



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:26 AM UTC

PDB ID : 4FC4 / pdb\_00004fc4  
Title : FNT family ion channel  
Authors : Lue, W.; Schwarzer, N.; Du, J.; Gerbig-Smentek, E.; Andrade, S.L.A.; Einsle, O.  
Deposited on : 2012-05-24  
Resolution : 2.40 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.

The types of validation reports are described at

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

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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)  
Xtrriage (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

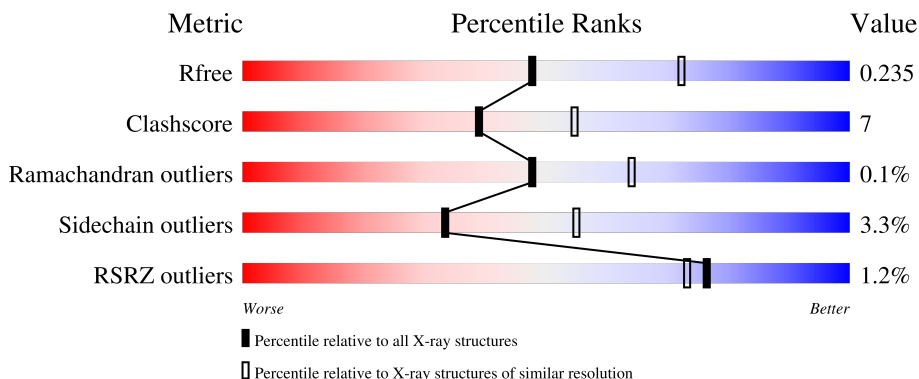
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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  $\geq 3$ , 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	261	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      76%      17%      .. 5%</p>
1	B	261	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">%      79%      15%      ..</p>
1	C	261	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">%      76%      19%      ..</p>
1	D	261	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">%      78%      16%      . 5%</p>
1	E	261	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">%      78%      16%      ..</p>

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Mol	Chain	Length	Quality of chain
1	F	261	
1	G	261	
1	H	261	
1	I	261	
1	J	261	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19016 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 Nitrite transporter NirC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	249	1874	1241	303	318	12	0	0	0
1	B	250	1881	1246	304	319	12	0	0	0
1	C	250	1881	1246	304	319	12	0	0	0
1	D	249	1873	1241	303	318	11	0	0	0
1	E	250	1881	1246	304	319	12	0	0	0
1	F	250	1881	1246	304	319	12	0	0	0
1	G	248	1866	1236	302	317	11	0	0	0
1	H	250	1881	1246	304	319	12	0	0	0
1	I	250	1881	1246	304	319	12	0	0	0
1	J	250	1881	1246	304	319	12	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	LEU	-	expression tag	UNP E8XE9
A	255	GLU	-	expression tag	UNP E8XE9
A	256	HIS	-	expression tag	UNP E8XE9
A	257	HIS	-	expression tag	UNP E8XE9
A	258	HIS	-	expression tag	UNP E8XE9
A	259	HIS	-	expression tag	UNP E8XE9
A	260	HIS	-	expression tag	UNP E8XE9
A	261	HIS	-	expression tag	UNP E8XE9
B	254	LEU	-	expression tag	UNP E8XE9

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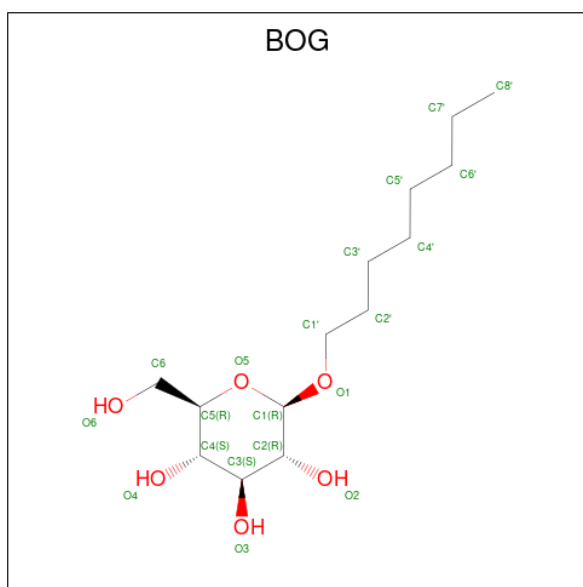
Chain	Residue	Modelled	Actual	Comment	Reference
B	255	GLU	-	expression tag	UNP E8XE9
B	256	HIS	-	expression tag	UNP E8XE9
B	257	HIS	-	expression tag	UNP E8XE9
B	258	HIS	-	expression tag	UNP E8XE9
B	259	HIS	-	expression tag	UNP E8XE9
B	260	HIS	-	expression tag	UNP E8XE9
B	261	HIS	-	expression tag	UNP E8XE9
C	254	LEU	-	expression tag	UNP E8XE9
C	255	GLU	-	expression tag	UNP E8XE9
C	256	HIS	-	expression tag	UNP E8XE9
C	257	HIS	-	expression tag	UNP E8XE9
C	258	HIS	-	expression tag	UNP E8XE9
C	259	HIS	-	expression tag	UNP E8XE9
C	260	HIS	-	expression tag	UNP E8XE9
C	261	HIS	-	expression tag	UNP E8XE9
D	254	LEU	-	expression tag	UNP E8XE9
D	255	GLU	-	expression tag	UNP E8XE9
D	256	HIS	-	expression tag	UNP E8XE9
D	257	HIS	-	expression tag	UNP E8XE9
D	258	HIS	-	expression tag	UNP E8XE9
D	259	HIS	-	expression tag	UNP E8XE9
D	260	HIS	-	expression tag	UNP E8XE9
D	261	HIS	-	expression tag	UNP E8XE9
E	254	LEU	-	expression tag	UNP E8XE9
E	255	GLU	-	expression tag	UNP E8XE9
E	256	HIS	-	expression tag	UNP E8XE9
E	257	HIS	-	expression tag	UNP E8XE9
E	258	HIS	-	expression tag	UNP E8XE9
E	259	HIS	-	expression tag	UNP E8XE9
E	260	HIS	-	expression tag	UNP E8XE9
E	261	HIS	-	expression tag	UNP E8XE9
F	254	LEU	-	expression tag	UNP E8XE9
F	255	GLU	-	expression tag	UNP E8XE9
F	256	HIS	-	expression tag	UNP E8XE9
F	257	HIS	-	expression tag	UNP E8XE9
F	258	HIS	-	expression tag	UNP E8XE9
F	259	HIS	-	expression tag	UNP E8XE9
F	260	HIS	-	expression tag	UNP E8XE9
F	261	HIS	-	expression tag	UNP E8XE9
G	254	LEU	-	expression tag	UNP E8XE9
G	255	GLU	-	expression tag	UNP E8XE9
G	256	HIS	-	expression tag	UNP E8XE9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	257	HIS	-	expression tag	UNP E8XEH9
G	258	HIS	-	expression tag	UNP E8XEH9
G	259	HIS	-	expression tag	UNP E8XEH9
G	260	HIS	-	expression tag	UNP E8XEH9
G	261	HIS	-	expression tag	UNP E8XEH9
H	254	LEU	-	expression tag	UNP E8XEH9
H	255	GLU	-	expression tag	UNP E8XEH9
H	256	HIS	-	expression tag	UNP E8XEH9
H	257	HIS	-	expression tag	UNP E8XEH9
H	258	HIS	-	expression tag	UNP E8XEH9
H	259	HIS	-	expression tag	UNP E8XEH9
H	260	HIS	-	expression tag	UNP E8XEH9
H	261	HIS	-	expression tag	UNP E8XEH9
I	254	LEU	-	expression tag	UNP E8XEH9
I	255	GLU	-	expression tag	UNP E8XEH9
I	256	HIS	-	expression tag	UNP E8XEH9
I	257	HIS	-	expression tag	UNP E8XEH9
I	258	HIS	-	expression tag	UNP E8XEH9
I	259	HIS	-	expression tag	UNP E8XEH9
I	260	HIS	-	expression tag	UNP E8XEH9
I	261	HIS	-	expression tag	UNP E8XEH9
J	254	LEU	-	expression tag	UNP E8XEH9
J	255	GLU	-	expression tag	UNP E8XEH9
J	256	HIS	-	expression tag	UNP E8XEH9
J	257	HIS	-	expression tag	UNP E8XEH9
J	258	HIS	-	expression tag	UNP E8XEH9
J	259	HIS	-	expression tag	UNP E8XEH9
J	260	HIS	-	expression tag	UNP E8XEH9
J	261	HIS	-	expression tag	UNP E8XEH9

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: 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	F	1	Total	C O	0	0
			20	14 6		


- Molecule 3 is water.

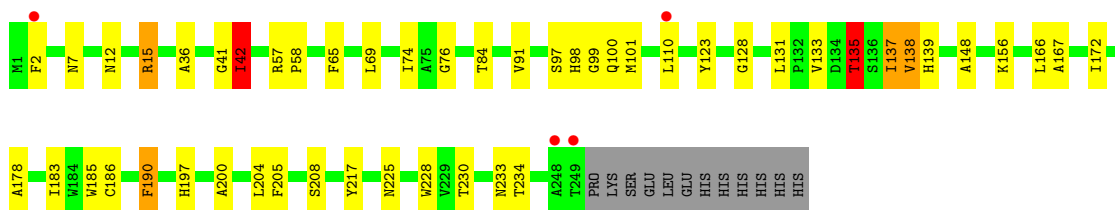
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	22	Total	O	0	0
			22	22		
3	C	11	Total	O	0	0
			11	11		
3	D	13	Total	O	0	0
			13	13		
3	E	15	Total	O	0	0
			15	15		
3	F	13	Total	O	0	0
			13	13		
3	G	11	Total	O	0	0
			11	11		
3	H	17	Total	O	0	0
			17	17		
3	I	40	Total	O	0	0
			40	40		
3	J	16	Total	O	0	0
			16	16		

### 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.

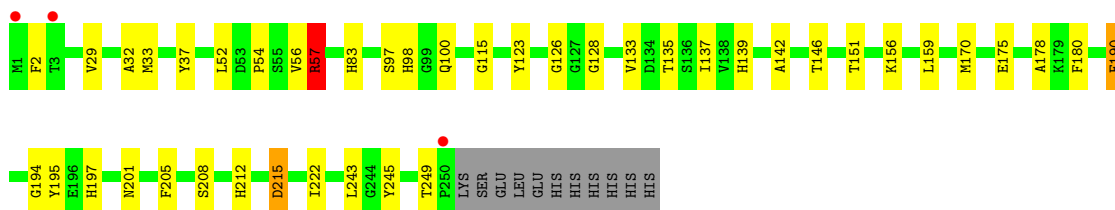
- Molecule 1: Nitrite transporter NirC

Chain A:  76% 17% 2% 5%




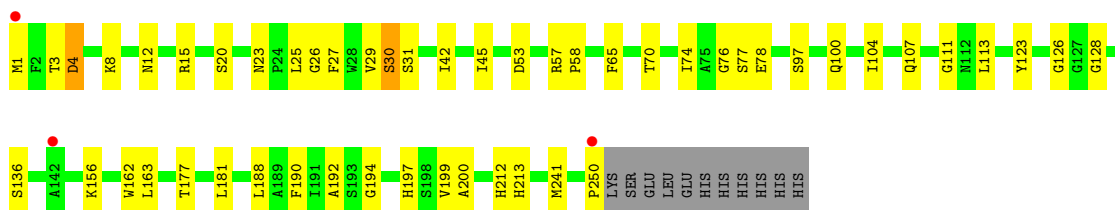
- Molecule 1: Nitrite transporter NirC

Chain B:  79% 15% 6% 1%




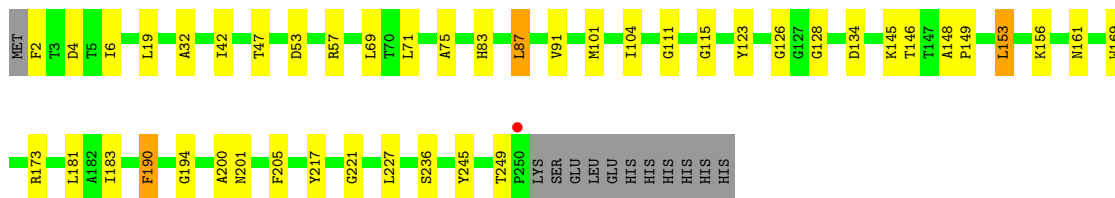
- Molecule 1: Nitrite transporter NirC

Chain C:  76% 19% 5% 0%

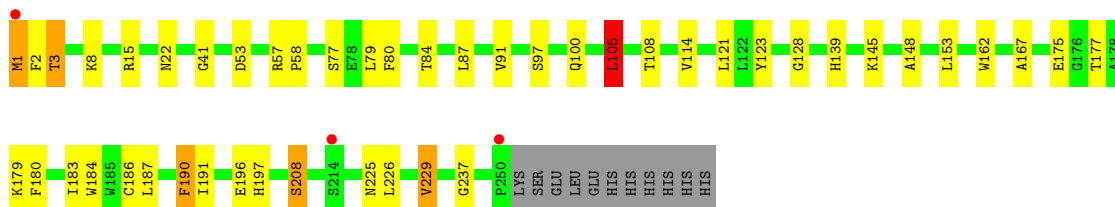
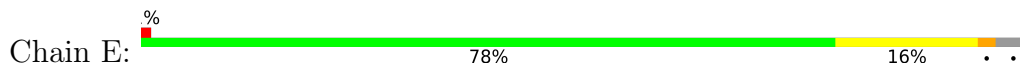


- Molecule 1: Nitrite transporter NirC

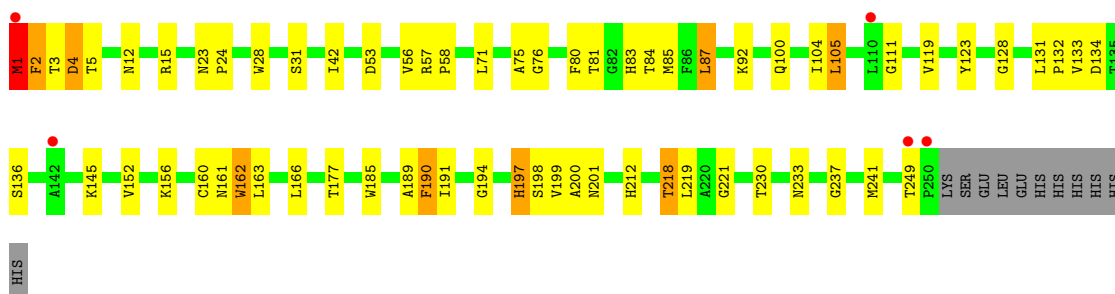
Chain D:  78% 16% 6% 0%



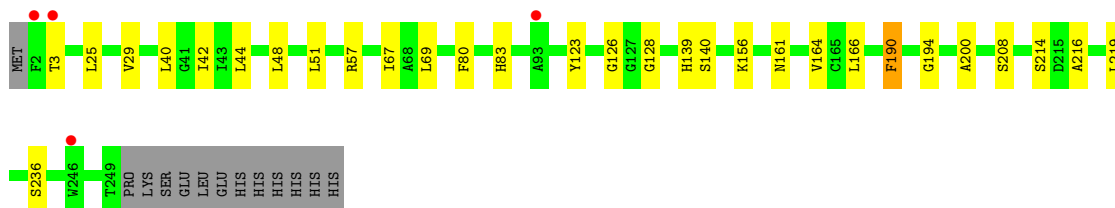
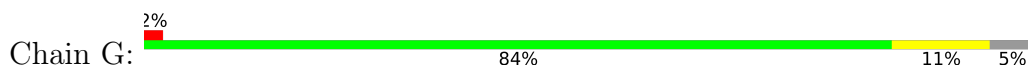
- Molecule 1: Nitrite transporter NirC



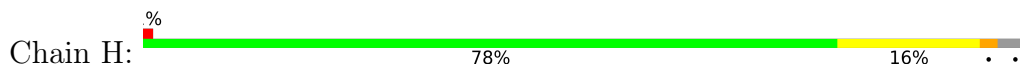
- Molecule 1: Nitrite transporter NirC



- Molecule 1: Nitrite transporter NirC

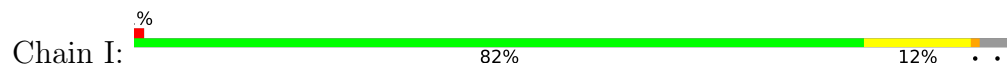


- Molecule 1: Nitrite transporter NirC

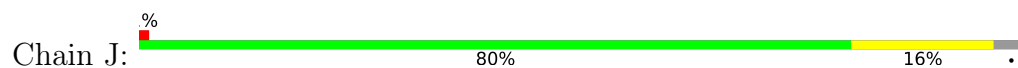




- Molecule 1: Nitrite transporter NirC



- Molecule 1: Nitrite transporter NirC



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.30Å 101.84Å 205.30Å 90.00° 101.24° 90.00°	Depositor
Resolution (Å)	87.75 – 2.40 87.75 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (87.75-2.40) 97.1 (87.75-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.40Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.192 , 0.236 0.192 , 0.235	Depositor DCC
$R_{free}$ test set	6772 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtrriage
Anisotropy	0.138	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 i

### 5.1 Standard geometry i

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	1.41	5/1928 (0.3%)	1.33	16/2638 (0.6%)
1	B	1.25	5/1936 (0.3%)	1.13	4/2650 (0.2%)
1	C	1.20	2/1936 (0.1%)	1.17	4/2650 (0.2%)
1	D	1.18	2/1928 (0.1%)	1.16	2/2640 (0.1%)
1	E	1.32	7/1936 (0.4%)	1.28	9/2650 (0.3%)
1	F	1.28	6/1936 (0.3%)	1.23	8/2650 (0.3%)
1	G	1.22	2/1920 (0.1%)	1.20	3/2628 (0.1%)
1	H	1.37	6/1936 (0.3%)	1.28	11/2650 (0.4%)
1	I	1.41	8/1936 (0.4%)	1.31	12/2650 (0.5%)
1	J	1.27	5/1936 (0.3%)	1.16	2/2650 (0.1%)
All	All	1.29	48/19328 (0.2%)	1.23	71/26456 (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	F	0	1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	83	HIS	CE1-NE2	7.04	1.39	1.32
1	H	197	HIS	ND1-CE1	6.96	1.39	1.32
1	G	83	HIS	CG-CD2	6.90	1.43	1.35
1	J	83	HIS	CG-CD2	6.80	1.43	1.35
1	E	197	HIS	CG-CD2	6.59	1.43	1.35
1	D	149	PRO	C-O	6.47	1.31	1.23
1	E	197	HIS	ND1-CE1	6.42	1.39	1.32
1	J	44	LEU	N-CA	6.22	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	212	HIS	ND1-CE1	6.16	1.38	1.32
1	A	204	LEU	C-O	6.08	1.31	1.24
1	F	197	HIS	CG-CD2	6.01	1.42	1.35
1	B	197	HIS	CG-CD2	6.00	1.42	1.35
1	F	197	HIS	ND1-CE1	5.95	1.38	1.32
1	I	224	HIS	CG-CD2	5.88	1.42	1.35
1	B	197	HIS	ND1-CE1	5.81	1.38	1.32
1	F	219	LEU	CA-C	5.77	1.60	1.52
1	A	98	HIS	CG-CD2	5.72	1.42	1.35
1	F	212	HIS	CG-CD2	5.71	1.42	1.35
1	B	98	HIS	CG-CD2	5.68	1.42	1.35
1	I	212	HIS	CG-CD2	5.68	1.42	1.35
1	H	31	SER	N-CA	5.64	1.53	1.46
1	B	212	HIS	CG-CD2	5.56	1.42	1.35
1	C	213	HIS	CG-CD2	5.55	1.42	1.35
1	E	77	SER	N-CA	5.54	1.53	1.46
1	D	53	ASP	CA-C	5.54	1.58	1.53
1	J	185	TRP	CD2-CE2	5.54	1.50	1.41
1	A	197	HIS	ND1-CE1	5.48	1.38	1.32
1	F	197	HIS	CE1-NE2	5.44	1.38	1.32
1	E	184	TRP	CG-CD2	5.35	1.53	1.43
1	F	133	VAL	CA-CB	5.29	1.59	1.53
1	A	185	TRP	CD2-CE2	5.28	1.50	1.41
1	I	139	HIS	CD2-NE2	-5.26	1.32	1.37
1	E	208	SER	C-O	5.25	1.30	1.24
1	J	197	HIS	CG-CD2	5.24	1.41	1.35
1	I	137	ILE	C-O	5.24	1.30	1.24
1	A	233	ASN	CA-C	5.23	1.59	1.52
1	H	212	HIS	CG-CD2	5.22	1.41	1.35
1	E	108	THR	N-CA	-5.21	1.40	1.46
1	I	197	HIS	CG-ND1	-5.20	1.32	1.38
1	H	174	THR	C-O	5.18	1.30	1.23
1	J	212	HIS	CG-CD2	5.18	1.41	1.35
1	H	209	TRP	CD2-CE2	5.17	1.50	1.41
1	H	184	TRP	CG-CD2	5.10	1.52	1.43
1	I	98	HIS	CG-CD2	5.09	1.41	1.35
1	C	212	HIS	CG-CD2	5.07	1.41	1.35
1	E	15	ARG	C-O	5.07	1.29	1.24
1	I	224	HIS	ND1-CE1	5.04	1.37	1.32
1	B	83	HIS	CG-CD2	5.04	1.41	1.35

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ALA	CA-C-N	-8.62	111.50	120.03
1	A	148	ALA	C-N-CA	-8.62	111.50	120.03
1	F	2	PHE	N-CA-C	8.41	123.92	112.90
1	E	105	LEU	CA-C-N	-7.65	111.84	119.56
1	E	105	LEU	C-N-CA	-7.65	111.84	119.56
1	G	57	ARG	CA-C-N	-7.48	111.05	119.28
1	G	57	ARG	C-N-CA	-7.48	111.05	119.28
1	I	137	ILE	N-CA-C	6.98	117.69	110.36
1	A	41	GLY	N-CA-C	-6.93	103.90	112.77
1	A	172	ILE	CB-CA-C	-6.92	102.80	112.14
1	A	138	VAL	N-CA-CB	6.90	119.93	110.54
1	A	15	ARG	NE-CZ-NH1	-6.79	114.71	121.50
1	H	57	ARG	CA-C-N	-6.67	111.94	119.28
1	H	57	ARG	C-N-CA	-6.67	111.94	119.28
1	F	56	VAL	N-CA-C	-6.61	106.80	113.47
1	J	43	ILE	N-CA-C	-6.48	104.01	110.62
1	A	230	THR	N-CA-C	-6.41	104.38	111.36
1	H	53	ASP	CA-C-N	-6.39	113.05	119.56
1	H	53	ASP	C-N-CA	-6.39	113.05	119.56
1	J	104	ILE	N-CA-C	6.31	116.94	110.82
1	F	162	TRP	N-CA-C	-6.29	104.04	111.03
1	E	148	ALA	CA-C-N	-6.29	113.47	120.14
1	E	148	ALA	C-N-CA	-6.29	113.47	120.14
1	A	137	ILE	N-CA-C	6.27	117.02	110.62
1	F	53	ASP	CB-CA-C	-5.95	98.44	110.17
1	F	134	ASP	N-CA-C	5.82	119.47	112.38
1	A	15	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	I	119	VAL	N-CA-C	5.80	116.58	110.72
1	H	219	LEU	N-CA-C	5.78	117.26	111.07
1	B	57	ARG	CA-C-N	-5.78	112.63	119.05
1	B	57	ARG	C-N-CA	-5.78	112.63	119.05
1	A	42	ILE	CG1-CB-CG2	-5.78	93.37	110.70
1	F	105	LEU	CA-C-N	-5.75	113.75	119.56
1	F	105	LEU	C-N-CA	-5.75	113.75	119.56
1	I	156	LYS	CD-CE-NZ	-5.75	93.49	111.90
1	I	57	ARG	CA-C-N	-5.72	112.70	119.05
1	I	57	ARG	C-N-CA	-5.72	112.70	119.05
1	A	183	ILE	N-CA-C	-5.69	104.97	110.72
1	I	99	GLY	N-CA-C	5.67	119.50	112.64
1	B	178	ALA	N-CA-C	-5.64	105.28	111.82
1	H	22	ASN	CA-C-N	-5.63	116.34	122.59
1	H	22	ASN	C-N-CA	-5.63	116.34	122.59
1	E	53	ASP	CA-C-N	-5.62	113.82	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	53	ASP	C-N-CA	-5.62	113.82	119.56
1	B	56	VAL	N-CA-C	-5.60	107.67	113.10
1	A	135	THR	N-CA-CB	-5.49	102.58	110.65
1	A	110	LEU	N-CA-C	5.49	117.34	111.36
1	C	163	LEU	N-CA-C	5.46	117.66	111.11
1	E	191	ILE	N-CA-C	-5.43	105.55	110.82
1	D	104	ILE	N-CA-C	5.42	115.62	110.53
1	I	168	ILE	N-CA-C	-5.39	105.27	110.72
1	C	23	ASN	CA-C-N	-5.37	113.38	119.28
1	C	23	ASN	C-N-CA	-5.37	113.38	119.28
1	E	41	GLY	N-CA-C	-5.35	106.19	113.37
1	H	148	ALA	CA-C-N	-5.34	114.46	119.85
1	H	148	ALA	C-N-CA	-5.34	114.46	119.85
1	H	2	PHE	N-CA-CB	5.33	119.50	110.49
1	I	136	SER	CA-C-N	5.30	127.44	120.60
1	I	136	SER	C-N-CA	5.30	127.44	120.60
1	I	23	ASN	CA-C-N	5.26	126.42	119.84
1	I	23	ASN	C-N-CA	5.26	126.42	119.84
1	I	145	LYS	N-CA-C	5.24	116.99	111.28
1	A	99	GLY	N-CA-C	5.17	118.89	112.64
1	A	74	ILE	N-CA-C	5.14	115.81	110.82
1	D	57	ARG	NE-CZ-NH1	-5.09	116.41	121.50
1	G	140	SER	N-CA-C	-5.09	105.43	111.69
1	H	84	THR	N-CA-CB	5.08	117.51	109.94
1	F	119	VAL	N-CA-C	5.08	115.31	110.53
1	C	53	ASP	CB-CA-C	-5.08	101.23	109.56
1	E	79	LEU	N-CA-C	5.05	116.92	107.99
1	A	228	TRP	N-CA-C	5.04	116.86	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	1	MET	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1874	0	1899	25	0
1	B	1881	0	1906	34	0
1	C	1881	0	1906	37	0
1	D	1873	0	1894	31	0
1	E	1881	0	1906	31	0
1	F	1881	0	1906	47	0
1	G	1866	0	1887	16	0
1	H	1881	0	1906	28	0
1	I	1881	0	1906	18	0
1	J	1881	0	1906	26	0
2	F	40	0	56	0	0
3	A	38	0	0	0	0
3	B	22	0	0	0	0
3	C	11	0	0	0	0
3	D	13	0	0	0	0
3	E	15	0	0	1	0
3	F	13	0	0	0	0
3	G	11	0	0	1	0
3	H	17	0	0	1	0
3	I	40	0	0	2	0
3	J	16	0	0	0	0
All	All	19016	0	19078	258	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 7.

All (258) 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:B:170:MET:HE3	1:C:74:ILE:HB	1.24	1.12
1:B:170:MET:CE	1:C:74:ILE:HB	1.81	1.09
1:F:218:THR:HG22	1:F:221:GLY:H	1.01	1.08
1:J:91:VAL:HG21	1:J:101:MET:HE3	1.41	1.02
1:C:12:ASN:OD1	1:C:15:ARG:NH2	1.95	0.99
1:E:97:SER:H	1:E:100:GLN:HE21	1.12	0.97
1:J:97:SER:H	1:J:100:GLN:HE21	1.16	0.92
1:F:218:THR:HG22	1:F:221:GLY:N	1.86	0.91
1:H:1:MET:HA	1:H:173:ARG:NH1	1.86	0.91
1:B:97:SER:H	1:B:100:GLN:HE21	1.12	0.90
1:F:85:MET:HE3	1:F:241:MET:HB3	1.55	0.89
1:F:218:THR:CG2	1:F:221:GLY:H	1.87	0.86
1:J:91:VAL:HG21	1:J:101:MET:CE	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:SER:H	1:F:233:ASN:HD21	1.26	0.82
1:J:91:VAL:CG2	1:J:101:MET:CE	2.57	0.82
1:B:133:VAL:HG12	1:B:135:THR:HG22	1.60	0.81
1:E:80:PHE:HE1	1:E:105:LEU:HD23	1.44	0.80
1:B:170:MET:HE1	1:C:70:THR:HG22	1.63	0.78
1:E:80:PHE:CE1	1:E:105:LEU:HD23	2.18	0.78
1:A:131:LEU:O	1:A:139:HIS:HE1	1.66	0.78
1:E:97:SER:H	1:E:100:GLN:NE2	1.82	0.78
1:F:160:CYS:SG	1:F:197:HIS:HB2	2.24	0.77
1:H:181:LEU:CD1	1:I:177:THR:HG23	2.14	0.77
1:H:1:MET:HA	1:H:173:ARG:HH12	1.51	0.74
1:F:12:ASN:OD1	1:F:15:ARG:NH2	2.19	0.74
1:C:100:GLN:O	1:C:104:ILE:HG12	1.86	0.73
1:J:91:VAL:CG2	1:J:101:MET:HE3	2.18	0.73
1:A:12:ASN:OD1	1:A:15:ARG:NH2	2.21	0.72
1:J:97:SER:H	1:J:100:GLN:NE2	1.86	0.71
1:H:181:LEU:HD11	1:I:177:THR:HG23	1.71	0.71
1:B:133:VAL:CG1	1:B:135:THR:HG22	2.21	0.70
1:C:25:LEU:O	1:C:29:VAL:HG12	1.90	0.70
1:F:81:THR:HB	1:F:161:ASN:ND2	2.08	0.69
1:B:97:SER:H	1:B:100:GLN:NE2	1.89	0.68
1:A:42:ILE:HD12	1:A:65:PHE:CE1	2.29	0.68
1:B:170:MET:HE3	1:C:74:ILE:CB	2.12	0.67
1:E:139:HIS:HD2	1:E:208:SER:OG	1.77	0.67
1:D:2:PHE:HD2	1:D:249:THR:HG22	1.60	0.67
1:C:42:ILE:HD11	1:C:200:ALA:HB1	1.77	0.66
1:F:57:ARG:HB3	1:F:58:PRO:HD3	1.77	0.66
1:B:170:MET:CE	1:C:74:ILE:CB	2.68	0.65
1:E:3:THR:HG21	1:H:4:ASP:OD1	1.97	0.64
1:C:31:SER:HB3	1:C:111:GLY:HA3	1.78	0.64
1:F:123:TYR:CE2	1:F:128:GLY:HA3	2.33	0.64
1:C:123:TYR:CE2	1:C:128:GLY:HA3	2.33	0.63
1:H:142:ALA:O	1:H:146:THR:HG23	1.99	0.63
1:H:181:LEU:HD11	1:I:177:THR:CG2	2.28	0.63
1:I:212:HIS:HD2	3:I:324:HOH:O	1.82	0.62
1:H:139:HIS:HD2	1:H:208:SER:OG	1.82	0.62
1:I:54:PRO:HA	1:I:57:ARG:HG3	1.81	0.62
1:C:162:TRP:HE1	1:C:241:MET:HE3	1.65	0.62
1:E:225:ASN:O	1:E:229:VAL:CG1	2.48	0.62
1:A:42:ILE:CD1	1:A:200:ALA:HB1	2.30	0.61
1:G:156:LYS:HE3	1:G:194:GLY:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:LYS:HD3	1:D:194:GLY:O	2.00	0.61
1:H:83:HIS:HB3	1:H:87:LEU:HD22	1.82	0.61
1:F:31:SER:HB3	1:F:111:GLY:HA3	1.81	0.61
1:B:156:LYS:HD2	1:C:126:GLY:O	2.01	0.61
1:E:225:ASN:O	1:E:229:VAL:HG12	2.02	0.60
1:B:170:MET:HE2	1:C:74:ILE:CG2	2.32	0.60
1:B:215:ASP:OD1	1:B:215:ASP:N	2.33	0.59
1:H:181:LEU:HD12	1:I:177:THR:HG23	1.84	0.59
1:J:87:LEU:HB3	1:J:101:MET:HG3	1.84	0.59
1:E:123:TYR:CE1	1:E:128:GLY:HA3	2.37	0.59
1:D:123:TYR:CZ	1:D:128:GLY:HA3	2.38	0.59
1:D:148:ALA:HB3	1:D:153:LEU:CD1	2.33	0.58
1:F:162:TRP:HE1	1:F:241:MET:HE3	1.68	0.58
1:C:15:ARG:NH1	1:C:78:GLU:OE2	2.37	0.58
1:D:71:LEU:O	1:D:75:ALA:HB3	2.03	0.58
1:B:139:HIS:HD2	1:B:208:SER:OG	1.87	0.57
1:C:30:SER:HB3	1:C:78:GLU:HG2	1.85	0.57
1:C:250:PRO:HG3	1:D:19:LEU:CD1	2.35	0.57
1:D:6:ILE:HD12	1:D:249:THR:HG21	1.85	0.57
1:F:241:MET:HA	1:F:241:MET:HE2	1.87	0.57
1:I:69:LEU:HG	1:I:73:ILE:HD12	1.86	0.57
1:C:162:TRP:NE1	1:C:241:MET:HE3	2.20	0.56
1:C:250:PRO:HG3	1:D:19:LEU:HD13	1.88	0.56
1:A:133:VAL:HG12	1:A:135:THR:HG22	1.88	0.56
1:A:42:ILE:HD12	1:A:65:PHE:HE1	1.70	0.55
1:F:156:LYS:HE2	1:G:126:GLY:O	2.05	0.55
1:F:1:MET:N	1:F:5:THR:H	2.04	0.55
1:F:185:TRP:HB3	1:G:67:ILE:HD12	1.87	0.55
1:D:181:LEU:HD12	1:E:177:THR:HG23	1.90	0.54
1:G:69:LEU:HD22	1:G:164:VAL:HG13	1.88	0.54
1:B:123:TYR:CZ	1:B:128:GLY:HA3	2.42	0.54
1:J:123:TYR:CZ	1:J:128:GLY:HA3	2.42	0.54
1:J:91:VAL:HG23	1:J:101:MET:HE2	1.90	0.54
1:I:97:SER:H	1:I:100:GLN:HE21	1.54	0.54
1:B:156:LYS:HE3	1:B:194:GLY:O	2.09	0.53
1:J:145:LYS:NZ	1:J:201:ASN:HD21	2.07	0.53
1:E:190:PHE:CD1	1:E:190:PHE:C	2.86	0.53
1:F:177:THR:HG23	1:J:181:LEU:HD22	1.89	0.53
1:F:1:MET:HG2	1:F:4:ASP:H	1.74	0.53
1:C:20:SER:OG	1:C:107:GLN:NE2	2.41	0.53
1:E:1:MET:N	3:E:313:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:TYR:CZ	1:C:128:GLY:HA3	2.44	0.52
1:G:42:ILE:HD11	1:G:200:ALA:HB1	1.91	0.52
1:D:145:LYS:NZ	1:D:201:ASN:HD21	2.06	0.52
1:G:139:HIS:HD2	1:G:208:SER:OG	1.92	0.52
1:A:2:PHE:HD2	1:A:7:ASN:HD21	1.58	0.52
1:B:170:MET:HE2	1:C:74:ILE:HG21	1.90	0.52
1:D:148:ALA:HB3	1:D:153:LEU:HD11	1.90	0.52
1:G:123:TYR:CZ	1:G:128:GLY:HA3	2.45	0.51
1:D:169:TRP:O	1:D:173:ARG:HG3	2.10	0.51
1:E:87:LEU:O	1:E:91:VAL:HG23	2.11	0.51
1:J:91:VAL:CG2	1:J:101:MET:HE2	2.41	0.51
1:A:166:LEU:HD21	1:B:37:TYR:CZ	2.46	0.51
1:A:156:LYS:HE3	1:B:126:GLY:O	2.11	0.51
1:B:142:ALA:O	1:B:146:THR:HG23	2.11	0.51
1:A:42:ILE:HD13	1:A:200:ALA:HB1	1.92	0.50
1:B:57:ARG:NH1	1:B:137:ILE:HG21	2.26	0.50
1:E:80:PHE:CE1	1:E:105:LEU:CD2	2.93	0.50
1:C:241:MET:HA	1:C:241:MET:HE2	1.93	0.50
1:G:214:SER:HB3	1:G:216:ALA:H	1.77	0.50
1:F:83:HIS:HB3	1:F:87:LEU:HD22	1.94	0.50
1:G:214:SER:HB2	3:G:310:HOH:O	2.12	0.50
1:E:167:ALA:HB2	1:E:186:CYS:HB2	1.94	0.49
1:J:153:LEU:HD13	1:J:225:ASN:HA	1.93	0.49
1:F:123:TYR:CZ	1:F:128:GLY:HA3	2.47	0.49
1:F:163:LEU:HG	1:G:40:LEU:HD13	1.93	0.49
1:F:198:SER:OG	1:F:233:ASN:ND2	2.46	0.49
1:J:57:ARG:HB2	1:J:58:PRO:HD3	1.95	0.49
1:H:190:PHE:CD1	1:H:190:PHE:C	2.91	0.49
1:D:2:PHE:CD2	1:D:249:THR:HG22	2.44	0.48
1:J:201:ASN:HB3	1:J:205:PHE:CE2	2.47	0.48
1:D:161:ASN:HB3	1:D:236:SER:OG	2.12	0.48
1:I:156:LYS:HE3	1:I:194:GLY:O	2.13	0.48
1:B:2:PHE:HB2	1:B:249:THR:HG22	1.95	0.48
1:D:83:HIS:HB3	1:D:87:LEU:HD22	1.95	0.48
1:I:123:TYR:CE2	1:I:128:GLY:HA3	2.49	0.48
1:B:170:MET:CE	1:C:74:ILE:CG2	2.91	0.48
1:F:152:VAL:CG1	1:F:156:LYS:HE3	2.44	0.48
1:H:123:TYR:CE2	1:H:128:GLY:HA3	2.48	0.48
1:A:97:SER:H	1:A:100:GLN:HE21	1.62	0.47
1:I:42:ILE:HD11	1:I:200:ALA:HB1	1.95	0.47
1:F:190:PHE:CD1	1:F:190:PHE:C	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:VAL:HG21	1:A:101:MET:HE2	1.96	0.47
1:C:57:ARG:HB2	1:C:58:PRO:HD3	1.95	0.47
1:A:42:ILE:HD11	1:A:200:ALA:HB1	1.95	0.47
1:A:139:HIS:HD2	1:A:208:SER:OG	1.96	0.47
1:F:197:HIS:CE1	1:F:199:VAL:HB	2.50	0.47
1:H:37:TYR:HB3	1:H:71:LEU:HB2	1.97	0.47
1:C:162:TRP:CD1	1:C:241:MET:HE3	2.49	0.47
1:F:145:LYS:NZ	1:F:201:ASN:HD21	2.12	0.47
1:J:145:LYS:HZ1	1:J:201:ASN:HD21	1.63	0.47
1:E:225:ASN:OD1	1:E:229:VAL:HG11	2.15	0.47
1:A:205:PHE:HA	1:A:217:TYR:OH	2.15	0.47
1:E:225:ASN:O	1:E:229:VAL:HG13	2.16	0.46
1:J:87:LEU:O	1:J:101:MET:HE2	2.14	0.46
1:D:32:ALA:HA	1:D:111:GLY:O	2.16	0.46
1:E:123:TYR:CZ	1:E:128:GLY:HA3	2.50	0.46
1:F:189:ALA:HA	1:G:44:LEU:HD13	1.97	0.46
1:A:2:PHE:HB2	1:A:7:ASN:ND2	2.30	0.46
1:F:1:MET:H2	1:F:2:PHE:HA	1.80	0.46
1:E:84:THR:OG1	1:E:237:GLY:HA3	2.16	0.46
1:J:225:ASN:O	1:J:229:VAL:HG23	2.15	0.46
1:A:76:GLY:HA3	1:E:2:PHE:HE1	1.81	0.46
1:H:156:LYS:HE3	1:H:194:GLY:O	2.16	0.46
1:D:32:ALA:O	1:D:115:GLY:HA3	2.16	0.46
1:D:148:ALA:HB3	1:D:153:LEU:HD13	1.97	0.46
1:E:57:ARG:HB2	1:E:58:PRO:HD3	1.97	0.46
1:B:29:VAL:O	1:B:33:MET:HG3	2.15	0.46
1:B:2:PHE:HE1	1:C:76:GLY:HA3	1.81	0.45
1:F:131:LEU:HB2	1:F:132:PRO:HD3	1.97	0.45
1:G:25:LEU:O	1:G:29:VAL:HG23	2.17	0.45
1:B:54:PRO:HA	1:B:57:ARG:HD3	1.99	0.45
1:D:134:ASP:OD1	1:D:134:ASP:N	2.49	0.45
1:B:190:PHE:CD1	1:B:190:PHE:C	2.94	0.45
1:E:1:MET:HG2	1:E:2:PHE:CZ	2.51	0.45
1:D:245:TYR:O	1:D:249:THR:HG23	2.17	0.45
1:C:4:ASP:O	1:C:8:LYS:HG3	2.17	0.45
1:A:57:ARG:HB2	1:A:58:PRO:HD3	1.99	0.45
1:E:3:THR:CG2	1:H:4:ASP:OD1	2.65	0.45
1:E:177:THR:O	1:E:180:PHE:HB2	2.16	0.45
1:J:160:CYS:HB2	1:J:195:TYR:HB3	1.99	0.45
1:A:123:TYR:CE2	1:A:128:GLY:HA3	2.52	0.45
1:C:97:SER:OG	1:C:100:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ASN:HB3	1:D:205:PHE:CE2	2.52	0.45
1:H:162:TRP:CH2	1:I:36:ALA:HB1	2.52	0.45
1:B:52:LEU:O	1:B:57:ARG:NH2	2.41	0.44
1:F:84:THR:OG1	1:F:237:GLY:HA3	2.17	0.44
1:E:179:LYS:O	1:E:183:ILE:HD12	2.16	0.44
1:G:123:TYR:CE2	1:G:128:GLY:HA3	2.51	0.44
1:I:164:VAL:HG12	3:I:330:HOH:O	2.16	0.44
1:F:81:THR:HB	1:F:161:ASN:HD21	1.78	0.44
1:I:245:TYR:O	1:I:249:THR:HG23	2.18	0.44
1:D:87:LEU:O	1:D:91:VAL:HG23	2.18	0.44
1:D:87:LEU:HB3	1:D:101:MET:HG3	1.99	0.44
1:F:92:LYS:HD3	1:F:92:LYS:HA	1.71	0.44
1:F:1:MET:HB3	1:F:4:ASP:HB2	1.99	0.44
1:J:213:HIS:HD2	1:J:214:SER:O	2.01	0.43
1:I:190:PHE:CD1	1:I:190:PHE:C	2.96	0.43
1:J:217:TYR:CZ	1:J:222:ILE:HD11	2.53	0.43
1:E:226:LEU:HD23	1:E:226:LEU:HA	1.89	0.43
1:F:76:GLY:HA3	1:J:2:PHE:HE1	1.83	0.43
1:C:57:ARG:CB	1:C:58:PRO:HD3	2.48	0.43
1:G:166:LEU:HD13	1:H:71:LEU:HD22	2.01	0.43
1:I:235:LEU:O	1:I:239:VAL:HB	2.18	0.43
1:H:121:LEU:HD23	1:H:121:LEU:HA	1.81	0.43
1:J:92:LYS:HE2	1:J:92:LYS:HA	2.01	0.43
1:F:152:VAL:HG12	1:F:156:LYS:HE3	2.00	0.43
1:I:105:LEU:HD23	1:I:105:LEU:HA	1.87	0.43
1:C:156:LYS:HD3	1:C:194:GLY:O	2.19	0.43
1:H:87:LEU:O	1:H:91:VAL:HG23	2.18	0.43
1:E:153:LEU:HD13	1:E:225:ASN:HA	2.01	0.43
1:F:105:LEU:HD23	1:F:105:LEU:HA	1.71	0.43
1:F:166:LEU:HD23	1:F:166:LEU:HA	1.93	0.43
1:B:245:TYR:O	1:B:249:THR:HG23	2.18	0.42
1:D:42:ILE:HD11	1:D:200:ALA:HB1	2.01	0.42
1:I:123:TYR:CZ	1:I:128:GLY:HA3	2.54	0.42
1:A:178:ALA:HB1	1:B:180:PHE:CE1	2.54	0.42
1:E:175:GLU:OE2	1:E:175:GLU:HA	2.20	0.42
1:H:55:SER:HB3	3:H:313:HOH:O	2.18	0.42
1:F:162:TRP:NE1	1:F:241:MET:HE3	2.35	0.42
1:H:225:ASN:O	1:H:229:VAL:HG23	2.19	0.42
1:F:100:GLN:O	1:F:104:ILE:HD12	2.20	0.42
1:C:27:PHE:CD1	1:C:27:PHE:C	2.98	0.42
1:E:145:LYS:NZ	1:E:196:GLU:OE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ILE:HD13	1:C:65:PHE:CD1	2.55	0.42
1:F:191:ILE:HD12	1:F:191:ILE:HG23	1.88	0.42
1:G:161:ASN:HB3	1:G:236:SER:OG	2.20	0.42
1:G:190:PHE:CD1	1:G:190:PHE:C	2.98	0.42
1:H:177:THR:O	1:H:180:PHE:HB2	2.20	0.42
1:B:57:ARG:NH1	1:B:137:ILE:CG2	2.83	0.42
1:F:23:ASN:ND2	1:J:250:PRO:HA	2.35	0.42
1:H:84:THR:OG1	1:H:237:GLY:HA3	2.19	0.42
1:A:36:ALA:HB1	1:E:162:TRP:CH2	2.56	0.41
1:H:165:CYS:CB	1:H:241:MET:HG3	2.50	0.41
1:J:131:LEU:O	1:J:139:HIS:HE1	2.03	0.41
1:B:205:PHE:CD2	1:B:222:ILE:HG23	2.55	0.41
1:C:156:LYS:HE2	1:D:126:GLY:O	2.20	0.41
1:F:24:PRO:O	1:F:28:TRP:HD1	2.04	0.41
1:F:80:PHE:CE2	1:F:230:THR:HG23	2.54	0.41
1:A:84:THR:HG21	1:A:234:THR:HA	2.02	0.41
1:C:197:HIS:CE1	1:C:199:VAL:HB	2.55	0.41
1:D:69:LEU:HB3	1:D:183:ILE:HG23	2.02	0.41
1:F:123:TYR:HE2	1:F:131:LEU:HD13	1.86	0.41
1:F:156:LYS:HD3	1:F:194:GLY:O	2.21	0.41
1:J:166:LEU:O	1:J:170:MET:HG3	2.19	0.41
1:B:32:ALA:O	1:B:115:GLY:HA3	2.20	0.41
1:F:71:LEU:O	1:F:75:ALA:HB3	2.20	0.41
1:D:123:TYR:CE2	1:D:128:GLY:HA3	2.55	0.41
1:F:42:ILE:HD11	1:F:200:ALA:HB1	2.02	0.41
1:A:131:LEU:O	1:A:139:HIS:CE1	2.58	0.41
1:B:159:LEU:HD13	1:B:195:TYR:CE1	2.56	0.41
1:D:190:PHE:CD1	1:D:190:PHE:C	2.98	0.41
1:H:32:ALA:O	1:H:115:GLY:HA3	2.20	0.41
1:C:192:ALA:O	1:D:47:THR:HG21	2.21	0.41
1:H:165:CYS:HB3	1:H:241:MET:HG3	2.03	0.41
1:C:26:GLY:HA2	1:C:29:VAL:CG1	2.50	0.40
1:E:1:MET:HB3	1:E:2:PHE:CD2	2.56	0.40
1:A:167:ALA:HB2	1:A:186:CYS:CB	2.51	0.40
1:A:190:PHE:CD1	1:A:190:PHE:C	3.00	0.40
1:B:201:ASN:HB3	1:B:205:PHE:CE2	2.56	0.40
1:D:146:THR:HB	1:D:221:GLY:HA3	2.03	0.40
1:H:131:LEU:H	1:H:132:PRO:HD3	1.86	0.40
1:D:205:PHE:HA	1:D:217:TYR:OH	2.21	0.40
1:H:1:MET:CA	1:H:173:ARG:HH12	2.28	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	247/261 (95%)	244 (99%)	3 (1%)	0	100	100
1	B	248/261 (95%)	242 (98%)	6 (2%)	0	100	100
1	C	248/261 (95%)	241 (97%)	6 (2%)	1 (0%)	30	43
1	D	247/261 (95%)	243 (98%)	4 (2%)	0	100	100
1	E	248/261 (95%)	238 (96%)	10 (4%)	0	100	100
1	F	248/261 (95%)	240 (97%)	8 (3%)	0	100	100
1	G	246/261 (94%)	240 (98%)	6 (2%)	0	100	100
1	H	248/261 (95%)	241 (97%)	6 (2%)	1 (0%)	30	43
1	I	248/261 (95%)	243 (98%)	5 (2%)	0	100	100
1	J	248/261 (95%)	243 (98%)	5 (2%)	0	100	100
All	All	2476/2610 (95%)	2415 (98%)	59 (2%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	2	PHE
1	C	77	SER

### 5.3.2 Protein sidechains [i](#)

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	191/203 (94%)	184 (96%)	7 (4%)	30	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	192/203 (95%)	186 (97%)	6 (3%)	35	57
1	C	192/203 (95%)	182 (95%)	10 (5%)	21	36
1	D	191/203 (94%)	186 (97%)	5 (3%)	40	63
1	E	192/203 (95%)	182 (95%)	10 (5%)	21	36
1	F	192/203 (95%)	184 (96%)	8 (4%)	26	45
1	G	190/203 (94%)	184 (97%)	6 (3%)	34	56
1	H	192/203 (95%)	189 (98%)	3 (2%)	55	76
1	I	192/203 (95%)	188 (98%)	4 (2%)	47	69
1	J	192/203 (95%)	187 (97%)	5 (3%)	40	63
All	All	1916/2030 (94%)	1852 (97%)	64 (3%)	33	55

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ILE
1	A	69	LEU
1	A	135	THR
1	A	137	ILE
1	A	138	VAL
1	A	190	PHE
1	A	225	ASN
1	B	57	ARG
1	B	151	THR
1	B	175	GLU
1	B	190	PHE
1	B	215	ASP
1	B	243	LEU
1	C	1	MET
1	C	3	THR
1	C	4	ASP
1	C	30	SER
1	C	113	LEU
1	C	136	SER
1	C	177	THR
1	C	181	LEU
1	C	188	LEU
1	C	190	PHE
1	D	4	ASP
1	D	87	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	153	LEU
1	D	190	PHE
1	D	227	LEU
1	E	1	MET
1	E	3	THR
1	E	8	LYS
1	E	22	ASN
1	E	105	LEU
1	E	114	VAL
1	E	121	LEU
1	E	187	LEU
1	E	190	PHE
1	E	229	VAL
1	F	1	MET
1	F	3	THR
1	F	4	ASP
1	F	87	LEU
1	F	136	SER
1	F	190	PHE
1	F	218	THR
1	F	249	THR
1	G	3	THR
1	G	48	LEU
1	G	51	LEU
1	G	80	PHE
1	G	190	PHE
1	G	219	LEU
1	H	8	LYS
1	H	87	LEU
1	H	190	PHE
1	I	57	ARG
1	I	71	LEU
1	I	181	LEU
1	I	190	PHE
1	J	51	LEU
1	J	69	LEU
1	J	121	LEU
1	J	135	THR
1	J	190	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	100	GLN
1	A	107	GLN
1	A	139	HIS
1	A	201	ASN
1	A	225	ASN
1	B	7	ASN
1	B	100	GLN
1	B	139	HIS
1	B	201	ASN
1	C	7	ASN
1	C	23	ASN
1	C	201	ASN
1	C	213	HIS
1	D	7	ASN
1	D	139	HIS
1	D	201	ASN
1	E	100	GLN
1	E	139	HIS
1	E	201	ASN
1	F	7	ASN
1	F	23	ASN
1	F	161	ASN
1	F	201	ASN
1	F	233	ASN
1	G	7	ASN
1	G	139	HIS
1	G	201	ASN
1	H	7	ASN
1	H	98	HIS
1	H	139	HIS
1	H	201	ASN
1	I	7	ASN
1	I	23	ASN
1	I	50	ASN
1	I	98	HIS
1	I	100	GLN
1	I	201	ASN
1	I	212	HIS
1	J	7	ASN
1	J	100	GLN
1	J	139	HIS
1	J	201	ASN

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Mol	Chain	Res	Type
1	J	213	HIS
1	J	224	HIS

### 5.3.3 RNA [i](#)

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 oligosaccharides 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	F	301	-	20,20,20	1.20	2 (10%)	25,25,25	1.62	5 (20%)
2	BOG	F	302	-	20,20,20	1.40	2 (10%)	25,25,25	2.49	9 (36%)

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	F	301	-	-	3/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	F	302	-	-	6/11/31/31	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	302	BOG	O1-C1	4.01	1.46	1.40
2	F	301	BOG	O1-C1	3.43	1.45	1.40
2	F	302	BOG	O5-C1	2.25	1.47	1.41
2	F	301	BOG	O5-C1	2.10	1.47	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	302	BOG	C1'-O1-C1	6.91	125.49	113.68
2	F	302	BOG	O1-C1-C2	5.88	117.20	108.27
2	F	301	BOG	C1-O5-C5	4.68	122.86	113.72
2	F	302	BOG	O5-C5-C6	4.06	116.49	106.44
2	F	302	BOG	O5-C1-C2	3.06	116.66	110.37
2	F	302	BOG	C6-C5-C4	2.99	120.35	113.02
2	F	302	BOG	O3-C3-C4	2.90	117.21	110.38
2	F	301	BOG	C4-C3-C2	-2.88	105.78	110.83
2	F	302	BOG	C1-O5-C5	-2.54	108.76	113.72
2	F	302	BOG	O5-C1-O1	2.23	115.31	110.04
2	F	302	BOG	O6-C6-C5	2.19	118.80	111.33
2	F	301	BOG	O3-C3-C4	2.15	115.45	110.38
2	F	301	BOG	O1-C1'-C2'	2.10	116.50	109.37
2	F	301	BOG	C1'-O1-C1	2.10	117.26	113.68

There are no chirality outliers.

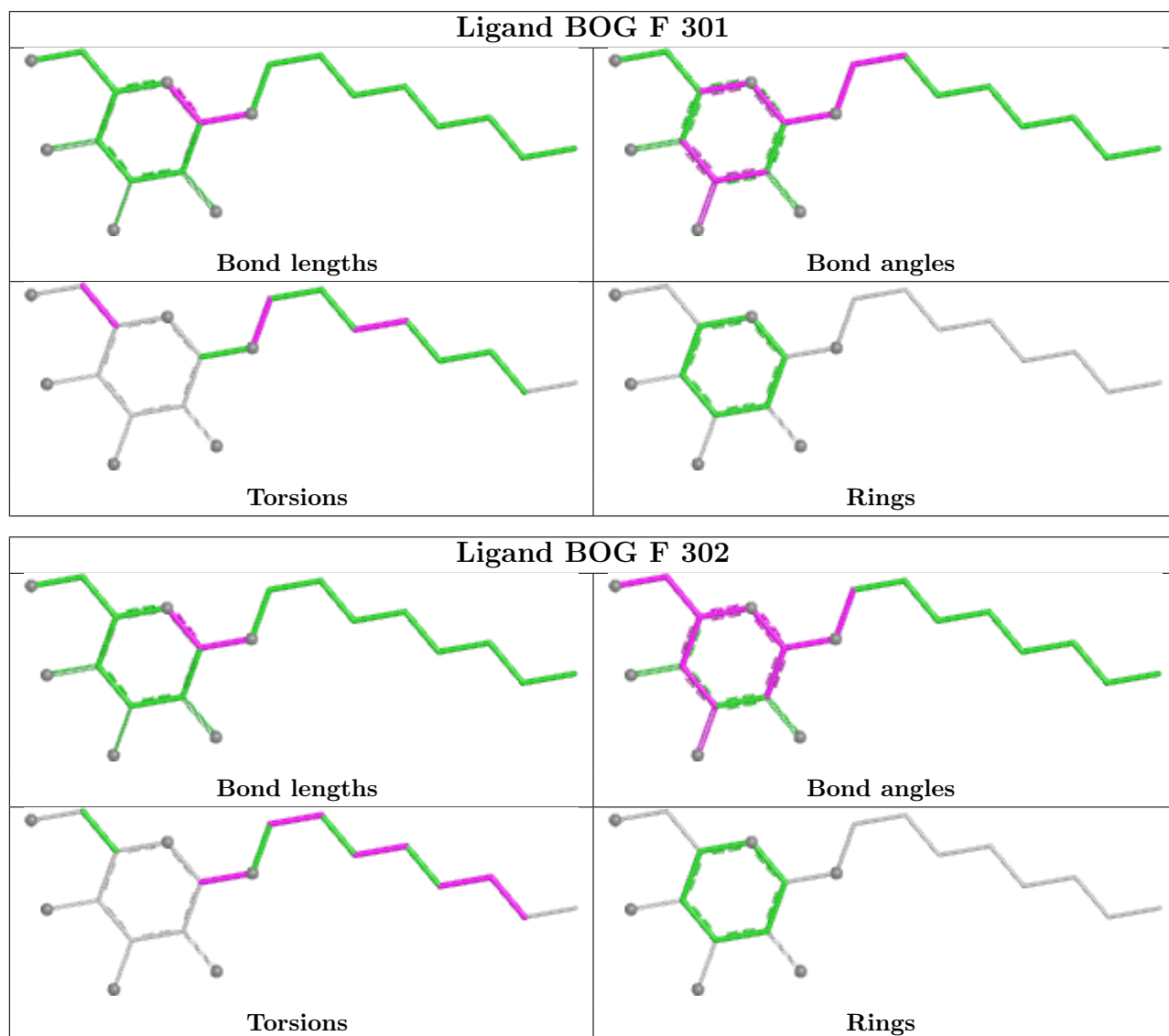
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	302	BOG	C2-C1-O1-C1'
2	F	302	BOG	O5-C1-O1-C1'
2	F	302	BOG	O1-C1'-C2'-C3'
2	F	301	BOG	C2'-C3'-C4'-C5'
2	F	301	BOG	C2'-C1'-O1-C1
2	F	302	BOG	C2'-C3'-C4'-C5'
2	F	302	BOG	C4'-C5'-C6'-C7'
2	F	301	BOG	O5-C5-C6-O6
2	F	302	BOG	C5'-C6'-C7'-C8'

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, 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	249/261 (95%)	-0.22	4 (1%) 70 66	31, 41, 55, 74	1 (0%)
1	B	250/261 (95%)	-0.24	3 (1%) 76 73	33, 47, 66, 94	0
1	C	250/261 (95%)	-0.08	3 (1%) 76 73	35, 52, 78, 107	0
1	D	249/261 (95%)	0.00	1 (0%) 88 86	36, 56, 77, 93	0
1	E	250/261 (95%)	-0.08	3 (1%) 76 73	32, 48, 63, 73	0
1	F	250/261 (95%)	-0.15	5 (2%) 65 60	32, 47, 71, 93	1 (0%)
1	G	248/261 (95%)	-0.07	4 (1%) 70 66	34, 51, 69, 87	0
1	H	250/261 (95%)	-0.23	3 (1%) 76 73	34, 46, 60, 76	0
1	I	250/261 (95%)	-0.23	2 (0%) 82 80	30, 40, 52, 101	0
1	J	250/261 (95%)	-0.37	2 (0%) 82 80	31, 46, 64, 90	0
All	All	2496/2610 (95%)	-0.17	30 (1%) 76 73	30, 47, 69, 107	2 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	250	PRO	5.9
1	G	3	THR	5.7
1	E	250	PRO	5.7
1	C	250	PRO	5.3
1	H	250	PRO	5.3
1	F	250	PRO	4.9
1	C	1	MET	4.5
1	D	250	PRO	4.1
1	J	1	MET	3.9
1	A	248	ALA	3.7
1	J	250	PRO	3.7
1	B	250	PRO	3.5
1	A	2	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	2	PHE	3.4
1	F	110	LEU	3.3
1	A	110	LEU	3.2
1	H	1	MET	3.1
1	F	1	MET	2.9
1	F	142	ALA	2.9
1	B	1	MET	2.9
1	I	2	PHE	2.8
1	G	246	TRP	2.8
1	G	93	ALA	2.7
1	F	249	THR	2.4
1	E	214	SER	2.2
1	H	216	ALA	2.2
1	C	142	ALA	2.1
1	A	249	THR	2.1
1	E	1	MET	2.1
1	B	3	THR	2.1

## 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

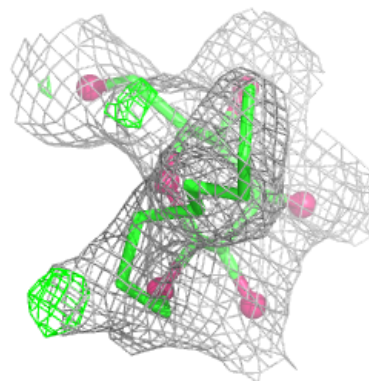
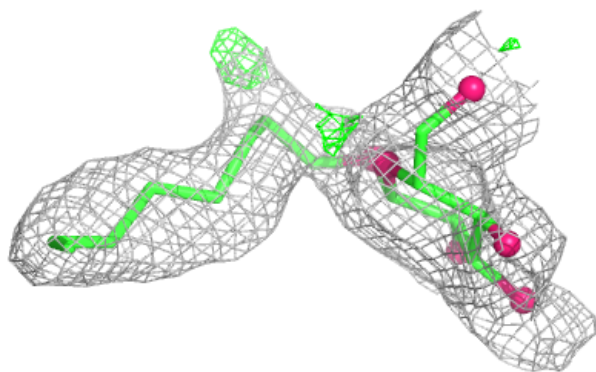
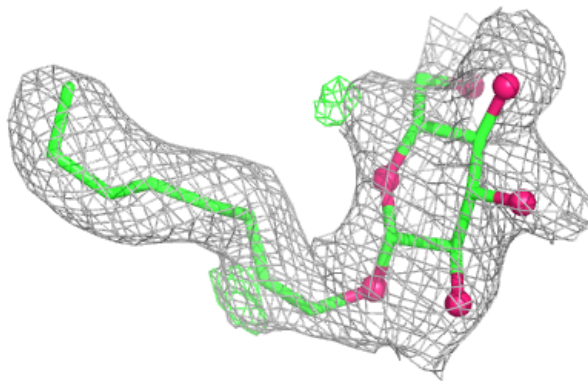
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BOG	F	301	20/20	0.75	0.18	53,90,108,114	0
2	BOG	F	302	20/20	0.82	0.21	54,83,114,116	0

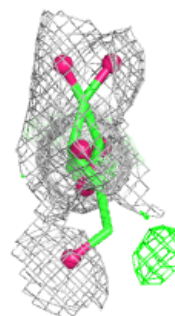
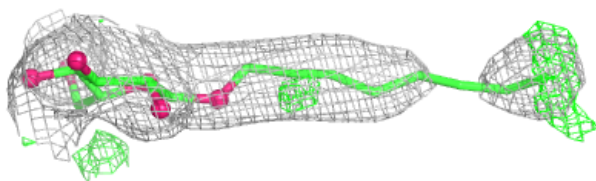
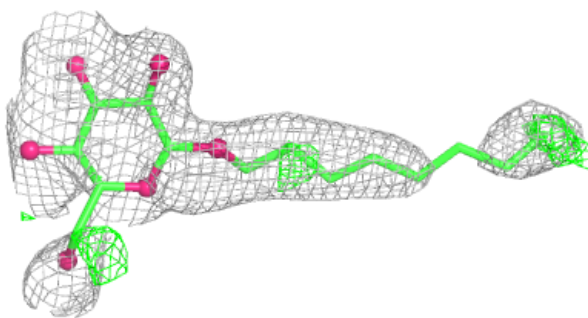
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around BOG F 301:**

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

**Electron density around BOG F 302:**

$2mF_o-DF_c$  (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.