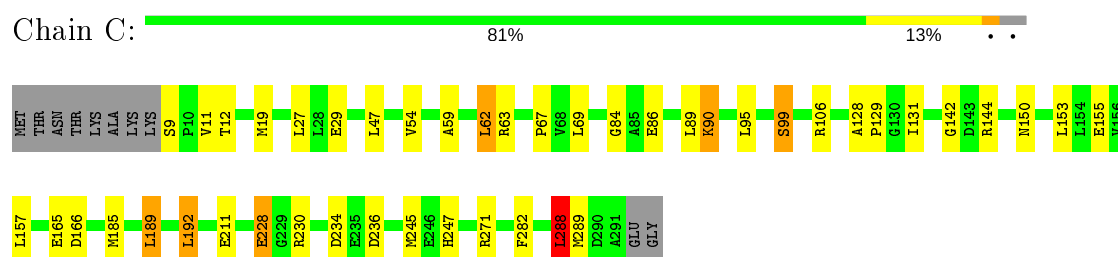
#### • Molecule 1: IMINE REDUCTASE



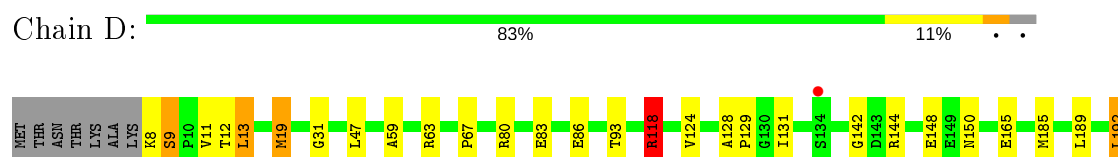
#### • Molecule 1: IMINE REDUCTASE



#### • Molecule 1: IMINE REDUCTASE

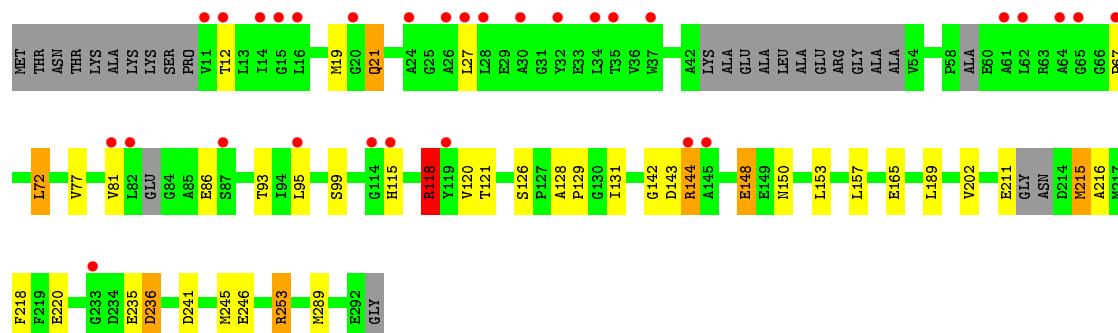
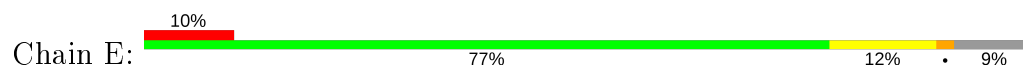


#### • Molecule 1: IMINE REDUCTASE

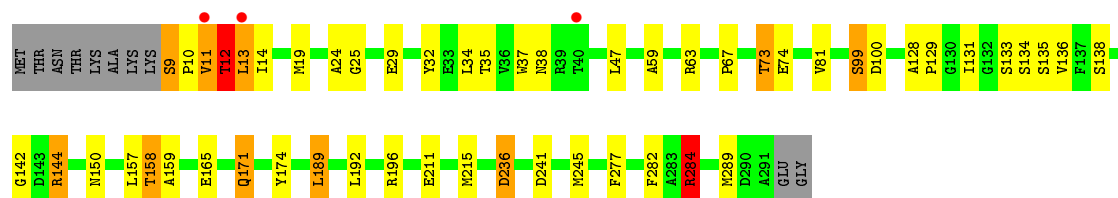
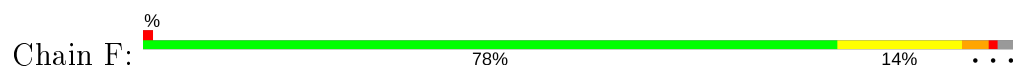




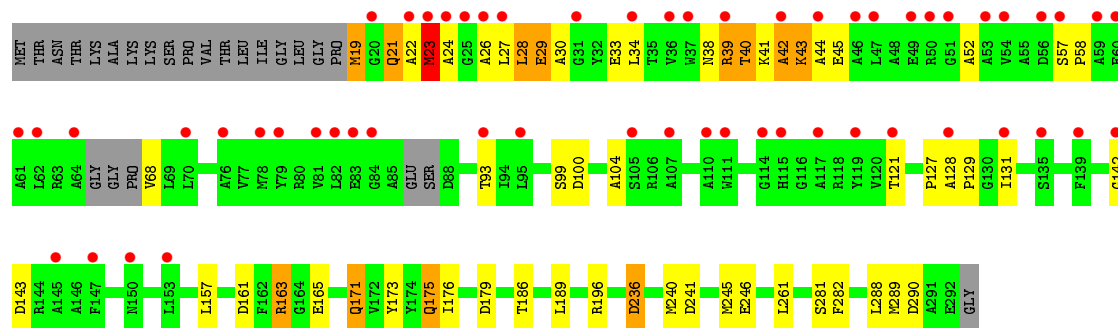
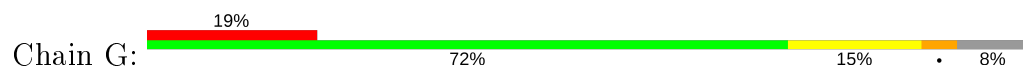
• Molecule 1: IMINE REDUCTASE



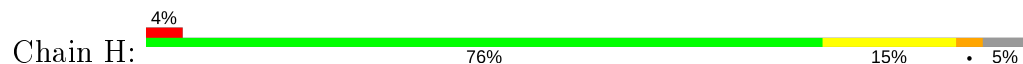
• Molecule 1: IMINE REDUCTASE

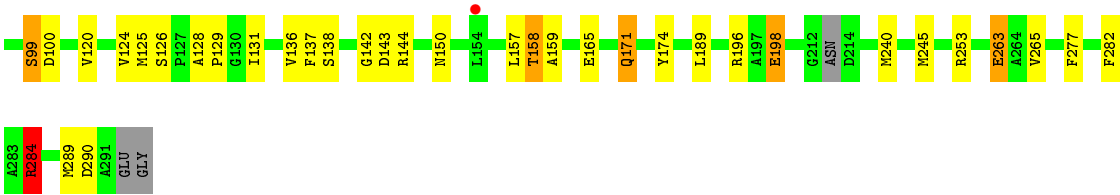


• Molecule 1: IMINE REDUCTASE



• Molecule 1: IMINE REDUCTASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.17Å 153.92Å 105.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.57 – 2.24 67.57 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.7 (67.57-2.24) 99.7 (67.57-2.24)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.25Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.230 , 0.266 0.235 , 0.269	Depositor DCC
$R_{free}$ test set	5458 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtrriage
Anisotropy	0.343	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16385	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6608e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.70	1/2107 (0.0%)	0.88	5/2867 (0.2%)
1	B	0.67	0/2051	0.89	7/2796 (0.3%)
1	C	0.73	2/2096 (0.1%)	0.88	7/2854 (0.2%)
1	D	0.67	0/2087	0.91	15/2843 (0.5%)
1	E	0.62	0/1902	0.81	6/2592 (0.2%)
1	F	0.79	3/2076 (0.1%)	0.97	12/2830 (0.4%)
1	G	0.63	0/1814	0.81	1/2476 (0.0%)
1	H	0.65	0/2003	0.85	3/2728 (0.1%)
All	All	0.69	6/16136 (0.0%)	0.88	56/21986 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	F	0	2
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	13	LEU	C-N	-14.37	1.00	1.34
1	F	133	SER	CB-OG	-5.72	1.34	1.42
1	C	99	SER	CB-OG	5.68	1.49	1.42
1	A	148	GLU	CG-CD	-5.47	1.43	1.51
1	F	10	PRO	N-CD	5.16	1.55	1.47
1	C	155	GLU	CD-OE2	-5.09	1.20	1.25

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	13	LEU	C-N-CA	13.77	156.13	121.70
1	F	13	LEU	O-C-N	-13.61	100.92	122.70
1	D	118	ARG	CG-CD-NE	12.66	138.39	111.80
1	B	14	ILE	C-N-CA	12.21	147.94	122.30
1	H	284	ARG	CG-CD-NE	11.05	135.00	111.80
1	A	19	MET	CG-SD-CE	10.80	117.47	100.20
1	H	284	ARG	NE-CZ-NH1	-10.18	115.21	120.30
1	B	50	ARG	NE-CZ-NH2	-9.57	115.51	120.30
1	F	12	THR	O-C-N	-8.81	108.60	122.70
1	A	62	LEU	CA-CB-CG	7.97	133.63	115.30
1	C	62	LEU	CA-CB-CG	7.62	132.82	115.30
1	D	196	ARG	CG-CD-NE	7.59	127.74	111.80
1	B	50	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	B	14	ILE	O-C-N	-7.51	110.43	123.20
1	C	144	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	D	196	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	C	155	GLU	OE1-CD-OE2	-7.37	114.46	123.30
1	F	11	VAL	C-N-CA	7.06	139.36	121.70
1	F	14	ILE	C-N-CA	7.06	137.12	122.30
1	F	133	SER	CB-CA-C	-6.79	97.21	110.10
1	D	118	ARG	CD-NE-CZ	6.50	132.69	123.60
1	F	13	LEU	CA-C-N	6.28	131.01	117.20
1	D	13	LEU	CB-CG-CD2	6.17	121.49	111.00
1	D	11	VAL	CB-CA-C	-6.15	99.72	111.40
1	F	284	ARG	CA-CB-CG	6.08	126.77	113.40
1	B	14	ILE	CA-C-N	6.04	128.28	116.20
1	E	118	ARG	CG-CD-NE	6.03	124.47	111.80
1	D	192	LEU	CB-CG-CD2	6.00	121.19	111.00
1	B	192	LEU	CB-CG-CD2	5.98	121.16	111.00
1	B	15	GLY	CA-C-N	-5.92	104.17	117.20
1	E	72	LEU	CA-CB-CG	5.90	128.87	115.30
1	C	11	VAL	CB-CA-C	-5.82	100.35	111.40
1	C	192	LEU	CB-CG-CD2	5.67	120.64	111.00
1	E	21	GLN	N-CA-CB	5.65	120.77	110.60
1	D	237	ARG	CA-CB-CG	5.62	125.77	113.40
1	F	9	SER	C-N-CD	5.62	140.20	128.40
1	F	19	MET	CG-SD-CE	-5.62	91.21	100.20
1	C	288	LEU	N-CA-CB	-5.57	99.25	110.40
1	G	23	MET	N-CA-CB	5.54	120.57	110.60
1	E	118	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	D	118	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	185	MET	CG-SD-CE	-5.47	91.45	100.20
1	A	177	LEU	CA-CB-CG	5.46	127.86	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	288	LEU	CA-CB-CG	5.42	127.76	115.30
1	D	118	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	92	ARG	CG-CD-NE	5.38	123.11	111.80
1	E	253	ARG	CG-CD-NE	5.34	123.02	111.80
1	F	144	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	D	19	MET	CG-SD-CE	-5.26	91.78	100.20
1	F	144	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	228	GLU	CB-CA-C	5.17	120.74	110.40
1	D	196	ARG	CD-NE-CZ	5.13	130.78	123.60
1	H	89	LEU	CB-CG-CD1	-5.10	102.34	111.00
1	D	240	MET	CA-CB-CG	5.06	121.91	113.30
1	E	253	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	34	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	15	GLY	Mainchain
1	F	12	THR	Mainchain
1	F	13	LEU	Mainchain

## 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	2067	0	2000	38	0
1	B	2013	0	1925	32	0
1	C	2056	0	1987	39	0
1	D	2047	0	1971	30	0
1	E	1869	0	1745	32	0
1	F	2036	0	1955	41	0
1	G	1784	0	1560	47	0
1	H	1966	0	1864	65	0
2	F	20	0	28	0	0
2	H	20	0	28	0	0
3	A	91	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	73	0	0	1	0
3	C	83	0	0	2	0
3	D	97	0	0	0	0
3	E	25	0	0	1	0
3	F	69	0	0	0	0
3	G	36	0	0	2	0
3	H	33	0	0	5	0
All	All	16385	0	15063	276	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 9.

All (276) 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:185:MET:CE	1:F:215:MET:CE	2.24	1.15
1:H:16:LEU:HD11	1:H:38:ASN:HB2	1.21	1.11
1:C:185:MET:HE3	1:F:215:MET:CE	1.83	1.09
1:E:77:VAL:O	1:E:81:VAL:HG12	1.54	1.07
1:C:185:MET:CE	1:F:215:MET:HE3	1.85	1.05
1:E:215:MET:CE	1:E:215:MET:HA	1.90	1.02
1:C:185:MET:HE3	1:F:215:MET:HE3	1.36	1.00
1:H:126:SER:HB2	1:H:136:VAL:HG21	1.00	0.98
1:H:126:SER:HB2	1:H:136:VAL:CG2	1.94	0.98
1:H:16:LEU:HD11	1:H:38:ASN:CB	1.97	0.95
1:H:126:SER:CB	1:H:136:VAL:HG21	1.96	0.94
1:H:136:VAL:HG13	1:H:158:THR:OG1	1.67	0.93
1:G:100:ASP:H	1:G:171:GLN:HE21	1.18	0.92
1:H:16:LEU:HD12	1:H:38:ASN:ND2	1.89	0.88
3:A:2043:HOH:O	1:H:198:GLU:HG2	1.74	0.87
1:G:186:THR:HG22	1:G:261:LEU:HD22	1.57	0.86
1:H:158:THR:HG23	1:H:159:ALA:O	1.77	0.85
1:G:28:LEU:O	1:G:30:ALA:N	2.09	0.85
1:E:215:MET:HA	1:E:215:MET:HE2	1.58	0.84
1:A:290:ASP:OD2	1:H:196:ARG:NH1	2.11	0.82
1:E:215:MET:HE3	1:E:215:MET:HA	1.63	0.79
1:H:263:GLU:HG3	3:H:2030:HOH:O	1.81	0.79
1:F:158:THR:HG23	1:F:159:ALA:O	1.84	0.76
1:G:99:SER:HA	1:G:171:GLN:NE2	2.02	0.75
1:C:185:MET:HE1	1:F:215:MET:CE	2.18	0.74
1:C:289:MET:HE1	1:F:189:LEU:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:284:ARG:HH11	1:H:284:ARG:CG	2.02	0.72
1:C:185:MET:HE1	1:F:215:MET:HE3	1.70	0.72
1:D:252:SER:O	1:D:257:VAL:HG12	1.90	0.72
1:F:11:VAL:O	1:F:34:LEU:HA	1.89	0.72
1:A:189:LEU:HB3	1:H:289:MET:HE1	1.71	0.72
1:D:128:ALA:HA	1:D:131:ILE:HD12	1.70	0.71
1:G:99:SER:HA	1:G:171:GLN:HE22	1.55	0.71
1:D:93:THR:OG1	1:D:118:ARG:NH1	2.25	0.69
1:B:144:ARG:NH1	1:B:148:GLU:OE2	2.25	0.69
1:F:100:ASP:O	1:F:171:GLN:HG3	1.92	0.69
1:C:106:ARG:NH1	1:C:166:ASP:OD2	2.26	0.68
1:G:21:GLN:O	1:G:24:ALA:N	2.26	0.68
1:D:230:ARG:HG3	1:D:231:PHE:H	1.59	0.68
1:D:144:ARG:NH1	1:D:148:GLU:OE2	2.26	0.67
1:H:16:LEU:CD1	1:H:38:ASN:CG	2.63	0.66
1:H:100:ASP:O	1:H:171:GLN:HG3	1.95	0.66
1:H:16:LEU:CD1	1:H:38:ASN:ND2	2.57	0.66
1:G:19:MET:CE	1:G:128:ALA:HA	2.26	0.66
1:C:185:MET:HE3	1:F:215:MET:HE1	1.73	0.65
1:E:93:THR:OG1	1:E:118:ARG:NH1	2.28	0.65
1:H:14:ILE:HG23	1:H:70:LEU:HD23	1.78	0.65
1:B:189:LEU:HB3	1:G:289:MET:HE1	1.77	0.65
1:C:185:MET:CE	1:F:215:MET:HE2	2.25	0.65
1:B:190:HIS:HD2	1:G:179:ASP:OD2	1.80	0.65
1:G:38:ASN:O	1:G:40:THR:N	2.30	0.64
1:H:284:ARG:HH11	1:H:284:ARG:HG2	1.62	0.64
1:H:16:LEU:CD1	1:H:38:ASN:HB2	2.14	0.64
1:C:189:LEU:HD22	1:F:282:PHE:CZ	2.33	0.64
1:F:136:VAL:HG23	1:F:158:THR:OG1	1.96	0.64
1:H:277:PHE:CE1	1:H:284:ARG:NH1	2.66	0.64
1:G:186:THR:HG22	1:G:261:LEU:CD2	2.27	0.63
1:H:95:LEU:HD23	1:H:120:VAL:HG22	1.79	0.63
1:A:289:MET:HE1	1:H:189:LEU:HB3	1.81	0.62
1:H:158:THR:HG22	3:H:2021:HOH:O	2.00	0.62
1:E:215:MET:CE	1:E:218:PHE:CD2	2.83	0.61
1:E:95:LEU:HD23	1:E:120:VAL:HG22	1.81	0.61
1:E:19:MET:HE1	1:E:126:SER:O	2.01	0.61
1:A:35:THR:CG2	3:A:2003:HOH:O	2.49	0.61
1:C:84:GLY:N	1:C:86:GLU:OE2	2.33	0.60
1:B:194:VAL:CG2	1:G:176:ILE:HG12	2.31	0.60
1:F:138:SER:OG	1:F:158:THR:HG21	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD22	1:H:282:PHE:CZ	2.38	0.59
1:H:16:LEU:CD1	1:H:38:ASN:CB	2.77	0.59
1:C:131:ILE:O	1:C:157:LEU:O	2.21	0.59
1:C:189:LEU:HB3	1:F:289:MET:HE1	1.85	0.59
1:G:100:ASP:H	1:G:171:GLN:NE2	1.93	0.59
1:B:259:THR:HG23	1:B:263:GLU:OE2	2.03	0.59
1:C:86:GLU:HA	1:C:89:LEU:HD13	1.85	0.59
1:G:19:MET:HE1	1:G:128:ALA:N	2.18	0.59
1:B:190:HIS:CD2	1:G:179:ASP:OD2	2.57	0.58
1:G:23:MET:O	1:G:26:ALA:N	2.36	0.58
1:C:90:LYS:N	1:C:90:LYS:HD3	2.17	0.58
1:C:106:ARG:NH1	1:C:166:ASP:OD1	2.36	0.58
1:B:131:ILE:O	1:B:157:LEU:O	2.22	0.58
1:A:40:THR:OG1	1:A:42:ALA:N	2.36	0.58
1:A:37:TRP:CZ3	1:A:81:VAL:CG2	2.87	0.58
1:G:131:ILE:O	1:G:157:LEU:O	2.22	0.58
1:A:240:MET:CE	1:H:18:PRO:CD	2.83	0.57
1:F:25:GLY:O	1:F:29:GLU:HG3	2.03	0.57
1:G:43:LYS:C	1:G:45:GLU:H	2.07	0.57
1:E:131:ILE:O	1:E:157:LEU:O	2.22	0.57
1:D:230:ARG:CG	1:D:231:PHE:H	2.18	0.57
1:E:215:MET:CE	1:E:215:MET:CA	2.74	0.57
1:A:131:ILE:O	1:A:157:LEU:O	2.23	0.56
1:H:86:GLU:HA	1:H:89:LEU:HD13	1.86	0.56
1:C:90:LYS:O	1:C:90:LYS:HD3	2.05	0.56
1:G:39:ARG:O	1:G:41:LYS:N	2.39	0.56
1:A:40:THR:OG1	1:A:42:ALA:HB2	2.06	0.56
1:B:25:GLY:O	1:B:29:GLU:HG3	2.05	0.56
1:F:131:ILE:O	1:F:157:LEU:O	2.24	0.56
1:F:73:THR:HG22	1:F:74:GLU:HG2	1.88	0.55
1:G:27:LEU:O	1:G:28:LEU:O	2.25	0.55
1:C:247:HIS:HD2	3:C:2069:HOH:O	1.88	0.55
1:F:158:THR:CG2	1:F:159:ALA:O	2.54	0.55
1:D:259:THR:HG23	1:D:263:GLU:OE1	2.06	0.55
1:H:131:ILE:O	1:H:157:LEU:O	2.25	0.55
1:E:86:GLU:CB	1:E:115:HIS:CD2	2.89	0.55
1:E:215:MET:CE	1:E:218:PHE:HD2	2.20	0.55
1:D:252:SER:HB3	1:D:257:VAL:HG13	1.87	0.55
1:H:131:ILE:CB	3:H:2020:HOH:O	2.55	0.54
1:A:67:PRO:HG3	1:A:150:ASN:OD1	2.07	0.54
1:A:37:TRP:CZ3	1:A:81:VAL:HG23	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:ARG:NH2	1:C:288:LEU:HD23	2.22	0.54
1:H:138:SER:OG	1:H:158:THR:HG21	2.07	0.54
1:G:19:MET:HE2	1:G:128:ALA:HA	1.90	0.54
1:A:240:MET:HE2	1:H:18:PRO:CD	2.37	0.54
1:C:27:LEU:CD2	1:C:153:LEU:HD11	2.38	0.53
1:D:237:ARG:HG2	1:D:240:MET:CE	2.38	0.53
1:H:42:ALA:C	1:H:44:ALA:H	2.11	0.53
1:E:215:MET:HE1	1:E:218:PHE:CD2	2.43	0.53
1:G:19:MET:HA	1:G:19:MET:HE2	1.90	0.53
1:G:19:MET:CE	1:G:128:ALA:CA	2.87	0.53
1:B:67:PRO:HG3	1:B:150:ASN:OD1	2.08	0.53
1:A:40:THR:OG1	1:A:42:ALA:CB	2.56	0.53
1:E:67:PRO:HG3	1:E:150:ASN:OD1	2.08	0.53
1:B:19:MET:HE1	3:B:2038:HOH:O	2.08	0.53
1:D:67:PRO:HG3	1:D:150:ASN:OD1	2.08	0.53
1:H:67:PRO:HG3	1:H:150:ASN:OD1	2.09	0.53
1:H:99:SER:HA	3:H:2017:HOH:O	2.08	0.53
1:C:282:PHE:CZ	1:F:189:LEU:HD22	2.44	0.52
1:A:144:ARG:O	1:A:148:GLU:OE1	2.26	0.52
1:C:19:MET:HE1	3:C:2034:HOH:O	2.09	0.52
1:H:253:ARG:NH2	1:H:263:GLU:OE2	2.43	0.52
1:C:90:LYS:O	1:C:90:LYS:HE2	2.09	0.52
1:D:8:LYS:HG2	1:D:31:GLY:O	2.10	0.52
1:F:67:PRO:HG3	1:F:150:ASN:OD1	2.08	0.52
1:C:67:PRO:HG3	1:C:150:ASN:OD1	2.09	0.52
1:C:289:MET:CE	1:F:189:LEU:HB3	2.39	0.52
1:G:281:SER:OG	1:G:282:PHE:N	2.42	0.52
1:H:158:THR:CG2	1:H:159:ALA:O	2.56	0.52
1:G:21:GLN:O	1:G:23:MET:N	2.42	0.52
1:D:8:LYS:CG	1:D:31:GLY:O	2.57	0.52
1:H:277:PHE:CZ	1:H:284:ARG:NH1	2.78	0.52
1:E:202:VAL:HG23	3:E:2014:HOH:O	2.10	0.51
1:G:171:GLN:OE1	1:G:171:GLN:HA	2.09	0.51
1:F:192:LEU:O	1:F:196:ARG:HG3	2.11	0.51
1:B:128:ALA:HB3	1:B:129:PRO:HD3	1.93	0.51
1:E:27:LEU:CD2	1:E:153:LEU:HD11	2.39	0.51
1:A:151:LYS:O	1:A:155:GLU:HG3	2.11	0.51
1:B:189:LEU:HD22	1:G:282:PHE:CZ	2.46	0.51
1:C:27:LEU:HD22	1:C:153:LEU:HD11	1.92	0.51
1:A:253:ARG:HD3	1:B:92:ARG:NH1	2.26	0.50
1:B:289:MET:HE1	1:G:189:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:TRP:CZ3	1:F:81:VAL:CG2	2.94	0.50
1:A:289:MET:HE1	1:H:189:LEU:CB	2.41	0.50
1:C:228:GLU:OE2	1:C:230:ARG:NH1	2.44	0.50
1:C:27:LEU:CD2	1:C:153:LEU:CD1	2.89	0.50
1:D:252:SER:HB3	1:D:257:VAL:CG1	2.41	0.50
1:E:27:LEU:CD2	1:E:153:LEU:CD1	2.90	0.50
1:F:24:ALA:HB1	1:F:47:LEU:HD22	1.94	0.50
1:G:163:ARG:HD3	1:G:173:TYR:CZ	2.47	0.50
1:A:196:ARG:NH1	1:H:290:ASP:OD2	2.45	0.50
1:H:95:LEU:CD2	1:H:120:VAL:CG2	2.90	0.50
1:D:144:ARG:NH1	1:D:148:GLU:CG	2.75	0.49
1:G:161:ASP:OD1	1:G:163:ARG:NH2	2.37	0.49
1:H:136:VAL:HG22	1:H:137:PHE:N	2.28	0.49
1:B:236:ASP:OD1	1:B:241:ASP:OD2	2.30	0.49
1:D:144:ARG:NH1	1:D:148:GLU:HG2	2.28	0.49
1:E:216:ALA:O	1:E:220:GLU:HG3	2.13	0.49
1:H:16:LEU:HD21	1:H:36:VAL:CG1	2.43	0.49
1:G:41:LYS:O	1:G:42:ALA:HB3	2.12	0.49
1:A:128:ALA:HB3	1:A:129:PRO:HD3	1.94	0.49
1:C:228:GLU:O	1:C:228:GLU:HG3	2.11	0.49
1:E:118:ARG:HG3	1:E:118:ARG:HH11	1.77	0.49
1:E:27:LEU:HD22	1:E:153:LEU:HD11	1.95	0.49
1:D:128:ALA:HB3	1:D:129:PRO:HD3	1.94	0.48
1:F:236:ASP:OD1	1:F:241:ASP:OD2	2.30	0.48
1:C:106:ARG:NH1	1:C:166:ASP:CG	2.67	0.48
1:C:69:LEU:HD23	1:C:95:LEU:HB2	1.96	0.48
1:D:257:VAL:HG23	1:E:289:MET:O	2.13	0.48
1:F:11:VAL:HG12	1:F:32:TYR:HB3	1.95	0.48
1:A:29:GLU:HG3	3:A:2010:HOH:O	2.14	0.48
1:D:289:MET:HE1	1:E:189:LEU:HB3	1.95	0.48
1:A:69:LEU:HD23	1:A:95:LEU:HB2	1.95	0.47
1:C:90:LYS:O	1:C:90:LYS:CD	2.62	0.47
1:D:144:ARG:HH12	1:D:148:GLU:CD	2.14	0.47
1:F:128:ALA:HB3	1:F:129:PRO:HD3	1.96	0.47
1:A:189:LEU:HB3	1:H:289:MET:CE	2.41	0.47
1:B:144:ARG:HH12	1:B:148:GLU:CD	2.16	0.47
1:C:185:MET:CE	1:F:215:MET:HE1	2.29	0.47
1:A:289:MET:CE	1:H:189:LEU:HB3	2.43	0.47
1:C:128:ALA:HB3	1:C:129:PRO:HD3	1.96	0.47
1:D:8:LYS:CG	1:D:9:SER:H	2.27	0.47
1:E:128:ALA:HB3	1:E:129:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ARG:NH1	1:B:148:GLU:HG2	2.30	0.47
1:F:37:TRP:CZ3	1:F:81:VAL:HG23	2.50	0.47
1:E:95:LEU:CD2	1:E:120:VAL:CG2	2.93	0.47
1:E:236:ASP:OD2	1:E:241:ASP:OD2	2.33	0.46
1:F:100:ASP:O	1:F:171:GLN:CG	2.60	0.46
1:G:236:ASP:OD2	1:G:241:ASP:OD2	2.33	0.46
1:E:120:VAL:HG12	1:E:143:ASP:N	2.29	0.46
1:H:120:VAL:HG12	1:H:143:ASP:N	2.30	0.46
1:A:240:MET:CE	1:H:18:PRO:HD2	2.46	0.46
1:B:189:LEU:HB3	1:G:289:MET:CE	2.46	0.46
1:H:128:ALA:HB3	1:H:129:PRO:HD3	1.97	0.46
1:A:240:MET:HE2	1:H:18:PRO:HD2	1.96	0.46
1:A:40:THR:HG1	1:A:42:ALA:N	2.13	0.46
1:B:194:VAL:HG12	1:B:257:VAL:HG21	1.98	0.46
1:B:83:GLU:HG3	1:D:80:ARG:NE	2.30	0.46
1:G:128:ALA:HB3	1:G:129:PRO:HD3	1.97	0.46
1:H:47:LEU:O	1:H:52:ALA:HB1	2.15	0.46
1:B:24:ALA:HB1	1:B:47:LEU:HD22	1.97	0.46
1:A:290:ASP:CG	1:H:196:ARG:HH11	2.19	0.46
1:A:286:VAL:HB	1:H:189:LEU:HD22	1.97	0.45
1:G:100:ASP:OD2	1:G:104:ALA:CB	2.64	0.45
1:B:251:THR:OG1	1:G:175:GLN:HG2	2.15	0.45
1:G:41:LYS:O	1:G:42:ALA:CB	2.64	0.45
1:D:142:GLY:O	1:D:165:GLU:HA	2.17	0.45
1:A:37:TRP:CH2	1:A:81:VAL:HG23	2.52	0.45
1:B:142:GLY:O	1:B:165:GLU:HA	2.17	0.45
1:B:144:ARG:NH1	1:B:148:GLU:CG	2.79	0.45
1:H:54:VAL:CG2	1:H:54:VAL:O	2.65	0.45
1:B:196:ARG:NH1	1:G:290:ASP:OD2	2.48	0.44
1:F:99:SER:HB2	1:F:174:TYR:CE2	2.52	0.44
1:H:100:ASP:O	1:H:171:GLN:CG	2.62	0.44
1:C:142:GLY:O	1:C:165:GLU:HA	2.17	0.44
1:F:37:TRP:CH2	1:F:81:VAL:HG23	2.53	0.44
1:B:194:VAL:HG22	1:G:176:ILE:HG12	1.97	0.44
1:D:230:ARG:HG3	1:D:231:PHE:N	2.28	0.44
1:E:144:ARG:NE	1:E:148:GLU:OE1	2.50	0.44
1:A:37:TRP:CZ3	1:A:81:VAL:HG21	2.52	0.44
1:H:142:GLY:O	1:H:165:GLU:HA	2.17	0.43
1:G:196:ARG:HA	3:G:2012:HOH:O	2.17	0.43
1:H:59:ALA:O	1:H:63:ARG:HG3	2.18	0.43
1:A:35:THR:HG22	3:A:2003:HOH:O	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ALA:O	1:B:63:ARG:HG3	2.19	0.43
1:F:142:GLY:O	1:F:165:GLU:HA	2.19	0.43
1:G:43:LYS:C	1:G:45:GLU:N	2.70	0.43
1:C:185:MET:HE2	1:F:215:MET:CE	2.39	0.43
1:A:186:THR:HG21	1:H:265:VAL:HG13	2.00	0.42
1:C:59:ALA:O	1:C:63:ARG:HG3	2.20	0.42
1:H:16:LEU:HD22	1:H:44:ALA:HB2	2.00	0.42
1:F:277:PHE:CE1	1:F:284:ARG:NH1	2.87	0.42
1:G:142:GLY:O	1:G:165:GLU:HA	2.19	0.42
1:G:28:LEU:O	1:G:29:GLU:C	2.55	0.42
1:D:59:ALA:O	1:D:63:ARG:HG3	2.20	0.42
1:B:83:GLU:HG3	1:D:80:ARG:CD	2.50	0.42
1:B:83:GLU:O	1:B:86:GLU:OE1	2.38	0.42
1:D:128:ALA:HA	1:D:131:ILE:CD1	2.44	0.42
1:E:95:LEU:HD23	1:E:120:VAL:CG2	2.49	0.42
1:H:42:ALA:C	1:H:44:ALA:N	2.73	0.42
1:A:142:GLY:O	1:A:165:GLU:HA	2.20	0.42
1:B:50:ARG:HD3	1:F:134:SER:HB3	2.02	0.42
1:F:59:ALA:O	1:F:63:ARG:HG3	2.19	0.42
1:H:95:LEU:CD2	1:H:120:VAL:HG22	2.48	0.42
1:A:153:LEU:HD23	1:A:153:LEU:C	2.41	0.41
1:D:19:MET:CE	1:D:124:VAL:HG11	2.50	0.41
1:E:95:LEU:CD2	1:E:120:VAL:HG22	2.49	0.41
1:G:68:VAL:CB	1:G:93:THR:O	2.68	0.41
1:H:99:SER:HB2	1:H:174:TYR:CE2	2.55	0.41
1:B:190:HIS:NE2	1:B:262:PRO:HG3	2.35	0.41
1:F:12:THR:HA	1:F:35:THR:O	2.20	0.41
1:A:144:ARG:HD2	1:A:162:PHE:CE2	2.55	0.41
1:E:142:GLY:O	1:E:165:GLU:HA	2.20	0.41
1:A:29:GLU:CG	3:A:2010:HOH:O	2.67	0.41
1:H:125:MET:O	1:H:136:VAL:HG23	2.21	0.41
1:G:19:MET:HE1	1:G:127:PRO:C	2.41	0.41
1:C:189:LEU:HB3	1:F:289:MET:CE	2.50	0.41
1:B:190:HIS:O	1:B:194:VAL:HG13	2.20	0.41
1:D:189:LEU:HB3	1:E:289:MET:HE1	2.02	0.41
1:H:95:LEU:HD22	1:H:120:VAL:CG2	2.51	0.41
1:D:83:GLU:O	1:D:86:GLU:OE1	2.39	0.41
1:E:77:VAL:O	1:E:81:VAL:CG1	2.46	0.41
1:G:143:ASP:CB	3:G:2008:HOH:O	2.69	0.41
1:H:240:MET:HG3	3:H:2028:HOH:O	2.20	0.40
1:H:136:VAL:CG1	1:H:158:THR:OG1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ALA:O	1:A:63:ARG:HG3	2.22	0.40
1:G:21:GLN:H	1:G:21:GLN:HG2	1.62	0.40
1:D:257:VAL:H	1:D:257:VAL:HG12	1.65	0.40
1:H:19:MET:CE	1:H:124:VAL:HG11	2.50	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	283/293 (97%)	279 (99%)	4 (1%)	0	100	100
1	B	278/293 (95%)	272 (98%)	5 (2%)	1 (0%)	34	35
1	C	281/293 (96%)	278 (99%)	3 (1%)	0	100	100
1	D	283/293 (97%)	280 (99%)	3 (1%)	0	100	100
1	E	257/293 (88%)	250 (97%)	6 (2%)	1 (0%)	34	35
1	F	281/293 (96%)	277 (99%)	4 (1%)	0	100	100
1	G	263/293 (90%)	240 (91%)	10 (4%)	13 (5%)	2	0
1	H	270/293 (92%)	267 (99%)	3 (1%)	0	100	100
All	All	2196/2344 (94%)	2143 (98%)	38 (2%)	15 (1%)	22	20

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	28	LEU
1	G	29	GLU
1	G	34	LEU
1	G	52	ALA
1	G	58	PRO
1	B	42	ALA

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Mol	Chain	Res	Type
1	G	33	GLU
1	G	39	ARG
1	G	40	THR
1	G	42	ALA
1	G	43	LYS
1	G	44	ALA
1	E	235	GLU
1	G	22	ALA
1	G	57	SER

### 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	199/214 (93%)	183 (92%)	16 (8%)	12	8
1	B	188/214 (88%)	178 (95%)	10 (5%)	22	21
1	C	200/214 (94%)	184 (92%)	16 (8%)	12	8
1	D	193/214 (90%)	183 (95%)	10 (5%)	23	22
1	E	169/214 (79%)	155 (92%)	14 (8%)	11	7
1	F	196/214 (92%)	183 (93%)	13 (7%)	16	14
1	G	137/214 (64%)	125 (91%)	12 (9%)	10	6
1	H	181/214 (85%)	168 (93%)	13 (7%)	14	11
All	All	1463/1712 (86%)	1359 (93%)	104 (7%)	14	11

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	27	LEU
1	A	29	GLU
1	A	34	LEU
1	A	35	THR
1	A	47	LEU

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Mol	Chain	Res	Type
1	A	54	VAL
1	A	62	LEU
1	A	99	SER
1	A	177	LEU
1	A	189	LEU
1	A	234	ASP
1	A	236	ASP
1	A	245	MET
1	A	270	ARG
1	A	288	LEU
1	B	16	LEU
1	B	83	GLU
1	B	99	SER
1	B	189	LEU
1	B	192	LEU
1	B	194	VAL
1	B	198	GLU
1	B	236	ASP
1	B	245	MET
1	B	279	GLU
1	C	9	SER
1	C	12	THR
1	C	29	GLU
1	C	47	LEU
1	C	54	VAL
1	C	62	LEU
1	C	90	LYS
1	C	99	SER
1	C	189	LEU
1	C	192	LEU
1	C	211	GLU
1	C	228	GLU
1	C	234	ASP
1	C	236	ASP
1	C	245	MET
1	C	288	LEU
1	D	9	SER
1	D	12	THR
1	D	13	LEU
1	D	47	LEU
1	D	118	ARG
1	D	192	LEU

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Mol	Chain	Res	Type
1	D	245	MET
1	D	249	VAL
1	D	259	THR
1	D	263	GLU
1	E	12	THR
1	E	21	GLN
1	E	72	LEU
1	E	99	SER
1	E	118	ARG
1	E	121	THR
1	E	144	ARG
1	E	148	GLU
1	E	211	GLU
1	E	215	MET
1	E	236	ASP
1	E	245	MET
1	E	246	GLU
1	E	253	ARG
1	F	9	SER
1	F	38	ASN
1	F	73	THR
1	F	99	SER
1	F	135	SER
1	F	144	ARG
1	F	158	THR
1	F	171	GLN
1	F	189	LEU
1	F	211	GLU
1	F	236	ASP
1	F	245	MET
1	F	284	ARG
1	G	19	MET
1	G	21	GLN
1	G	23	MET
1	G	121	THR
1	G	163	ARG
1	G	171	GLN
1	G	175	GLN
1	G	236	ASP
1	G	240	MET
1	G	245	MET
1	G	246	GLU

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Mol	Chain	Res	Type
1	G	288	LEU
1	H	9	SER
1	H	12	THR
1	H	14	ILE
1	H	16	LEU
1	H	54	VAL
1	H	99	SER
1	H	144	ARG
1	H	158	THR
1	H	171	GLN
1	H	198	GLU
1	H	245	MET
1	H	263	GLU
1	H	284	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	175	GLN
1	A	247	HIS
1	B	75	HIS
1	B	171	GLN
1	B	190	HIS
1	C	171	GLN
1	D	75	HIS
1	D	171	GLN
1	D	175	GLN
1	F	38	ASN
1	F	75	HIS
1	F	171	GLN
1	F	213	ASN
1	G	75	HIS
1	G	171	GLN
1	G	213	ASN
1	H	38	ASN
1	H	171	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	H	1000	-	20,20,20	1.81	4 (20%)	25,25,25	2.09	5 (20%)
2	BOG	F	1000	-	20,20,20	1.25	1 (5%)	25,25,25	1.15	2 (8%)

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	H	1000	-	-	6/11/31/31	0/1/1/1
2	BOG	F	1000	-	-	6/11/31/31	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1000	BOG	O1-C1	5.93	1.50	1.40
2	F	1000	BOG	O1-C1	3.85	1.46	1.40
2	H	1000	BOG	C4-C3	2.97	1.59	1.52
2	H	1000	BOG	O5-C1	2.41	1.48	1.41
2	H	1000	BOG	C3-C2	2.20	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1000	BOG	O5-C1-O1	7.61	128.00	109.97
2	F	1000	BOG	C6'-C5'-C4'	-2.88	99.80	114.42
2	H	1000	BOG	C6'-C5'-C4'	-2.80	100.23	114.42
2	H	1000	BOG	C3'-C2'-C1'	-2.69	101.55	113.49
2	F	1000	BOG	C3'-C2'-C1'	-2.69	101.56	113.49
2	H	1000	BOG	C1'-O1-C1	2.23	117.54	113.84
2	H	1000	BOG	O5-C5-C6	2.01	111.43	106.44

There are no chirality outliers.

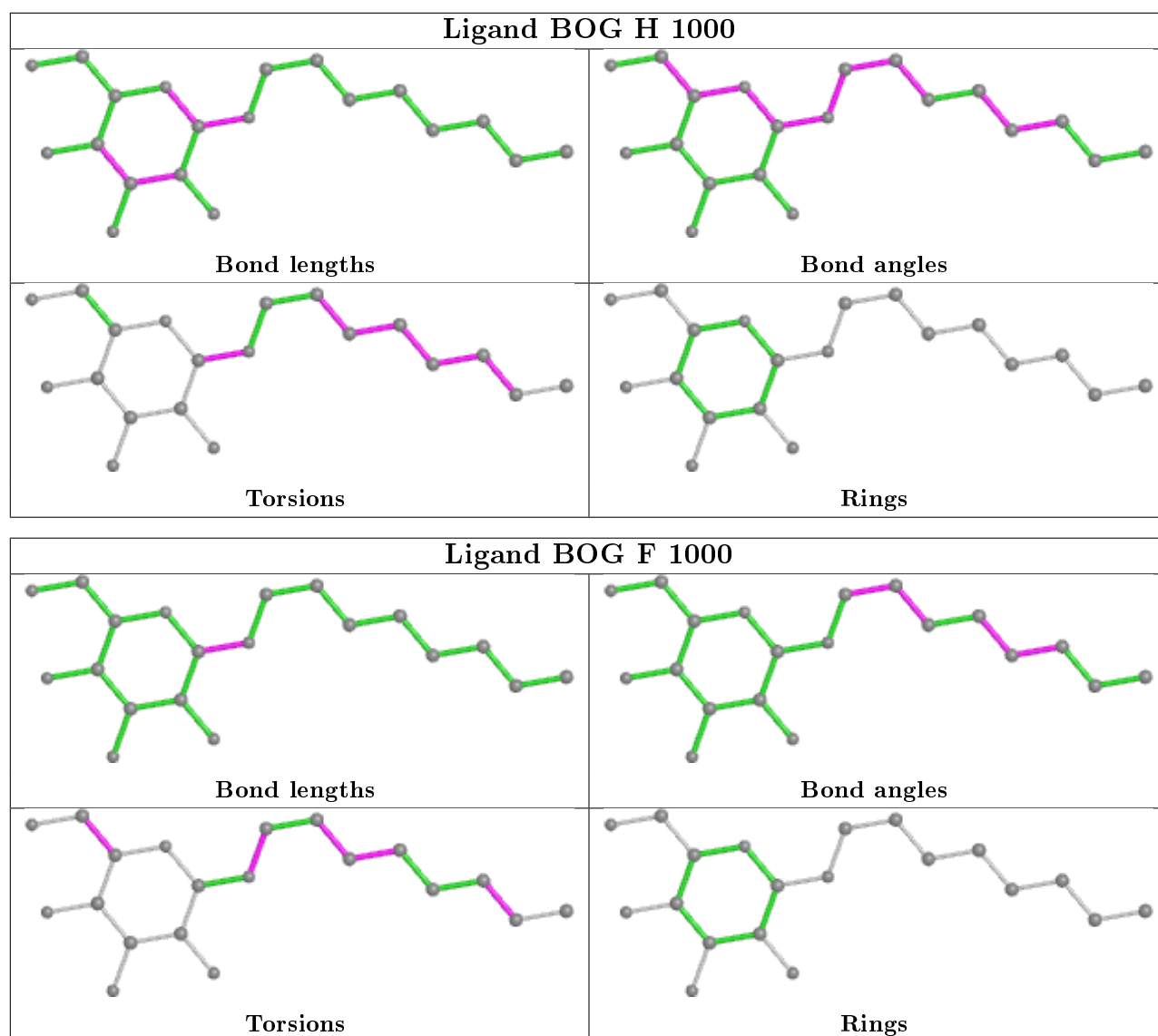
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1000	BOG	O5-C1-O1-C1'
2	F	1000	BOG	C2'-C3'-C4'-C5'
2	H	1000	BOG	C4'-C5'-C6'-C7'
2	H	1000	BOG	C2'-C3'-C4'-C5'
2	F	1000	BOG	C1'-C2'-C3'-C4'
2	H	1000	BOG	C1'-C2'-C3'-C4'
2	H	1000	BOG	C5'-C6'-C7'-C8'
2	F	1000	BOG	C5'-C6'-C7'-C8'
2	F	1000	BOG	C2'-C1'-O1-C1
2	F	1000	BOG	C4-C5-C6-O6
2	F	1000	BOG	O5-C5-C6-O6
2	H	1000	BOG	C3'-C4'-C5'-C6'

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	13:LEU	C	14:ILE	N	1.01

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	285/293 (97%)	-0.15	2 (0%) 87 87	26, 43, 70, 102	0
1	B	282/293 (96%)	-0.21	0 100 100	26, 45, 76, 102	0
1	C	283/293 (96%)	-0.22	0 100 100	25, 40, 66, 88	0
1	D	285/293 (97%)	-0.25	1 (0%) 92 93	26, 40, 72, 93	0
1	E	267/293 (91%)	0.46	30 (11%) 5 4	25, 56, 96, 117	0
1	F	283/293 (96%)	-0.16	3 (1%) 80 81	23, 40, 76, 102	0
1	G	269/293 (91%)	0.88	56 (20%) 1 0	27, 70, 124, 141	0
1	H	278/293 (94%)	0.25	11 (3%) 38 38	28, 56, 92, 109	0
All	All	2232/2344 (95%)	0.07	103 (4%) 32 32	23, 46, 94, 141	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	37	TRP	8.0
1	G	44	ALA	6.5
1	G	145	ALA	6.1
1	G	54	VAL	6.1
1	H	27	LEU	5.8
1	G	142	GLY	5.7
1	G	128	ALA	5.0
1	G	84	GLY	5.0
1	G	36	VAL	5.0
1	G	51	GLY	4.9
1	E	145	ALA	4.7
1	E	24	ALA	4.7
1	E	114	GLY	4.6
1	E	65	GLY	4.6
1	H	30	ALA	4.5
1	G	64	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	110	ALA	4.2
1	G	62	LEU	4.1
1	E	11	VAL	4.1
1	G	50	ARG	4.1
1	G	147	PHE	4.1
1	G	26	ALA	4.0
1	G	114	GLY	4.0
1	F	40	THR	4.0
1	G	24	ALA	4.0
1	G	27	LEU	3.9
1	E	67	PRO	3.8
1	G	76	ALA	3.8
1	G	39	ARG	3.8
1	A	42	ALA	3.6
1	G	46	ALA	3.5
1	E	119	TYR	3.5
1	G	150	ASN	3.5
1	G	105	SER	3.3
1	E	34	LEU	3.3
1	E	26	ALA	3.3
1	E	14	ILE	3.3
1	G	20	GLY	3.3
1	G	82	LEU	3.2
1	E	64	ALA	3.2
1	H	46	ALA	3.2
1	G	117	ALA	3.1
1	G	95	LEU	3.1
1	E	30	ALA	3.1
1	G	47	LEU	3.1
1	E	61	ALA	3.1
1	G	22	ALA	3.1
1	G	23	MET	3.0
1	H	154	LEU	3.0
1	H	26	ALA	2.9
1	G	49	GLU	2.9
1	G	53	ALA	2.9
1	G	57	SER	2.8
1	G	70	LEU	2.8
1	H	52	ALA	2.8
1	E	87	SER	2.8
1	E	12	THR	2.8
1	G	119	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	82	LEU	2.8
1	E	16	LEU	2.7
1	G	131	ILE	2.7
1	G	42	ALA	2.7
1	G	59	ALA	2.7
1	G	78	MET	2.7
1	E	81	VAL	2.7
1	G	79	TYR	2.7
1	E	32	TYR	2.6
1	G	107	ALA	2.6
1	A	229	GLY	2.6
1	H	95	LEU	2.5
1	G	81	VAL	2.5
1	G	25	GLY	2.5
1	G	93	THR	2.5
1	G	121	THR	2.5
1	G	83	GLU	2.5
1	G	61	ALA	2.4
1	G	153	LEU	2.4
1	D	134	SER	2.4
1	E	233	GLY	2.4
1	G	135	SER	2.4
1	E	15	GLY	2.4
1	E	95	LEU	2.3
1	G	31	GLY	2.3
1	E	35	THR	2.3
1	H	54	VAL	2.3
1	E	144	ARG	2.2
1	F	13	LEU	2.2
1	G	34	LEU	2.2
1	E	115	HIS	2.2
1	F	11	VAL	2.2
1	E	37	TRP	2.2
1	H	31	GLY	2.2
1	E	27	LEU	2.1
1	G	139	PHE	2.1
1	H	48	ALA	2.1
1	E	28	LEU	2.1
1	E	20	GLY	2.1
1	G	60	GLU	2.1
1	G	111	TRP	2.1
1	H	93	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	115	HIS	2.0
1	E	62	LEU	2.0
1	G	56	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 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, 95<sup>th</sup> 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.

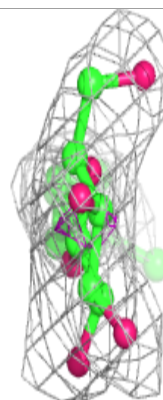
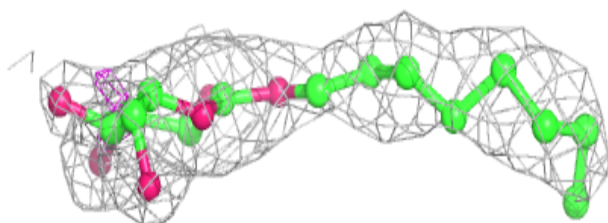
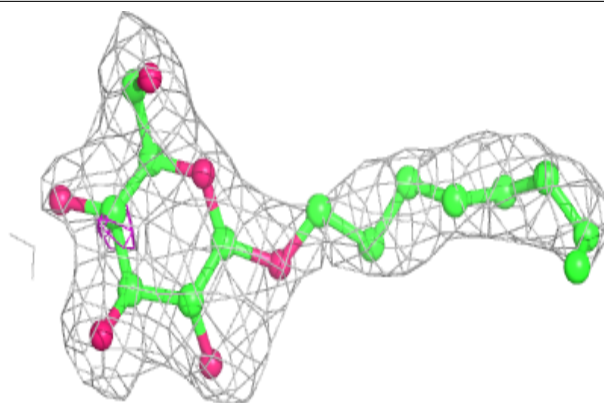
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BOG	H	1000	20/20	0.82	0.19	45,53,68,73	0
2	BOG	F	1000	20/20	0.94	0.12	36,46,69,69	0

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.

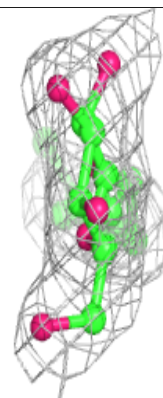
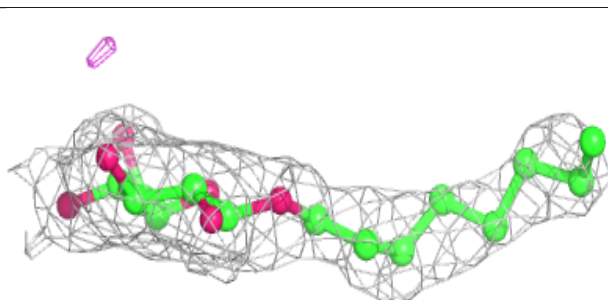
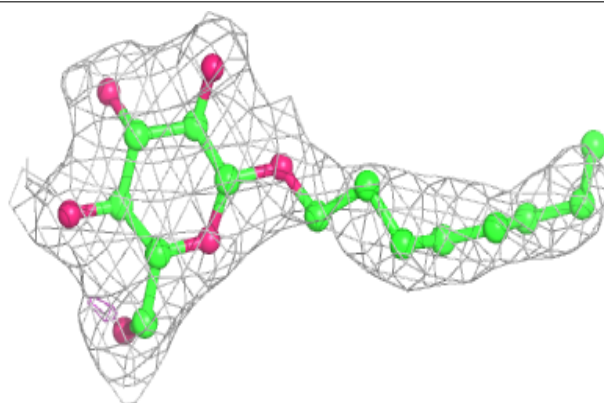


**Electron density around BOG H 1000:**

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

**Electron density around BOG F 1000:**

$2mF_o-DF_c$  (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.