



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 07:32 AM BST

PDB ID : 3TE0
Title : Crystal structure of HSC K148E
Authors : Czyzewski, B.K.; Wang, D.-N.
Deposited on : 2011-08-11
Resolution : 2.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

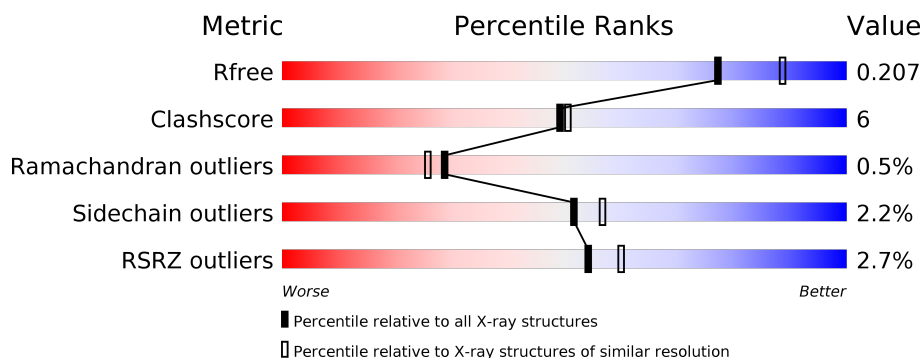
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 ≥ 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	268	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>...</div> </div> </div>
1	B	268	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>..</div> </div> </div>
1	C	268	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>...</div> </div> </div>
1	D	268	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>...</div> </div> </div>
1	E	268	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>..</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BOG	A	267	-	-	-	X
2	BOG	B	268	-	-	-	X
2	BOG	D	267	-	-	-	X
2	BOG	E	267	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10217 atoms, of which 112 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 formate/nitrite transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	1	0
			1903	1246	299	344	14			
1	B	257	Total	C	N	O	S	0	2	0
			1912	1254	300	344	14			
1	C	266	Total	C	N	O	S	0	0	0
			1969	1289	310	356	14			
1	D	257	Total	C	N	O	S	0	1	0
			1907	1249	300	344	14			
1	E	256	Total	C	N	O	S	0	2	0
			1902	1246	297	345	14			

There are 60 discrepancies between the modelled and reference sequences:

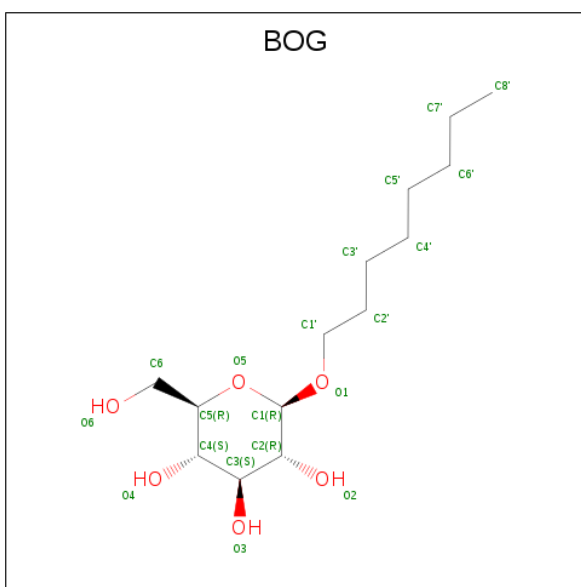
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP Q186B7
A	-1	GLY	-	expression tag	UNP Q186B7
A	0	ARG	-	expression tag	UNP Q186B7
A	1	ALA	-	expression tag	UNP Q186B7
A	148	GLU	LYS	engineered mutation	UNP Q186B7
A	259	ALA	-	expression tag	UNP Q186B7
A	260	ALA	-	expression tag	UNP Q186B7
A	261	ALA	-	expression tag	UNP Q186B7
A	262	GLU	-	expression tag	UNP Q186B7
A	263	ASN	-	expression tag	UNP Q186B7
A	264	LEU	-	expression tag	UNP Q186B7
A	265	TYR	-	expression tag	UNP Q186B7
B	-2	MET	-	expression tag	UNP Q186B7
B	-1	GLY	-	expression tag	UNP Q186B7
B	0	ARG	-	expression tag	UNP Q186B7
B	1	ALA	-	expression tag	UNP Q186B7
B	148	GLU	LYS	engineered mutation	UNP Q186B7
B	259	ALA	-	expression tag	UNP Q186B7
B	260	ALA	-	expression tag	UNP Q186B7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	261	ALA	-	expression tag	UNP Q186B7
B	262	GLU	-	expression tag	UNP Q186B7
B	263	ASN	-	expression tag	UNP Q186B7
B	264	LEU	-	expression tag	UNP Q186B7
B	265	TYR	-	expression tag	UNP Q186B7
C	-2	MET	-	expression tag	UNP Q186B7
C	-1	GLY	-	expression tag	UNP Q186B7
C	0	ARG	-	expression tag	UNP Q186B7
C	1	ALA	-	expression tag	UNP Q186B7
C	148	GLU	LYS	engineered mutation	UNP Q186B7
C	259	ALA	-	expression tag	UNP Q186B7
C	260	ALA	-	expression tag	UNP Q186B7
C	261	ALA	-	expression tag	UNP Q186B7
C	262	GLU	-	expression tag	UNP Q186B7
C	263	ASN	-	expression tag	UNP Q186B7
C	264	LEU	-	expression tag	UNP Q186B7
C	265	TYR	-	expression tag	UNP Q186B7
D	-2	MET	-	expression tag	UNP Q186B7
D	-1	GLY	-	expression tag	UNP Q186B7
D	0	ARG	-	expression tag	UNP Q186B7
D	1	ALA	-	expression tag	UNP Q186B7
D	148	GLU	LYS	engineered mutation	UNP Q186B7
D	259	ALA	-	expression tag	UNP Q186B7
D	260	ALA	-	expression tag	UNP Q186B7
D	261	ALA	-	expression tag	UNP Q186B7
D	262	GLU	-	expression tag	UNP Q186B7
D	263	ASN	-	expression tag	UNP Q186B7
D	264	LEU	-	expression tag	UNP Q186B7
D	265	TYR	-	expression tag	UNP Q186B7
E	-2	MET	-	expression tag	UNP Q186B7
E	-1	GLY	-	expression tag	UNP Q186B7
E	0	ARG	-	expression tag	UNP Q186B7
E	1	ALA	-	expression tag	UNP Q186B7
E	148	GLU	LYS	engineered mutation	UNP Q186B7
E	259	ALA	-	expression tag	UNP Q186B7
E	260	ALA	-	expression tag	UNP Q186B7
E	261	ALA	-	expression tag	UNP Q186B7
E	262	GLU	-	expression tag	UNP Q186B7
E	263	ASN	-	expression tag	UNP Q186B7
E	264	LEU	-	expression tag	UNP Q186B7
E	265	TYR	-	expression tag	UNP Q186B7

- Molecule 2 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			48	14	28	6		
2	B	1	Total	C	H	O	0	0
			48	14	28	6		
2	D	1	Total	C	H	O	0	0
			48	14	28	6		
2	E	1	Total	C	H	O	0	0
			48	14	28	6		

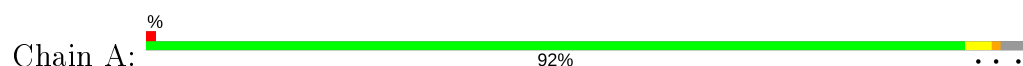
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	97	Total	O	0	0
			97	97		
3	B	86	Total	O	0	0
			86	86		
3	C	86	Total	O	0	0
			86	86		
3	D	75	Total	O	0	0
			75	75		
3	E	88	Total	O	0	0
			88	88		

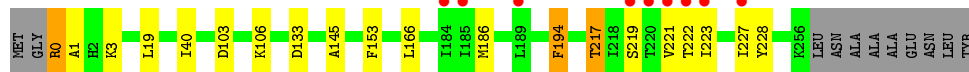
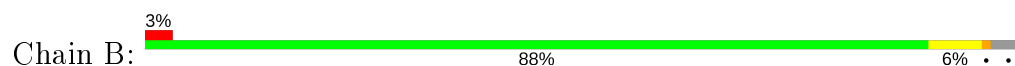
3 Residue-property plots

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

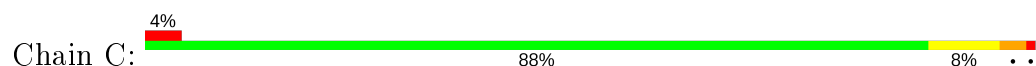
- Molecule 1: formate/nitrite transporter



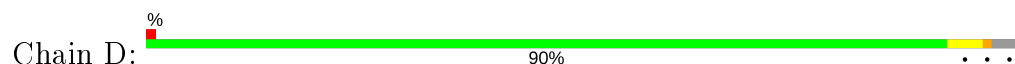
- Molecule 1: formate/nitrite transporter



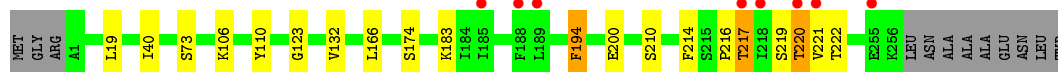
- Molecule 1: formate/nitrite transporter



- Molecule 1: formate/nitrite transporter



- Molecule 1: formate/nitrite transporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.44Å 118.47Å 150.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 2.09 49.72 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.72-2.09) 95.3 (49.72-2.09)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.168 , 0.199 0.187 , 0.207	Depositor DCC
R_{free} test set	5262 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10217	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.48	0/1935	0.52	0/2624
1	B	0.46	0/1947	0.49	0/2639
1	C	0.46	0/2002	0.52	0/2715
1	D	0.47	0/1939	0.51	0/2628
1	E	0.51	0/1934	0.52	0/2622
All	All	0.48	0/9757	0.51	0/13228

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	260	ALA	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	1903	0	1993	13	0
1	B	1912	0	2015	19	0
1	C	1969	0	2064	53	0
1	D	1907	0	2004	15	0
1	E	1902	0	1995	21	0
2	A	20	28	28	3	0
2	B	20	28	28	3	0
2	D	20	28	28	1	0
2	E	20	28	28	4	0
3	A	97	0	0	0	0
3	B	86	0	0	2	0
3	C	86	0	0	5	0
3	D	75	0	0	2	0
3	E	88	0	0	3	0
All	All	10105	112	10183	117	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 6.

All (117) 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:258:ASN:HA	1:C:260:ALA:N	1.22	1.47
1:C:258:ASN:CA	1:C:260:ALA:H	1.40	1.33
1:C:258:ASN:ND2	1:C:258:ASN:O	1.68	1.26
1:B:106:LYS:HG3	2:B:268:BOG:H61	1.15	1.15
1:C:0:ARG:CB	1:C:1:ALA:HA	1.78	1.10
1:C:0:ARG:HB2	1:C:1:ALA:HA	1.34	1.08
1:C:0:ARG:HG3	1:C:0:ARG:HH11	1.18	1.07
1:C:258:ASN:H	1:C:259:ALA:HB3	1.18	1.07
1:C:258:ASN:C	1:C:258:ASN:HD22	1.56	1.03
1:A:106:LYS:HG3	2:A:267:BOG:H61	1.47	0.93
1:C:222:THR:HG22	1:C:225:GLY:H	1.34	0.91
1:C:221:VAL:O	1:C:222:THR:HB	1.70	0.89
1:D:218:ILE:HD12	1:D:219:SER:H	1.37	0.89
1:B:0:ARG:HG3	1:B:1:ALA:H	1.38	0.88
1:A:221:VAL:O	1:A:222:THR:HB	1.73	0.86
1:C:258:ASN:N	1:C:259:ALA:HB3	1.88	0.86
1:E:106:LYS:HD2	2:E:267:BOG:H61	1.58	0.86
1:B:106:LYS:HG3	2:B:268:BOG:C6	2.05	0.83
1:B:0:ARG:HG3	1:B:1:ALA:N	1.93	0.82
1:C:0:ARG:NH2	1:C:3:LYS:H	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:0:ARG:CB	1:C:1:ALA:CA	2.59	0.81
1:C:0:ARG:HH11	1:C:0:ARG:CG	1.95	0.80
1:C:258:ASN:O	3:C:323:HOH:O	2.00	0.79
1:C:258:ASN:CA	1:C:260:ALA:N	2.15	0.77
1:A:0:ARG:HD3	1:A:0:ARG:O	1.84	0.77
1:C:217:THR:HG23	1:C:217:THR:O	1.84	0.77
1:D:218:ILE:HD12	1:D:219:SER:N	1.99	0.77
1:C:0:ARG:NH1	3:C:392:HOH:O	2.16	0.77
1:D:215:SER:OG	1:D:217:THR:HG23	1.84	0.77
1:C:0:ARG:HB3	1:C:1:ALA:HA	1.65	0.76
1:B:145:ALA:HB1	1:B:221:VAL:HG11	1.67	0.75
1:B:106:LYS:CG	2:B:268:BOG:H61	2.08	0.74
1:A:0:ARG:HD3	1:A:0:ARG:C	2.08	0.73
1:C:146:ALA:HA	1:C:221:VAL:HG12	1.72	0.72
1:C:0:ARG:HG3	1:C:0:ARG:NH1	1.98	0.70
1:C:257:LEU:O	1:C:258:ASN:CG	2.30	0.70
1:B:0:ARG:NH1	1:B:3:LYS:H	1.90	0.70
1:D:132:VAL:O	1:D:217:THR:HG21	1.95	0.66
1:C:216:PRO:HD2	3:C:412:HOH:O	1.96	0.66
1:E:110:TYR:CZ	2:E:267:BOG:H3'1	2.30	0.66
1:E:220:THR:HG23	1:E:220:THR:O	1.95	0.65
1:B:0:ARG:HH11	1:B:3:LYS:H	1.44	0.64
1:D:219:SER:HA	3:D:328:HOH:O	1.98	0.64
1:B:133:ASP:HA	1:B:217:THR:HG21	1.79	0.63
1:D:255:GLU:OE1	1:D:255:GLU:N	2.29	0.63
1:B:145:ALA:CB	1:B:221:VAL:HG11	2.28	0.62
1:B:186:MET:SD	1:E:73[B]:SER:OG	2.57	0.62
1:C:218:ILE:HG22	1:C:220:THR:HG22	1.81	0.62
1:E:221:VAL:O	3:E:324:HOH:O	2.16	0.60
1:D:221:VAL:HG13	1:D:222:THR:H	1.67	0.59
1:A:0:ARG:HG2	1:A:2:HIS:CD2	2.38	0.58
1:C:0:ARG:NH1	1:C:0:ARG:CG	2.58	0.58
1:C:222:THR:HG22	1:C:225:GLY:N	2.15	0.57
1:B:133:ASP:O	1:B:217:THR:HG21	2.04	0.56
1:C:219:SER:O	1:C:221:VAL:HG22	2.05	0.56
1:E:106:LYS:CD	2:E:267:BOG:H61	2.34	0.56
1:C:146:ALA:HA	1:C:221:VAL:CG1	2.36	0.56
1:C:219:SER:C	1:C:221:VAL:H	2.09	0.56
1:C:76:ILE:HG13	1:C:187:ILE:HD11	1.87	0.56
1:A:222:THR:HG22	1:A:225:GLY:H	1.70	0.55
1:A:194:PHE:C	1:A:194:PHE:CD1	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:PHE:O	1:E:216:PRO:HD3	2.07	0.55
1:C:219:SER:O	1:C:220:THR:HG23	2.05	0.55
1:C:217:THR:CG2	1:C:217:THR:O	2.55	0.54
1:E:220:THR:CG2	1:E:220:THR:O	2.56	0.53
1:C:258:ASN:ND2	1:C:258:ASN:C	2.32	0.53
1:E:123:GLY:HA3	1:E:210[B]:SER:OG	2.08	0.53
1:C:0:ARG:HB3	1:C:1:ALA:CA	2.30	0.52
1:C:264:LEU:O	1:C:265:TYR:CD2	2.62	0.52
1:C:219:SER:O	1:C:221:VAL:N	2.43	0.52
1:E:221:VAL:O	1:E:222:THR:HG23	2.10	0.52
1:C:255:GLU:O	1:C:258:ASN:ND2	2.43	0.51
1:C:264:LEU:O	1:C:265:TYR:CG	2.63	0.51
1:C:216:PRO:O	1:C:218:ILE:N	2.41	0.51
1:C:218:ILE:CG2	1:C:220:THR:HG22	2.42	0.49
1:A:221:VAL:O	1:A:222:THR:CB	2.47	0.49
1:C:4:GLU:HG2	3:C:370:HOH:O	2.12	0.48
1:C:151:MET:HB3	1:C:151:MET:HE2	1.64	0.48
1:D:254:LYS:HD2	1:D:255:GLU:OE1	2.13	0.48
1:A:106:LYS:CG	2:A:267:BOG:H61	2.34	0.47
1:C:219:SER:O	1:C:220:THR:CG2	2.62	0.47
1:A:166:LEU:HD21	1:B:40:ILE:HG21	1.97	0.47
1:C:219:SER:OG	3:C:359:HOH:O	2.20	0.47
1:D:215:SER:HG	1:D:217:THR:HG23	1.80	0.46
1:E:132:VAL:O	1:E:217:THR:HG21	2.15	0.46
1:E:174:SER:HA	1:E:183:LYS:HG2	1.98	0.46
1:D:110:TYR:CE2	2:D:267:BOG:H4'1	2.51	0.46
1:C:258:ASN:HA	1:C:260:ALA:CA	2.31	0.46
1:B:194:PHE:CD1	1:B:194:PHE:C	2.89	0.45
1:C:40:ILE:HG21	1:E:166:LEU:HD21	1.98	0.45
1:B:19:LEU:HD21	3:B:307:HOH:O	2.15	0.45
1:C:174:SER:HA	1:C:183:LYS:HG2	1.99	0.45
1:E:221:VAL:C	1:E:222:THR:HG23	2.37	0.45
1:A:174:SER:HA	1:A:183:LYS:HG2	1.99	0.44
1:C:257:LEU:O	1:C:258:ASN:CB	2.64	0.44
1:A:110:TYR:CZ	2:A:267:BOG:H3'1	2.53	0.44
1:D:42:ILE:HD11	1:D:204:ALA:HB1	1.98	0.44
1:C:219:SER:C	1:C:221:VAL:N	2.71	0.44
1:B:133:ASP:CA	1:B:217:THR:HG21	2.47	0.44
1:D:221:VAL:HG13	1:D:222:THR:N	2.32	0.44
1:E:221:VAL:HG12	1:E:222:THR:N	2.33	0.44
1:E:219:SER:OG	1:E:220:THR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:LYS:NZ	3:D:314:HOH:O	2.52	0.43
1:B:166:LEU:HD21	1:E:40:ILE:HG21	2.00	0.42
1:E:194:PHE:C	1:E:194:PHE:CD1	2.93	0.42
1:B:153:PHE:N	1:B:228:TYR:OH	2.53	0.42
1:B:103:ASP:OD2	3:B:442:HOH:O	2.21	0.42
1:C:219:SER:C	1:C:220:THR:CG2	2.88	0.42
1:A:174:SER:HB2	1:A:183:LYS:HD3	2.01	0.42
1:E:200:GLU:OE2	3:E:305:HOH:O	2.21	0.41
1:C:91:SER:OG	1:C:246:GLY:HA3	2.20	0.41
1:D:174:SER:HA	1:D:183:LYS:HG2	2.02	0.41
1:D:194:PHE:C	1:D:194:PHE:CD1	2.93	0.41
1:E:110:TYR:CE1	2:E:267:BOG:H3'1	2.55	0.41
1:C:42:ILE:HD11	1:C:204:ALA:HB1	2.03	0.41
1:E:19:LEU:HD21	3:E:286:HOH:O	2.21	0.41
1:C:194:PHE:C	1:C:194:PHE:CD1	2.94	0.41

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	256/268 (96%)	251 (98%)	5 (2%)	0	100	100
1	B	257/268 (96%)	253 (98%)	4 (2%)	0	100	100
1	C	264/268 (98%)	252 (96%)	6 (2%)	6 (2%)	6	2
1	D	256/268 (96%)	251 (98%)	4 (2%)	1 (0%)	34	32
1	E	256/268 (96%)	253 (99%)	3 (1%)	0	100	100
All	All	1289/1340 (96%)	1260 (98%)	22 (2%)	7 (0%)	29	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	220	THR
1	C	258	ASN
1	C	218	ILE
1	C	259	ALA
1	D	221	VAL
1	C	222	THR
1	C	217	THR

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	207/214 (97%)	203 (98%)	4 (2%)	57	63
1	B	209/214 (98%)	202 (97%)	7 (3%)	38	40
1	C	213/214 (100%)	207 (97%)	6 (3%)	43	47
1	D	208/214 (97%)	205 (99%)	3 (1%)	67	73
1	E	208/214 (97%)	205 (99%)	3 (1%)	67	73
All	All	1045/1070 (98%)	1022 (98%)	23 (2%)	52	57

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	ARG
1	A	194	PHE
1	A	221	VAL
1	A	222	THR
1	B	0	ARG
1	B	194	PHE
1	B	217	THR
1	B	219	SER
1	B	222	THR
1	B	223	ILE
1	B	227	ILE
1	C	0	ARG
1	C	194	PHE

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Mol	Chain	Res	Type
1	C	220	THR
1	C	221	VAL
1	C	222	THR
1	C	258	ASN
1	D	194	PHE
1	D	217	THR
1	D	218	ILE
1	E	194	PHE
1	E	217	THR
1	E	220	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	258	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BOG	B	268	-	20,20,20	0.46	0	25,25,25	0.57	0
2	BOG	D	267	-	20,20,20	0.45	0	25,25,25	0.59	0
2	BOG	A	267	-	20,20,20	0.47	0	25,25,25	0.59	0
2	BOG	E	267	-	20,20,20	0.45	0	25,25,25	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	B	268	-	-	2/11/31/31	0/1/1/1
2	BOG	D	267	-	-	3/11/31/31	0/1/1/1
2	BOG	A	267	-	-	0/11/31/31	0/1/1/1
2	BOG	E	267	-	-	1/11/31/31	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	268	BOG	O5-C1-O1-C1'
2	D	267	BOG	O5-C5-C6-O6
2	D	267	BOG	C4-C5-C6-O6
2	B	268	BOG	C2'-C3'-C4'-C5'
2	D	267	BOG	O5-C1-O1-C1'
2	E	267	BOG	O5-C1-O1-C1'

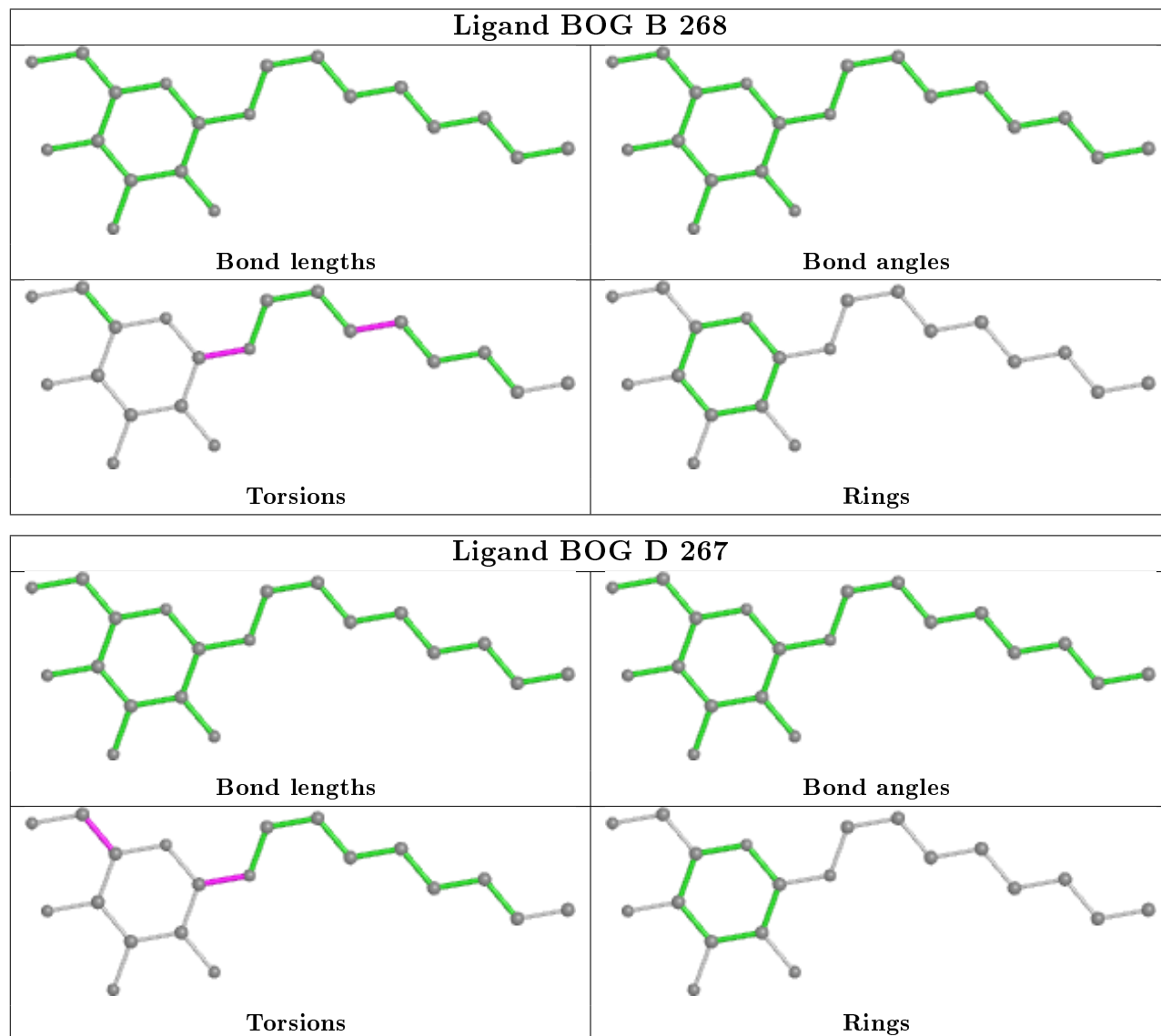
There are no ring outliers.

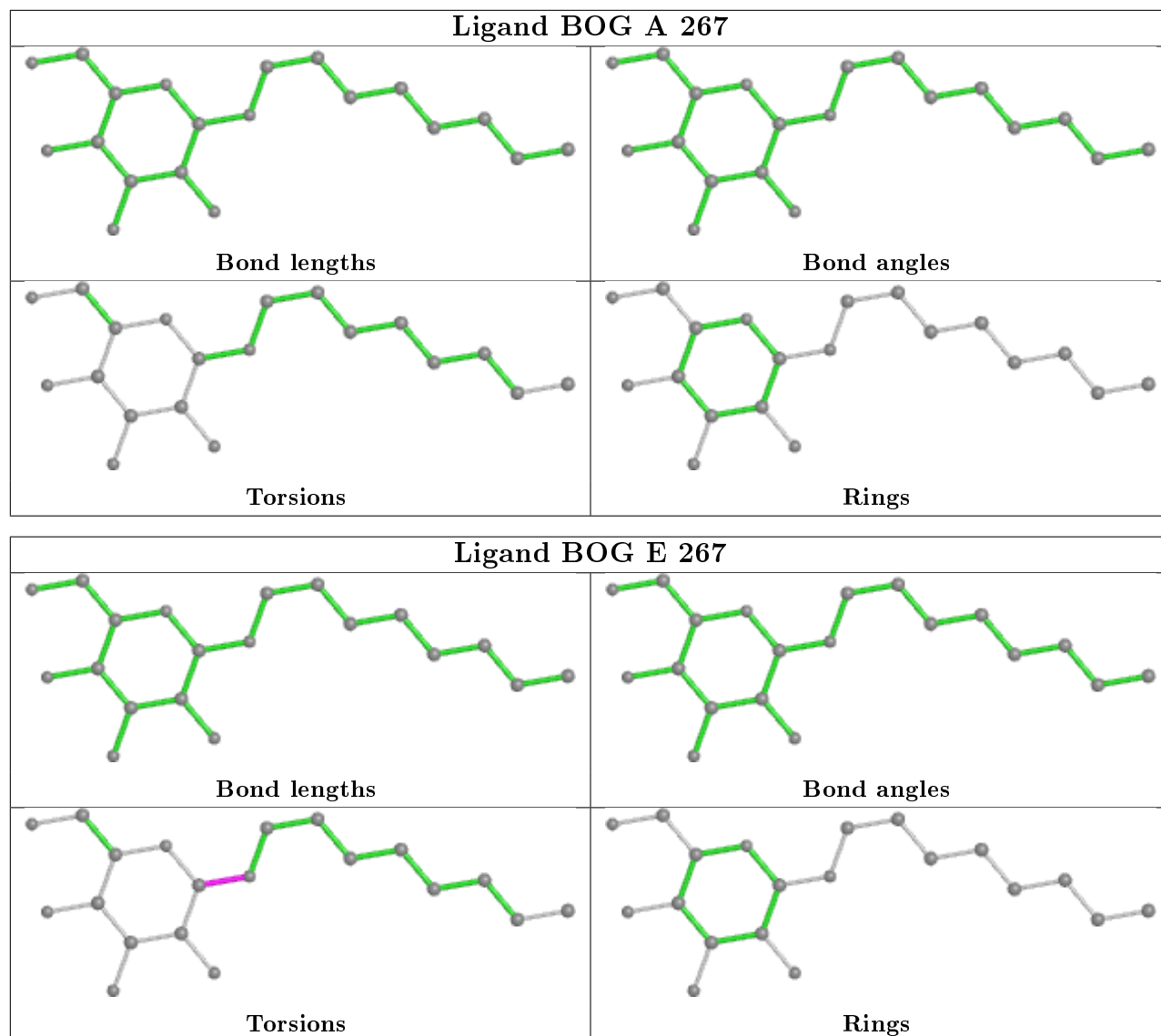
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	268	BOG	3	0
2	D	267	BOG	1	0
2	A	267	BOG	3	0
2	E	267	BOG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	257/268 (95%)	-0.29	3 (1%) 79 82	24, 35, 56, 92	0
1	B	257/268 (95%)	-0.27	9 (3%) 44 50	23, 34, 65, 82	0
1	C	266/268 (99%)	-0.07	11 (4%) 37 43	23, 36, 67, 124	0
1	D	257/268 (95%)	-0.26	4 (1%) 72 75	22, 34, 56, 95	0
1	E	256/268 (95%)	-0.37	8 (3%) 49 55	24, 33, 56, 85	0
All	All	1293/1340 (96%)	-0.25	35 (2%) 54 60	22, 35, 60, 124	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	219	SER	8.8
1	C	265	TYR	6.9
1	B	222	THR	6.6
1	B	221	VAL	5.4
1	B	220	THR	5.4
1	C	149	ALA	4.3
1	C	216	PRO	3.5
1	A	17	ILE	3.5
1	C	221	VAL	3.5
1	C	220	THR	3.3
1	B	219	SER	3.1
1	D	218	ILE	3.0
1	C	66	LEU	2.9
1	C	264	LEU	2.6
1	B	223	ILE	2.5
1	E	221	VAL	2.5
1	B	185	ILE	2.5
1	D	184	ILE	2.5
1	A	221	VAL	2.5
1	E	220	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	66	LEU	2.3
1	C	146	ALA	2.3
1	B	227	ILE	2.3
1	E	188	PHE	2.3
1	C	188	PHE	2.3
1	B	189	LEU	2.3
1	E	218	ILE	2.2
1	E	255	GLU	2.1
1	C	22	THR	2.1
1	D	185	ILE	2.0
1	D	256	LYS	2.0
1	B	184	ILE	2.0
1	E	185	ILE	2.0
1	E	189	LEU	2.0
1	E	217	THR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

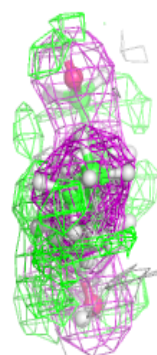
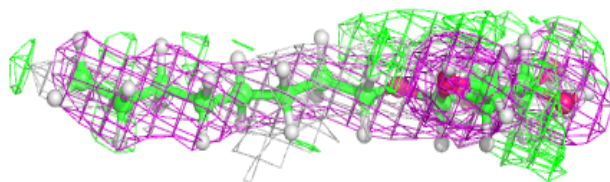
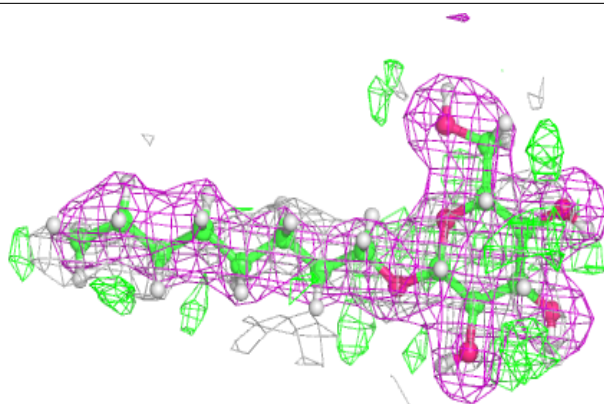
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BOG	D	267	20/20	0.48	0.68	10,10,10,10	0
2	BOG	E	267	20/20	0.57	0.61	10,10,10,10	0
2	BOG	B	268	20/20	0.58	0.58	10,10,10,10	0
2	BOG	A	267	20/20	0.64	0.67	10,10,10,10	0

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.

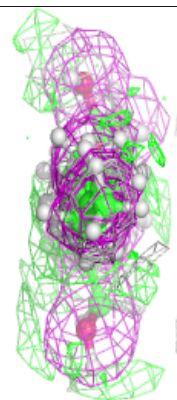
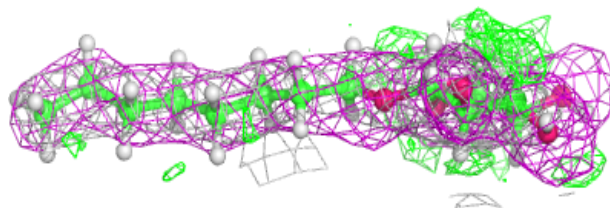
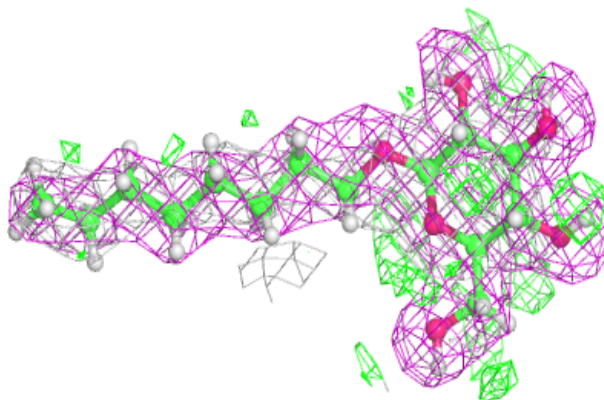
Electron density around BOG D 267:

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



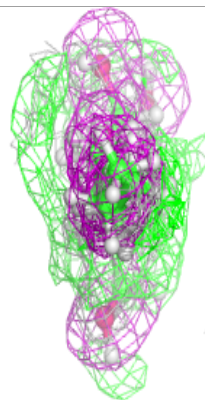
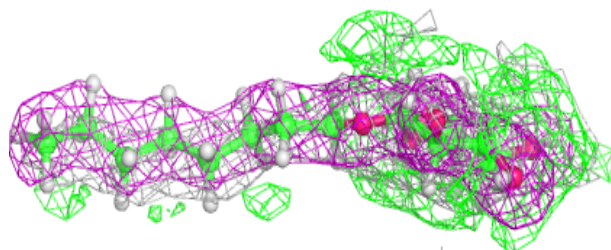
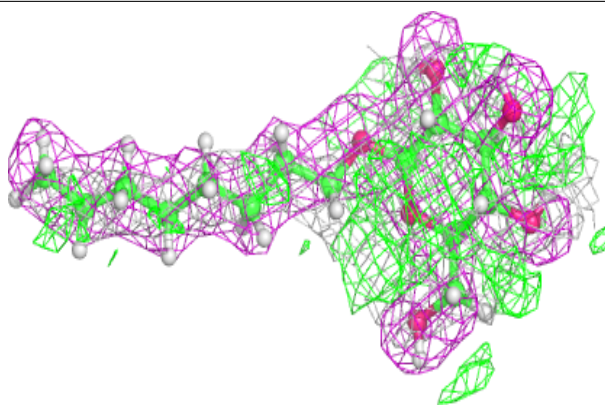
Electron density around BOG E 267:

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

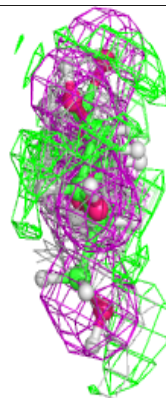
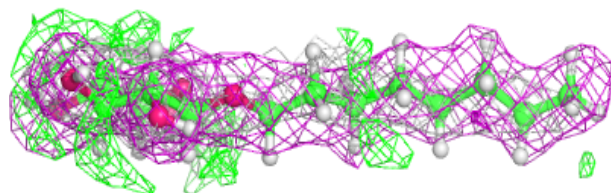
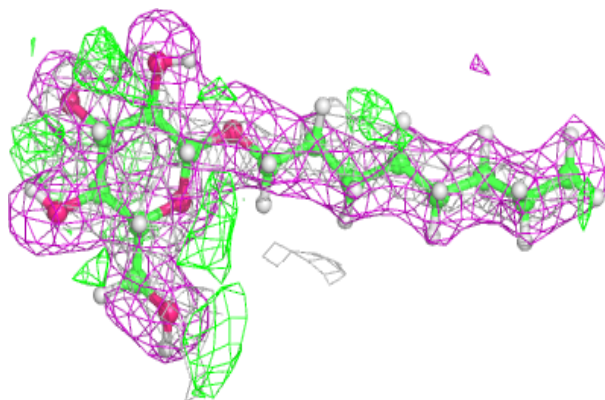


Electron density around BOG B 268:

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

**Electron density around BOG A 267:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.