



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:45 AM GMT

PDB ID : 3POX  
Title : Crystal Structure of E.coli OmpF porin in lipidic cubic phase: space group P1  
Authors : Efremov, R.G.; Sazanov, L.A.  
Deposited on : 2010-11-23  
Resolution : 2.00 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

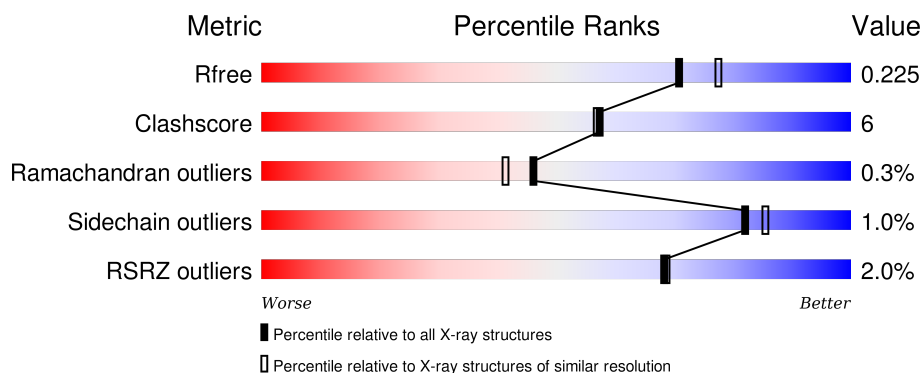
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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	340	<div> <div></div> <div>88%12%</div> </div>
1	B	340	<div> <div>3%</div> <div>86%13%</div> </div>
1	C	340	<div> <div>2%</div> <div>90%10%</div> </div>
1	D	340	<div> <div>2%</div> <div>90%10%</div> </div>
1	E	340	<div> <div></div> <div>89%10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	340	

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	OLC	A	343	-	-	-	X
2	OLC	A	344	-	-	-	X
2	OLC	A	346	-	-	-	X
2	OLC	A	347	-	-	-	X
2	OLC	A	349	-	-	-	X
2	OLC	A	350	-	-	-	X
2	OLC	A	354	-	-	-	X
2	OLC	A	356	-	-	-	X
2	OLC	A	357	-	-	-	X
2	OLC	A	358	-	-	-	X
2	OLC	A	359	-	-	-	X
2	OLC	A	361	-	-	-	X
2	OLC	A	363	-	-	-	X
2	OLC	B	342	-	-	-	X
2	OLC	B	345	-	-	-	X
2	OLC	B	346	-	-	-	X
2	OLC	B	350	-	-	-	X
2	OLC	B	351	-	-	-	X
2	OLC	B	352	-	-	-	X
2	OLC	B	353	-	-	-	X
2	OLC	C	342	-	-	-	X
2	OLC	C	345	-	-	-	X
2	OLC	C	348	-	-	-	X
2	OLC	C	349	-	-	-	X
2	OLC	C	350	-	-	-	X
2	OLC	C	352	-	-	-	X
2	OLC	C	357	-	-	-	X
2	OLC	C	358	-	-	-	X
2	OLC	C	359	-	-	-	X
2	OLC	C	360	-	-	-	X
2	OLC	C	361	-	-	-	X
2	OLC	C	362	-	-	-	X
2	OLC	C	363	-	-	-	X
2	OLC	D	342	-	-	-	X
2	OLC	D	344	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OLC	D	346	-	-	-	X
2	OLC	D	348	-	-	-	X
2	OLC	D	349	-	-	-	X
2	OLC	E	341	-	-	-	X
2	OLC	E	342	-	-	-	X
2	OLC	E	343	-	-	-	X
2	OLC	E	345	-	-	-	X
2	OLC	E	347	-	-	-	X
2	OLC	E	348	-	-	-	X
2	OLC	F	341	-	-	-	X
2	OLC	F	342	-	-	-	X
2	OLC	F	343	-	-	-	X
2	OLC	F	345	-	-	-	X
2	OLC	F	346	-	-	-	X
4	SCN	E	352	-	-	-	X

## 2 Entry composition [i](#)

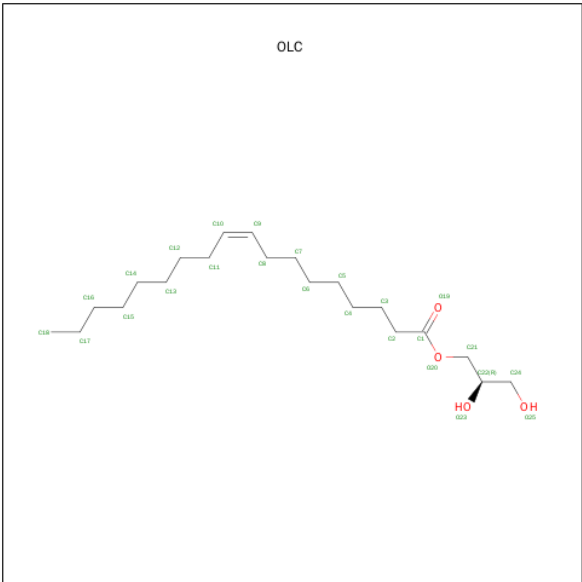
There are 5 unique types of molecules in this entry. The entry contains 18507 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OmpF protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	B	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	C	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	D	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	E	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	F	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			

- Molecule 2 is (2R)-2,3-DIHYDROXYPROPYL (9Z)-OCTADEC-9-ENOATE (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 14 14	0	0
2	A	1	Total C 14 14	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 14 14	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 12 12	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 8 8	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C 16 16	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 8 8	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C 12 12	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 14 14	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 14 14	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C 12 12	0	0
2	D	1	Total C 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 25 21 4	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C 10 10	0	0
2	D	1	Total C 12 12	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C O 25 21 4	0	0
2	E	1	Total C O 25 21 4	0	0
2	E	1	Total C 8 8	0	0
2	E	1	Total C 12 12	0	0
2	E	1	Total C 12 12	0	0
2	E	1	Total C 14 14	0	0
2	E	1	Total C 10 10	0	0
2	E	1	Total C O 25 21 4	0	0
2	E	1	Total C 12 12	0	0
2	F	1	Total C 8 8	0	0
2	F	1	Total C 14 14	0	0
2	F	1	Total C 8 8	0	0
2	F	1	Total C 10 10	0	0
2	F	1	Total C 12 12	0	0

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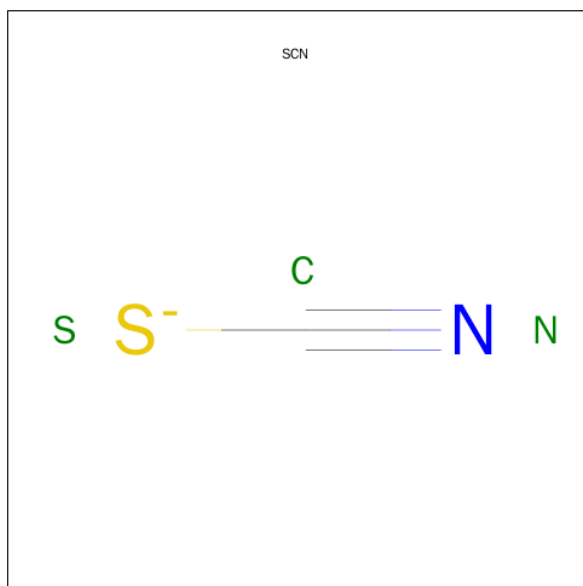
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C 8 8	0	0
2	F	1	Total C 14 14	0	0
2	F	1	Total C 14 14	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	4	Total K 4 4	0	0
3	E	3	Total K 3 3	0	0
3	B	3	Total K 3 3	0	0
3	C	4	Total K 4 4	0	0
3	A	3	Total K 3 3	0	0
3	F	3	Total K 3 3	0	0

- Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).

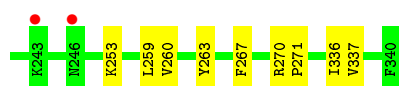


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N S 3 1 1 1	0	0
4	B	1	Total C N S 3 1 1 1	0	0
4	D	1	Total C N S 3 1 1 1	0	0
4	E	1	Total C N S 3 1 1 1	0	0
4	E	1	Total C N S 3 1 1 1	0	0
4	F	1	Total C N S 3 1 1 1	0	0

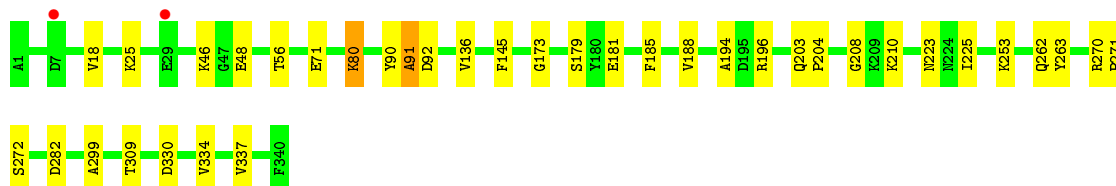
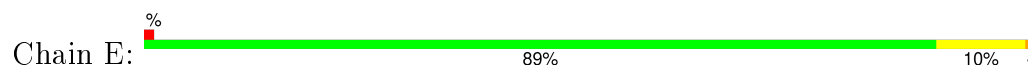
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	267	Total O 267 267	0	0
5	B	236	Total O 236 236	0	0
5	C	257	Total O 257 257	0	0
5	D	272	Total O 272 272	0	0
5	E	278	Total O 278 278	0	0
5	F	212	Total O 212 212	0	0

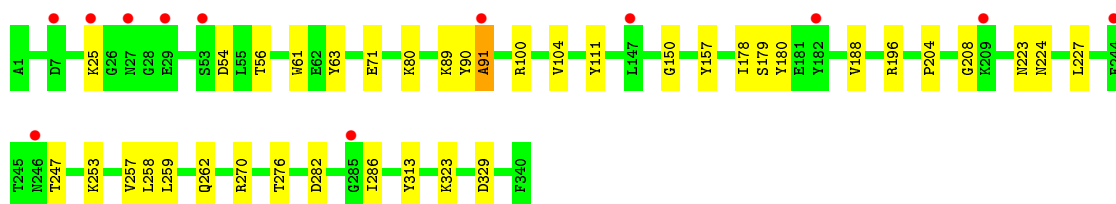
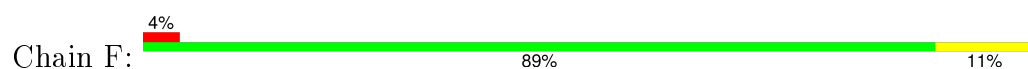




- Molecule 1: OmpF protein



- Molecule 1: OmpF protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.57Å 86.02Å 116.56Å 83.28° 78.46° 89.89°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-2.00) 93.5 (20.00-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.188 , 0.225 0.187 , 0.225	Depositor DCC
$R_{free}$ test set	9833 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 64.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 196184 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18507	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: K, OLC, SCN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.44	0/2683	0.56	0/3628
1	B	0.39	0/2683	0.54	0/3628
1	C	0.40	0/2683	0.55	0/3628
1	D	0.40	0/2683	0.55	0/3628
1	E	0.43	0/2683	0.57	0/3628
1	F	0.36	0/2683	0.53	0/3628
All	All	0.40	0/16098	0.55	0/21768

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2627	0	2444	35	0
1	B	2627	0	2444	36	0
1	C	2627	0	2444	27	0
1	D	2627	0	2444	26	0
1	E	2627	0	2444	26	0
1	F	2627	0	2444	28	0
2	A	342	0	531	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	205	0	321	5	0
2	C	323	0	499	18	0
2	D	109	0	167	8	0
2	E	118	0	183	19	0
2	F	88	0	135	9	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	D	3	0	0	0	0
4	E	6	0	0	0	0
4	F	3	0	0	0	0
5	A	267	0	0	2	0
5	B	236	0	0	4	0
5	C	257	0	0	1	0
5	D	272	0	0	1	0
5	E	278	0	0	2	0
5	F	212	0	0	0	0
All	All	18507	0	16500	201	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 (201) 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:179:SER:HB2	1:B:188:VAL:HG22	1.53	0.90
2:A:341:OLC:H2	2:A:361:OLC:O19	1.73	0.88
1:A:297:VAL:HG12	2:A:361:OLC:H13	1.58	0.85
1:A:258:LEU:CD1	1:A:276:THR:HG23	2.07	0.84
2:A:359:OLC:H24	1:B:172:ASP:OD1	1.79	0.83
1:C:179:SER:CB	1:C:188:VAL:HG12	2.09	0.83
2:C:363:OLC:H22	5:C:546:HOH:O	1.77	0.82
1:C:172:ASP:OD1	2:C:359:OLC:H24	1.80	0.81
2:A:360:OLC:C12	2:A:365:OLC:H3	2.12	0.79
1:E:334:VAL:CG2	2:E:347:OLC:H9	2.13	0.79
1:C:179:SER:HB2	1:C:188:VAL:HG12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:348:OLC:H7A	2:C:349:OLC:H2A	1.66	0.77
2:E:346:OLC:H3	2:F:347:OLC:H6A	1.68	0.74
1:F:178:ILE:HG13	2:F:342:OLC:H4	1.68	0.74
2:B:344:OLC:H9	2:B:345:OLC:H21	1.68	0.73
1:E:334:VAL:HG22	2:E:347:OLC:H9	1.70	0.73
2:A:360:OLC:C11	2:A:365:OLC:H3	2.19	0.73
1:D:18:VAL:HG13	1:D:337:VAL:HG22	1.71	0.73
1:B:71:GLU:HB3	1:C:80:LYS:HD2	1.71	0.72
1:F:179:SER:HB2	1:F:188:VAL:HG22	1.71	0.72
1:C:18:VAL:HG13	1:C:337:VAL:HG22	1.73	0.70
1:C:111:TYR:OH	1:C:188:VAL:HG13	1.92	0.70
1:B:111:TYR:OH	1:B:188:VAL:HG23	1.92	0.70
1:F:54:ASP:HB3	1:F:91:ALA:HB2	1.73	0.69
2:A:360:OLC:H11A	2:A:365:OLC:H3	1.75	0.69
1:D:160:LYS:HE2	5:D:1294:HOH:O	1.93	0.69
2:C:353:OLC:H2A	2:C:363:OLC:H18	1.75	0.68
1:C:179:SER:HB3	1:C:188:VAL:HG12	1.75	0.67
1:F:258:LEU:CD1	1:F:276:THR:HG23	2.25	0.67
1:B:179:SER:CB	1:B:188:VAL:HG22	2.25	0.66
1:E:262:GLN:HG2	1:E:272:SER:HB2	1.78	0.65
1:B:334:VAL:CG2	2:C:359:OLC:H12	2.28	0.64
1:E:330:ASP:H	2:E:344:OLC:C1	2.09	0.64
1:D:178:ILE:HG13	2:D:342:OLC:H11	1.78	0.64
1:E:334:VAL:HG23	2:E:347:OLC:H12A	1.78	0.63
1:A:271:PRO:HB3	2:A:361:OLC:H18B	1.81	0.63
1:F:179:SER:CB	1:F:188:VAL:HG22	2.30	0.62
2:A:361:OLC:H18	2:A:365:OLC:C1	2.30	0.61
1:B:258:LEU:CD1	1:B:276:THR:HG23	2.30	0.61
1:E:299:ALA:HB3	2:E:347:OLC:H18B	1.79	0.61
1:A:196:ARG:HD3	1:A:208:GLY:O	1.99	0.61
1:A:179:SER:HB3	1:A:188:VAL:HG22	1.83	0.61
1:F:286:ILE:HG23	1:F:323:LYS:HD3	1.83	0.60
1:A:111:TYR:OH	1:A:188:VAL:HG23	2.01	0.60
2:E:347:OLC:C11	2:E:348:OLC:H3	2.32	0.59
1:A:179:SER:CB	1:A:188:VAL:HG22	2.30	0.59
1:A:334:VAL:HG12	2:A:359:OLC:H8A	1.84	0.59
1:E:334:VAL:CG2	2:E:347:OLC:H12A	2.33	0.58
1:D:267:PHE:HB2	2:D:349:OLC:H22	1.84	0.58
1:D:80:LYS:HD2	1:F:71:GLU:HB3	1.84	0.58
1:A:258:LEU:HD12	1:A:276:THR:HG23	1.85	0.57
1:A:309:THR:OG1	2:A:359:OLC:H11A	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:347:OLC:H11A	2:E:348:OLC:H3	1.86	0.57
1:B:180:TYR:CE1	2:B:350:OLC:H5	2.40	0.57
1:E:253:LYS:HE2	1:E:282:ASP:OD2	2.04	0.57
2:C:347:OLC:H5	2:C:358:OLC:O19	2.04	0.57
1:F:157:TYR:CZ	2:F:347:OLC:H8	2.40	0.56
1:B:71:GLU:CB	1:C:80:LYS:HD2	2.35	0.56
2:A:356:OLC:H7	1:C:334:VAL:HG12	1.87	0.56
1:A:263:TYR:O	1:A:271:PRO:HD2	2.05	0.56
1:F:259:LEU:HD11	2:F:344:OLC:H7A	1.86	0.56
1:E:299:ALA:HB3	2:E:347:OLC:C18	2.36	0.56
1:F:257:VAL:O	1:F:258:LEU:HD13	2.05	0.56
1:F:258:LEU:HD12	1:F:276:THR:HG23	1.88	0.56
2:F:341:OLC:C1	2:F:342:OLC:H2A	2.36	0.56
1:B:204:PRO:HG2	1:B:247:THR:HG23	1.88	0.55
1:A:100:ARG:NH2	1:C:71:GLU:HG3	2.20	0.55
1:F:196:ARG:HD3	1:F:208:GLY:O	2.06	0.55
2:A:341:OLC:H4	2:A:361:OLC:H3A	1.88	0.55
1:C:191:TYR:HE2	2:C:352:OLC:H5	1.71	0.55
2:E:347:OLC:H11A	2:E:348:OLC:C3	2.38	0.54
1:D:178:ILE:HG12	2:D:342:OLC:H14	1.89	0.54
1:F:253:LYS:HE2	1:F:282:ASP:OD2	2.07	0.54
1:A:92:ASP:O	1:A:145:PHE:HA	2.08	0.54
1:A:257:VAL:O	1:A:258:LEU:HD13	2.08	0.53
1:B:196:ARG:HD3	1:B:208:GLY:O	2.08	0.53
1:C:266:ASP:N	2:C:362:OLC:H24	2.23	0.53
1:B:334:VAL:HG22	2:C:359:OLC:H12	1.91	0.53
2:E:347:OLC:C10	2:E:348:OLC:H3	2.38	0.53
1:E:46:LYS:HG2	5:E:1092:HOH:O	2.08	0.52
1:A:180:TYR:HB2	2:A:349:OLC:H12A	1.90	0.52
1:D:61:TRP:CZ2	1:D:63:TYR:HB2	2.45	0.52
1:F:111:TYR:OH	1:F:188:VAL:HG23	2.10	0.52
1:F:223:ASN:O	1:F:224:ASN:HB2	2.10	0.52
1:E:263:TYR:O	1:E:271:PRO:HD2	2.10	0.52
1:E:179:SER:HB3	1:E:188:VAL:HG23	1.92	0.52
1:D:235:ARG:HD3	1:D:253:LYS:HG2	1.93	0.51
1:B:71:GLU:HG3	1:C:100:ARG:NH2	2.26	0.51
1:B:313:TYR:CE2	1:B:332:VAL:HG22	2.46	0.51
1:D:259:LEU:HB3	2:D:346:OLC:H6A	1.93	0.51
2:E:347:OLC:H10	2:E:348:OLC:H3	1.91	0.51
1:B:111:TYR:OH	1:B:188:VAL:CG2	2.58	0.51
1:B:54:ASP:HB3	1:B:91:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ARG:HD3	1:C:208:GLY:O	2.10	0.50
1:A:71:GLU:HG3	1:B:100:ARG:NH2	2.26	0.50
1:E:48:GLU:HG3	1:E:56:THR:CG2	2.42	0.50
2:C:360:OLC:H12A	2:C:360:OLC:H8A	1.93	0.50
1:E:92:ASP:O	1:E:145:PHE:HA	2.12	0.50
1:A:173:GLY:HA3	1:A:194:ALA:HB2	1.93	0.50
1:C:61:TRP:CZ2	1:C:63:TYR:HB2	2.47	0.50
1:A:271:PRO:HB2	2:A:343:OLC:H2	1.94	0.50
1:F:178:ILE:CG1	2:F:342:OLC:H4	2.39	0.50
1:F:111:TYR:CZ	1:F:188:VAL:HG23	2.47	0.49
1:C:111:TYR:CZ	1:C:188:VAL:HG13	2.47	0.49
1:E:18:VAL:HG13	1:E:337:VAL:HG22	1.95	0.49
2:A:349:OLC:H21	5:A:425:HOH:O	2.13	0.49
1:C:25:LYS:HE3	1:C:329:ASP:CG	2.33	0.49
1:C:263:TYR:O	1:C:271:PRO:HD2	2.14	0.48
2:C:347:OLC:H3	2:C:358:OLC:O19	2.13	0.48
1:F:204:PRO:HG2	1:F:247:THR:HG23	1.95	0.48
1:C:266:ASP:H	2:C:362:OLC:H24	1.79	0.48
1:A:143:ASN:HA	1:A:148:VAL:O	2.13	0.48
1:D:336:ILE:HB	2:E:341:OLC:H9	1.95	0.48
1:A:271:PRO:CB	2:A:361:OLC:H18B	2.41	0.48
2:E:343:OLC:H2A	2:E:344:OLC:H5	1.96	0.48
1:B:223:ASN:O	1:B:224:ASN:HB2	2.13	0.47
1:E:270:ARG:NH2	5:E:641:HOH:O	2.47	0.47
1:D:142:SER:HA	1:D:152:ASN:OD1	2.14	0.47
1:F:180:TYR:HB2	2:F:343:OLC:C1	2.45	0.47
1:B:255:GLN:NE2	5:B:956:HOH:O	2.48	0.47
1:B:263:TYR:O	1:B:271:PRO:HD2	2.13	0.47
1:C:25:LYS:HE3	1:C:329:ASP:OD1	2.14	0.47
1:B:143:ASN:HA	1:B:148:VAL:O	2.15	0.47
1:A:187:ILE:HG12	2:A:349:OLC:H16	1.95	0.47
1:B:313:TYR:CD2	1:B:332:VAL:HG22	2.49	0.47
1:B:7:ASP:HB2	5:B:661:HOH:O	2.15	0.47
1:E:196:ARG:HD3	1:E:208:GLY:O	2.15	0.46
1:B:259:LEU:HD11	2:B:351:OLC:H8	1.97	0.46
1:A:258:LEU:HD11	1:A:276:THR:HG23	1.91	0.46
2:B:351:OLC:O19	2:B:351:OLC:C4	2.62	0.46
1:A:147:LEU:HD11	2:A:353:OLC:H3	1.98	0.46
1:B:92:ASP:O	1:B:145:PHE:HA	2.15	0.46
1:F:56:THR:HB	1:F:89:LYS:HG2	1.96	0.46
1:A:61:TRP:CZ2	1:A:63:TYR:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:TYR:CZ	1:A:188:VAL:HG23	2.51	0.45
2:A:361:OLC:H22	5:A:397:HOH:O	2.16	0.45
1:B:234:THR:O	1:B:235:ARG:HD3	2.17	0.45
1:B:111:TYR:CZ	1:B:188:VAL:HG23	2.51	0.45
1:A:179:SER:HB2	1:A:188:VAL:HG22	1.97	0.45
1:C:191:TYR:CE2	2:C:352:OLC:H5	2.52	0.45
1:D:270:ARG:O	1:D:270:ARG:HG2	2.17	0.45
1:D:48:GLU:HG3	1:D:56:THR:CG2	2.46	0.45
1:B:257:VAL:O	1:B:258:LEU:HD13	2.16	0.45
2:C:363:OLC:H5A	2:C:363:OLC:H8A	1.61	0.45
1:B:220:TYR:OH	2:B:345:OLC:H21A	2.17	0.44
1:B:61:TRP:CZ2	1:B:63:TYR:HB2	2.53	0.44
1:F:150:GLY:O	1:F:180:TYR:HA	2.17	0.44
1:B:50:GLN:NE2	5:B:1263:HOH:O	2.50	0.44
1:E:223:ASN:O	1:E:225:ILE:HG13	2.17	0.44
1:D:231:TYR:HB2	2:D:348:OLC:H3	1.99	0.44
1:D:178:ILE:CG1	2:D:342:OLC:H14	2.47	0.44
1:B:30:ASN:ND2	1:B:327:GLY:HA2	2.32	0.44
1:D:263:TYR:O	1:D:271:PRO:HD2	2.17	0.44
1:D:187:ILE:HG13	1:D:218:LEU:HD23	2.00	0.44
1:C:119:GLY:HA2	1:C:294:TYR:OH	2.18	0.43
1:A:98:TYR:CE1	2:A:356:OLC:H4A	2.53	0.43
1:C:218:LEU:HG	2:C:349:OLC:H9	1.99	0.43
1:C:267:PHE:HB2	2:C:360:OLC:H21	1.99	0.43
1:C:142:SER:HA	1:C:152:ASN:OD1	2.18	0.43
2:A:345:OLC:H3	2:A:362:OLC:H4	2.00	0.43
1:D:100:ARG:NH2	1:F:71:GLU:HG3	2.34	0.43
1:F:227:LEU:HB3	2:F:345:OLC:H5A	1.99	0.43
1:A:258:LEU:O	1:A:259:LEU:HD23	2.17	0.43
1:C:27:ASN:OD1	1:C:29:GLU:HB2	2.19	0.43
1:E:181:GLU:HA	1:E:185:PHE:O	2.19	0.43
1:F:61:TRP:CZ2	1:F:63:TYR:HB2	2.54	0.43
1:D:71:GLU:HG2	1:E:80:LYS:HG3	2.00	0.42
1:D:228:ALA:HB3	1:D:260:VAL:CG2	2.49	0.42
1:F:262:GLN:OE1	1:F:270:ARG:NH1	2.48	0.42
1:E:309:THR:HG21	2:E:348:OLC:H5A	2.01	0.42
1:F:25:LYS:HE3	1:F:329:ASP:OD1	2.19	0.42
1:C:253:LYS:HE2	1:C:282:ASP:OD2	2.19	0.42
1:B:104:VAL:HG22	1:B:177:SER:HB3	2.02	0.42
1:D:13:LEU:HD12	1:D:44:GLY:O	2.20	0.42
1:E:71:GLU:HG3	1:F:100:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:HG13	1:A:156:GLN:CD	2.40	0.42
1:E:173:GLY:HA3	1:E:194:ALA:HB2	2.02	0.42
1:B:254:THR:HA	1:B:279:LYS:O	2.20	0.42
1:B:204:PRO:HB2	1:B:247:THR:HG21	2.02	0.41
1:E:25:LYS:HD3	2:E:344:OLC:H2	2.02	0.41
1:A:305:LYS:NZ	5:B:661:HOH:O	2.52	0.41
1:E:90:TYR:O	1:E:91:ALA:C	2.58	0.41
1:E:203:GLN:HA	1:E:204:PRO:HD3	1.94	0.41
1:F:54:ASP:HB2	1:F:90:TYR:HE1	1.85	0.41
1:A:315:ILE:HG12	2:A:361:OLC:H3	2.03	0.41
2:C:352:OLC:H10	2:C:363:OLC:H15A	2.03	0.41
1:D:191:TYR:CE1	2:D:345:OLC:H5A	2.56	0.41
1:D:48:GLU:HG3	1:D:56:THR:HG21	2.03	0.41
2:A:344:OLC:C10	2:A:344:OLC:H6	2.51	0.40
1:D:90:TYR:O	1:D:91:ALA:C	2.60	0.40
2:E:346:OLC:H5	2:F:347:OLC:C9	2.51	0.40
1:A:203:GLN:HA	1:A:204:PRO:HD3	1.92	0.40
2:E:342:OLC:H4	2:E:342:OLC:H7	1.89	0.40
1:A:46:LYS:HB3	1:A:46:LYS:HE2	1.77	0.40
1:D:95:SER:O	1:D:139:TYR:HA	2.21	0.40
2:A:360:OLC:H11A	2:A:365:OLC:C3	2.47	0.40
2:C:348:OLC:H7A	2:C:349:OLC:C2	2.45	0.40
1:D:178:ILE:CG1	2:D:342:OLC:H11	2.48	0.40
1:A:269:LEU:HG	1:A:271:PRO:HD3	2.03	0.40
1:A:48:GLU:HG2	1:A:56:THR:CG2	2.52	0.40
1:B:253:LYS:O	1:B:280:ALA:HA	2.22	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	338/340 (99%)	325 (96%)	12 (4%)	1 (0%)	46	41
1	B	338/340 (99%)	323 (96%)	14 (4%)	1 (0%)	46	41
1	C	338/340 (99%)	324 (96%)	13 (4%)	1 (0%)	46	41
1	D	338/340 (99%)	327 (97%)	10 (3%)	1 (0%)	46	41
1	E	338/340 (99%)	325 (96%)	12 (4%)	1 (0%)	46	41
1	F	338/340 (99%)	321 (95%)	16 (5%)	1 (0%)	46	41
All	All	2028/2040 (99%)	1945 (96%)	77 (4%)	6 (0%)	46	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	91	ALA
1	A	91	ALA
1	F	91	ALA
1	D	91	ALA
1	B	91	ALA
1	C	91	ALA

### 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	263/263 (100%)	260 (99%)	3 (1%)	80	83
1	B	263/263 (100%)	261 (99%)	2 (1%)	86	89
1	C	263/263 (100%)	260 (99%)	3 (1%)	80	83
1	D	263/263 (100%)	262 (100%)	1 (0%)	93	95
1	E	263/263 (100%)	260 (99%)	3 (1%)	80	83
1	F	263/263 (100%)	260 (99%)	3 (1%)	80	83
All	All	1578/1578 (100%)	1563 (99%)	15 (1%)	82	85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	A	97	ASP
1	A	136	VAL
1	B	80	LYS
1	B	136	VAL
1	C	121	ASP
1	C	136	VAL
1	C	313	TYR
1	D	136	VAL
1	E	80	LYS
1	E	136	VAL
1	E	210	LYS
1	F	80	LYS
1	F	104	VAL
1	F	313	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	60	GLN
1	B	30	ASN
1	B	50	GLN
1	B	60	GLN
1	C	30	ASN
1	C	50	GLN
1	C	60	GLN
1	D	30	ASN
1	D	60	GLN
1	E	60	GLN
1	F	30	ASN
1	F	60	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 114 ligands modelled in this entry, 20 are monoatomic - leaving 94 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	OLC	A	341	-	7,7,24	0.22	0	6,6,25	0.45	0
2	OLC	A	342	-	7,7,24	0.22	0	6,6,25	0.57	0
2	OLC	A	343	-	7,7,24	0.23	0	6,6,25	0.57	0
2	OLC	A	344	-	9,9,24	1.19	1 (11%)	8,8,25	0.98	1 (12%)
2	OLC	A	345	-	7,7,24	0.27	0	6,6,25	0.48	0
2	OLC	A	346	-	24,24,24	1.52	4 (16%)	25,25,25	1.23	2 (8%)
2	OLC	A	347	-	7,7,24	0.24	0	6,6,25	0.52	0
2	OLC	A	348	-	9,9,24	1.16	1 (11%)	8,8,25	0.99	1 (12%)
2	OLC	A	349	-	24,24,24	1.49	4 (16%)	25,25,25	1.11	2 (8%)
2	OLC	A	350	-	13,13,24	1.11	1 (7%)	11,12,25	0.95	1 (9%)
2	OLC	A	351	-	13,13,24	1.08	1 (7%)	11,12,25	0.95	1 (9%)
2	OLC	A	352	-	9,9,24	1.16	1 (11%)	8,8,25	0.95	1 (12%)
2	OLC	A	353	-	7,7,24	0.20	0	6,6,25	0.54	0
2	OLC	A	354	-	7,7,24	0.24	0	6,6,25	0.52	0
2	OLC	A	355	-	9,9,24	1.16	1 (11%)	8,8,25	1.01	1 (12%)
2	OLC	A	356	-	24,24,24	1.49	4 (16%)	25,25,25	1.27	2 (8%)
2	OLC	A	357	-	9,9,24	1.17	1 (11%)	8,8,25	0.93	1 (12%)
2	OLC	A	358	-	24,24,24	1.50	4 (16%)	25,25,25	1.16	2 (8%)
2	OLC	A	359	-	24,24,24	1.44	4 (16%)	25,25,25	1.03	2 (8%)
2	OLC	A	360	-	11,11,24	1.16	1 (9%)	10,10,25	1.27	1 (10%)
2	OLC	A	361	-	24,24,24	1.58	4 (16%)	25,25,25	1.35	2 (8%)
2	OLC	A	362	-	13,13,24	1.13	1 (7%)	11,12,25	1.05	1 (9%)
2	OLC	A	363	-	11,11,24	1.27	1 (9%)	10,10,25	1.15	1 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	A	364	-	11,11,24	1.21	1 (9%)	10,10,25	1.40	1 (10%)
2	OLC	A	365	-	7,7,24	0.44	0	6,6,25	0.78	0
4	SCN	A	369	-	2,2,2	1.96	1 (50%)	1,1,1	0.18	0
2	OLC	B	341	-	4,4,24	0.21	0	3,3,25	0.44	0
2	OLC	B	342	-	13,13,24	1.07	1 (7%)	11,12,25	0.99	2 (18%)
2	OLC	B	343	-	7,7,24	0.22	0	6,6,25	0.46	0
2	OLC	B	344	-	9,9,24	1.17	1 (11%)	8,8,25	0.94	1 (12%)
2	OLC	B	345	-	24,24,24	1.50	4 (16%)	25,25,25	1.07	1 (4%)
2	OLC	B	346	-	24,24,24	1.50	4 (16%)	25,25,25	1.40	2 (8%)
2	OLC	B	347	-	13,13,24	1.09	1 (7%)	11,12,25	1.04	1 (9%)
2	OLC	B	348	-	13,13,24	1.06	1 (7%)	11,12,25	1.02	1 (9%)
2	OLC	B	349	-	7,7,24	0.24	0	6,6,25	0.47	0
2	OLC	B	350	-	24,24,24	1.51	4 (16%)	25,25,25	1.09	1 (4%)
2	OLC	B	351	-	24,24,24	1.41	4 (16%)	25,25,25	1.11	1 (4%)
2	OLC	B	352	-	15,15,24	0.98	1 (6%)	14,14,25	1.23	2 (14%)
2	OLC	B	353	-	7,7,24	0.34	0	6,6,25	0.46	0
2	OLC	B	354	-	7,7,24	0.43	0	6,6,25	0.67	0
4	SCN	B	358	-	2,2,2	1.90	1 (50%)	1,1,1	0.15	0
2	OLC	C	341	-	9,9,24	1.15	1 (11%)	8,8,25	1.00	1 (12%)
2	OLC	C	342	-	7,7,24	0.22	0	6,6,25	0.57	0
2	OLC	C	343	-	7,7,24	0.22	0	6,6,25	0.52	0
2	OLC	C	344	-	7,7,24	0.28	0	6,6,25	0.45	0
2	OLC	C	345	-	11,11,24	1.19	1 (9%)	10,10,25	1.33	1 (10%)
2	OLC	C	346	-	9,9,24	1.15	1 (11%)	8,8,25	1.11	1 (12%)
2	OLC	C	347	-	9,9,24	1.16	1 (11%)	8,8,25	1.08	1 (12%)
2	OLC	C	348	-	11,11,24	1.18	1 (9%)	10,10,25	1.35	1 (10%)
2	OLC	C	349	-	9,9,24	1.14	1 (11%)	8,8,25	1.16	1 (12%)
2	OLC	C	350	-	13,13,24	1.08	1 (7%)	11,12,25	0.99	1 (9%)
2	OLC	C	351	-	7,7,24	0.24	0	6,6,25	0.49	0
2	OLC	C	352	-	11,11,24	1.16	1 (9%)	10,10,25	1.46	1 (10%)
2	OLC	C	353	-	9,9,24	1.16	1 (11%)	8,8,25	1.00	1 (12%)
2	OLC	C	354	-	9,9,24	1.15	1 (11%)	8,8,25	1.01	1 (12%)
2	OLC	C	355	-	9,9,24	1.14	1 (11%)	8,8,25	1.02	1 (12%)
2	OLC	C	356	-	7,7,24	0.26	0	6,6,25	0.40	0
2	OLC	C	357	-	13,13,24	1.15	1 (7%)	11,12,25	0.84	0
2	OLC	C	358	-	24,24,24	1.50	4 (16%)	25,25,25	1.22	1 (4%)
2	OLC	C	359	-	24,24,24	1.49	4 (16%)	25,25,25	1.36	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	C	360	3	24,24,24	1.52	4 (16%)	25,25,25	1.05	1 (4%)
2	OLC	C	361	-	11,11,24	1.21	1 (9%)	10,10,25	1.21	1 (10%)
2	OLC	C	362	-	24,24,24	1.49	4 (16%)	25,25,25	1.41	2 (8%)
2	OLC	C	363	-	24,24,24	1.47	4 (16%)	25,25,25	1.40	3 (12%)
2	OLC	C	364	-	11,11,24	1.20	1 (9%)	10,10,25	1.49	2 (20%)
2	OLC	D	341	-	4,4,24	0.25	0	3,3,25	0.35	0
2	OLC	D	342	-	24,24,24	1.50	4 (16%)	25,25,25	1.10	2 (8%)
2	OLC	D	343	-	7,7,24	0.22	0	6,6,25	0.55	0
2	OLC	D	344	-	7,7,24	0.21	0	6,6,25	0.50	0
2	OLC	D	345	-	9,9,24	1.14	1 (11%)	8,8,25	1.07	1 (12%)
2	OLC	D	346	-	11,11,24	1.20	1 (9%)	10,10,25	1.44	2 (20%)
2	OLC	D	347	-	7,7,24	0.31	0	6,6,25	0.49	0
2	OLC	D	348	-	7,7,24	0.17	0	6,6,25	0.82	0
2	OLC	D	349	3	24,24,24	1.40	4 (16%)	25,25,25	1.25	3 (12%)
4	SCN	D	354	-	2,2,2	1.85	1 (50%)	1,1,1	0.17	0
2	OLC	E	341	-	24,24,24	1.49	4 (16%)	25,25,25	1.41	3 (12%)
2	OLC	E	342	-	7,7,24	0.23	0	6,6,25	0.60	0
2	OLC	E	343	-	11,11,24	1.20	1 (9%)	10,10,25	1.25	2 (20%)
2	OLC	E	344	-	11,11,24	1.15	1 (9%)	10,10,25	1.37	2 (20%)
2	OLC	E	345	-	13,13,24	1.10	1 (7%)	11,12,25	0.92	1 (9%)
2	OLC	E	346	-	9,9,24	1.15	1 (11%)	8,8,25	1.00	1 (12%)
2	OLC	E	347	-	24,24,24	1.52	4 (16%)	25,25,25	1.21	4 (16%)
2	OLC	E	348	-	11,11,24	1.28	1 (9%)	10,10,25	1.47	1 (10%)
4	SCN	E	352	-	2,2,2	1.96	1 (50%)	1,1,1	0.20	0
4	SCN	E	353	-	2,2,2	1.94	1 (50%)	1,1,1	0.27	0
2	OLC	F	341	-	7,7,24	0.25	0	6,6,25	0.47	0
2	OLC	F	342	-	13,13,24	1.12	1 (7%)	11,12,25	0.92	1 (9%)
2	OLC	F	343	-	7,7,24	0.22	0	6,6,25	0.63	0
2	OLC	F	344	-	9,9,24	1.14	1 (11%)	8,8,25	1.03	1 (12%)
2	OLC	F	345	-	11,11,24	1.17	1 (9%)	10,10,25	1.37	1 (10%)
2	OLC	F	346	-	7,7,24	0.22	0	6,6,25	0.64	0
2	OLC	F	347	-	13,13,24	1.08	1 (7%)	11,12,25	0.96	1 (9%)
2	OLC	F	348	-	13,13,24	1.16	1 (7%)	11,12,25	0.97	0
4	SCN	F	352	-	2,2,2	1.83	1 (50%)	1,1,1	0.10	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	OLC	A	341	-	-	0/5/5/24	0/0/0/0
2	OLC	A	342	-	-	0/5/5/24	0/0/0/0
2	OLC	A	343	-	-	0/5/5/24	0/0/0/0
2	OLC	A	344	-	-	0/7/7/24	0/0/0/0
2	OLC	A	345	-	-	0/5/5/24	0/0/0/0
2	OLC	A	346	-	-	0/24/24/24	0/0/0/0
2	OLC	A	347	-	-	0/5/5/24	0/0/0/0
2	OLC	A	348	-	-	0/7/7/24	0/0/0/0
2	OLC	A	349	-	-	0/24/24/24	0/0/0/0
2	OLC	A	350	-	-	0/11/11/24	0/0/0/0
2	OLC	A	351	-	-	0/11/11/24	0/0/0/0
2	OLC	A	352	-	-	0/7/7/24	0/0/0/0
2	OLC	A	353	-	-	0/5/5/24	0/0/0/0
2	OLC	A	354	-	-	0/5/5/24	0/0/0/0
2	OLC	A	355	-	-	0/7/7/24	0/0/0/0
2	OLC	A	356	-	-	0/24/24/24	0/0/0/0
2	OLC	A	357	-	-	0/7/7/24	0/0/0/0
2	OLC	A	358	-	-	0/24/24/24	0/0/0/0
2	OLC	A	359	-	-	0/24/24/24	0/0/0/0
2	OLC	A	360	-	-	0/9/9/24	0/0/0/0
2	OLC	A	361	-	-	0/24/24/24	0/0/0/0
2	OLC	A	362	-	-	0/11/11/24	0/0/0/0
2	OLC	A	363	-	-	0/9/9/24	0/0/0/0
2	OLC	A	364	-	-	0/9/9/24	0/0/0/0
2	OLC	A	365	-	-	0/5/5/24	0/0/0/0
4	SCN	A	369	-	-	0/0/0/0	0/0/0/0
2	OLC	B	341	-	-	0/2/2/24	0/0/0/0
2	OLC	B	342	-	-	0/11/11/24	0/0/0/0
2	OLC	B	343	-	-	0/5/5/24	0/0/0/0
2	OLC	B	344	-	-	0/7/7/24	0/0/0/0
2	OLC	B	345	-	-	0/24/24/24	0/0/0/0
2	OLC	B	346	-	-	0/24/24/24	0/0/0/0
2	OLC	B	347	-	-	0/11/11/24	0/0/0/0
2	OLC	B	348	-	-	0/11/11/24	0/0/0/0
2	OLC	B	349	-	-	0/5/5/24	0/0/0/0
2	OLC	B	350	-	-	0/24/24/24	0/0/0/0
2	OLC	B	351	-	-	0/24/24/24	0/0/0/0
2	OLC	B	352	-	-	0/13/13/24	0/0/0/0
2	OLC	B	353	-	-	0/5/5/24	0/0/0/0
2	OLC	B	354	-	-	0/5/5/24	0/0/0/0
4	SCN	B	358	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	341	-	-	0/7/7/24	0/0/0/0
2	OLC	C	342	-	-	0/5/5/24	0/0/0/0
2	OLC	C	343	-	-	0/5/5/24	0/0/0/0
2	OLC	C	344	-	-	0/5/5/24	0/0/0/0
2	OLC	C	345	-	-	0/9/9/24	0/0/0/0
2	OLC	C	346	-	-	0/7/7/24	0/0/0/0
2	OLC	C	347	-	-	0/7/7/24	0/0/0/0
2	OLC	C	348	-	-	0/9/9/24	0/0/0/0
2	OLC	C	349	-	-	0/7/7/24	0/0/0/0
2	OLC	C	350	-	-	0/11/11/24	0/0/0/0
2	OLC	C	351	-	-	0/5/5/24	0/0/0/0
2	OLC	C	352	-	-	0/9/9/24	0/0/0/0
2	OLC	C	353	-	-	0/7/7/24	0/0/0/0
2	OLC	C	354	-	-	0/7/7/24	0/0/0/0
2	OLC	C	355	-	-	0/7/7/24	0/0/0/0
2	OLC	C	356	-	-	0/5/5/24	0/0/0/0
2	OLC	C	357	-	-	0/11/11/24	0/0/0/0
2	OLC	C	358	-	-	0/24/24/24	0/0/0/0
2	OLC	C	359	-	-	0/24/24/24	0/0/0/0
2	OLC	C	360	3	-	0/24/24/24	0/0/0/0
2	OLC	C	361	-	-	0/9/9/24	0/0/0/0
2	OLC	C	362	-	-	0/24/24/24	0/0/0/0
2	OLC	C	363	-	-	0/24/24/24	0/0/0/0
2	OLC	C	364	-	-	0/9/9/24	0/0/0/0
2	OLC	D	341	-	-	0/2/2/24	0/0/0/0
2	OLC	D	342	-	-	0/24/24/24	0/0/0/0
2	OLC	D	343	-	-	0/5/5/24	0/0/0/0
2	OLC	D	344	-	-	0/5/5/24	0/0/0/0
2	OLC	D	345	-	-	0/7/7/24	0/0/0/0
2	OLC	D	346	-	-	0/9/9/24	0/0/0/0
2	OLC	D	347	-	-	0/5/5/24	0/0/0/0
2	OLC	D	348	-	-	0/5/5/24	0/0/0/0
2	OLC	D	349	3	-	0/24/24/24	0/0/0/0
4	SCN	D	354	-	-	0/0/0/0	0/0/0/0
2	OLC	E	341	-	-	0/24/24/24	0/0/0/0
2	OLC	E	342	-	-	0/5/5/24	0/0/0/0
2	OLC	E	343	-	-	0/9/9/24	0/0/0/0
2	OLC	E	344	-	-	0/9/9/24	0/0/0/0
2	OLC	E	345	-	-	0/11/11/24	0/0/0/0
2	OLC	E	346	-	-	0/7/7/24	0/0/0/0
2	OLC	E	347	-	-	0/24/24/24	0/0/0/0
2	OLC	E	348	-	-	0/9/9/24	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SCN	E	352	-	-	0/0/0/0	0/0/0/0
4	SCN	E	353	-	-	0/0/0/0	0/0/0/0
2	OLC	F	341	-	-	0/5/5/24	0/0/0/0
2	OLC	F	342	-	-	0/11/11/24	0/0/0/0
2	OLC	F	343	-	-	0/5/5/24	0/0/0/0
2	OLC	F	344	-	-	0/7/7/24	0/0/0/0
2	OLC	F	345	-	-	0/9/9/24	0/0/0/0
2	OLC	F	346	-	-	0/5/5/24	0/0/0/0
2	OLC	F	347	-	-	0/11/11/24	0/0/0/0
2	OLC	F	348	-	-	0/11/11/24	0/0/0/0
4	SCN	F	352	-	-	0/0/0/0	0/0/0/0

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	358	OLC	C11-C10	-3.94	1.32	1.50
2	E	341	OLC	C11-C10	-3.90	1.33	1.50
2	B	350	OLC	C8-C9	-3.88	1.33	1.50
2	B	350	OLC	C11-C10	-3.88	1.33	1.50
2	E	341	OLC	C8-C9	-3.87	1.33	1.50
2	C	359	OLC	C11-C10	-3.82	1.33	1.50
2	A	356	OLC	C11-C10	-3.82	1.33	1.50
2	A	349	OLC	C11-C10	-3.82	1.33	1.50
2	A	346	OLC	C11-C10	-3.82	1.33	1.50
2	C	358	OLC	C8-C9	-3.79	1.33	1.50
2	E	347	OLC	C8-C9	-3.78	1.33	1.50
2	B	345	OLC	C11-C10	-3.77	1.33	1.50
2	A	358	OLC	C11-C10	-3.77	1.33	1.50
2	B	346	OLC	C11-C10	-3.77	1.33	1.50
2	A	358	OLC	C8-C9	-3.77	1.33	1.50
2	C	359	OLC	C8-C9	-3.73	1.33	1.50
2	B	346	OLC	C8-C9	-3.72	1.33	1.50
2	A	349	OLC	C8-C9	-3.72	1.33	1.50
2	C	363	OLC	C8-C9	-3.68	1.33	1.50
2	A	346	OLC	C8-C9	-3.68	1.34	1.50
2	B	345	OLC	C8-C9	-3.67	1.34	1.50
2	A	361	OLC	C11-C10	-3.66	1.34	1.50
2	A	356	OLC	C8-C9	-3.65	1.34	1.50
2	C	362	OLC	C11-C10	-3.64	1.34	1.50
2	D	342	OLC	C8-C9	-3.62	1.34	1.50
2	C	363	OLC	C11-C10	-3.60	1.34	1.50
2	C	362	OLC	C8-C9	-3.57	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	342	OLC	C11-C10	-3.56	1.34	1.50
2	E	347	OLC	C11-C10	-3.55	1.34	1.50
2	C	360	OLC	C8-C9	-3.52	1.34	1.50
2	A	361	OLC	C8-C9	-3.50	1.34	1.50
2	C	360	OLC	C11-C10	-3.50	1.34	1.50
2	A	359	OLC	C11-C10	-3.49	1.34	1.50
2	B	351	OLC	C8-C9	-3.49	1.34	1.50
2	A	359	OLC	C8-C9	-3.47	1.34	1.50
2	B	351	OLC	C11-C10	-3.36	1.35	1.50
2	D	349	OLC	C8-C9	-3.27	1.35	1.50
2	D	349	OLC	C11-C10	-3.22	1.36	1.50
2	B	346	OLC	C9-C10	2.43	1.45	1.31
2	A	356	OLC	C9-C10	2.44	1.45	1.31
2	C	358	OLC	C9-C10	2.45	1.45	1.31
2	C	363	OLC	C9-C10	2.46	1.45	1.31
2	B	350	OLC	C9-C10	2.50	1.46	1.31
2	E	341	OLC	C9-C10	2.51	1.46	1.31
2	B	345	OLC	C9-C10	2.53	1.46	1.31
2	E	347	OLC	C9-C10	2.54	1.46	1.31
4	F	352	SCN	C-S	2.55	1.80	1.63
4	D	354	SCN	C-S	2.56	1.80	1.63
2	A	349	OLC	C9-C10	2.56	1.46	1.31
2	A	358	OLC	C9-C10	2.56	1.46	1.31
2	C	359	OLC	C9-C10	2.57	1.46	1.31
2	A	359	OLC	C9-C10	2.58	1.46	1.31
2	A	346	OLC	C9-C10	2.61	1.46	1.31
2	D	342	OLC	C9-C10	2.62	1.46	1.31
4	B	358	SCN	C-S	2.63	1.80	1.63
4	E	353	SCN	C-S	2.69	1.80	1.63
2	C	362	OLC	C9-C10	2.70	1.47	1.31
4	A	369	SCN	C-S	2.71	1.81	1.63
4	E	352	SCN	C-S	2.72	1.81	1.63
2	B	351	OLC	C9-C10	2.72	1.47	1.31
2	A	361	OLC	C9-C10	2.73	1.47	1.31
2	C	360	OLC	C9-C10	2.77	1.47	1.31
2	D	349	OLC	C9-C10	3.01	1.49	1.31
2	F	344	OLC	C10-C9	3.31	1.51	1.28
2	D	345	OLC	C10-C9	3.32	1.51	1.28
2	C	341	OLC	C10-C9	3.32	1.51	1.28
2	C	353	OLC	C10-C9	3.32	1.51	1.28
2	C	355	OLC	C10-C9	3.32	1.51	1.28
2	C	347	OLC	C10-C9	3.33	1.51	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	346	OLC	C10-C9	3.33	1.51	1.28
2	E	346	OLC	C10-C9	3.33	1.51	1.28
2	C	354	OLC	C10-C9	3.33	1.51	1.28
2	C	349	OLC	C10-C9	3.34	1.51	1.28
2	A	352	OLC	C10-C9	3.35	1.52	1.28
2	A	355	OLC	C10-C9	3.35	1.52	1.28
2	A	348	OLC	C10-C9	3.35	1.52	1.28
2	B	344	OLC	C10-C9	3.35	1.52	1.28
2	A	357	OLC	C10-C9	3.39	1.52	1.28
2	A	344	OLC	C10-C9	3.44	1.52	1.28
2	B	352	OLC	C9-C10	3.56	1.52	1.31
2	B	348	OLC	C9-C10	3.65	1.52	1.31
2	D	349	OLC	O20-C1	3.66	1.44	1.33
2	C	352	OLC	C9-C10	3.68	1.53	1.31
2	E	344	OLC	C9-C10	3.68	1.53	1.31
2	F	345	OLC	C9-C10	3.69	1.53	1.31
2	B	342	OLC	C9-C10	3.70	1.53	1.31
2	A	351	OLC	C9-C10	3.70	1.53	1.31
2	C	350	OLC	C9-C10	3.70	1.53	1.31
2	A	360	OLC	C9-C10	3.70	1.53	1.31
2	C	348	OLC	C9-C10	3.71	1.53	1.31
2	F	347	OLC	C9-C10	3.73	1.53	1.31
2	B	347	OLC	C9-C10	3.73	1.53	1.31
2	C	345	OLC	C9-C10	3.73	1.53	1.31
2	E	345	OLC	C9-C10	3.76	1.53	1.31
2	A	350	OLC	C9-C10	3.77	1.53	1.31
2	E	343	OLC	C9-C10	3.78	1.53	1.31
2	F	342	OLC	C9-C10	3.79	1.53	1.31
2	A	364	OLC	C9-C10	3.80	1.53	1.31
2	D	346	OLC	C9-C10	3.80	1.53	1.31
2	B	351	OLC	O20-C1	3.80	1.44	1.33
2	A	362	OLC	C9-C10	3.81	1.53	1.31
2	C	364	OLC	C9-C10	3.83	1.53	1.31
2	C	357	OLC	C9-C10	3.87	1.54	1.31
2	C	361	OLC	C9-C10	3.90	1.54	1.31
2	F	348	OLC	C9-C10	3.94	1.54	1.31
2	E	348	OLC	C9-C10	3.95	1.54	1.31
2	C	358	OLC	O20-C1	3.97	1.45	1.33
2	E	341	OLC	O20-C1	3.97	1.45	1.33
2	C	359	OLC	O20-C1	3.97	1.45	1.33
2	A	363	OLC	C9-C10	3.99	1.54	1.31
2	A	349	OLC	O20-C1	3.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	359	OLC	O20-C1	4.00	1.45	1.33
2	B	350	OLC	O20-C1	4.07	1.45	1.33
2	A	358	OLC	O20-C1	4.10	1.45	1.33
2	C	363	OLC	O20-C1	4.11	1.45	1.33
2	C	362	OLC	O20-C1	4.14	1.45	1.33
2	B	345	OLC	O20-C1	4.24	1.46	1.33
2	A	356	OLC	O20-C1	4.25	1.46	1.33
2	A	346	OLC	O20-C1	4.27	1.46	1.33
2	B	346	OLC	O20-C1	4.33	1.46	1.33
2	D	342	OLC	O20-C1	4.37	1.46	1.33
2	E	347	OLC	O20-C1	4.43	1.46	1.33
2	C	360	OLC	O20-C1	4.53	1.47	1.33
2	A	361	OLC	O20-C1	4.75	1.47	1.33

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	348	OLC	C11-C10-C9	-4.22	107.76	127.06
2	C	352	OLC	C11-C10-C9	-3.99	108.80	127.06
2	C	364	OLC	C11-C10-C9	-3.78	109.76	127.06
2	A	364	OLC	C11-C10-C9	-3.67	110.26	127.06
2	C	345	OLC	C11-C10-C9	-3.64	110.42	127.06
2	D	346	OLC	C11-C10-C9	-3.61	110.55	127.06
2	C	348	OLC	C11-C10-C9	-3.57	110.73	127.06
2	F	345	OLC	C11-C10-C9	-3.54	110.89	127.06
2	C	362	OLC	O20-C1-O19	-3.46	114.55	123.49
2	E	344	OLC	C11-C10-C9	-3.35	111.73	127.06
2	A	361	OLC	O20-C1-O19	-3.34	114.87	123.49
2	A	360	OLC	C11-C10-C9	-3.17	112.59	127.06
2	C	363	OLC	O20-C1-O19	-3.16	115.34	123.49
2	D	349	OLC	O20-C1-O19	-3.03	115.67	123.49
2	E	343	OLC	C11-C10-C9	-3.01	113.29	127.06
2	A	363	OLC	C11-C10-C9	-2.88	113.88	127.06
2	E	341	OLC	C3-C2-C1	-2.83	102.47	113.59
2	C	361	OLC	C11-C10-C9	-2.80	114.24	127.06
2	B	346	OLC	O20-C1-O19	-2.64	116.68	123.49
2	A	362	OLC	C8-C9-C10	-2.61	107.15	125.34
2	C	359	OLC	O20-C1-O19	-2.55	116.92	123.49
2	A	356	OLC	O20-C1-O19	-2.54	116.95	123.49
2	C	349	OLC	C8-C9-C10	-2.51	110.08	127.08
2	D	345	OLC	C8-C9-C10	-2.48	110.29	127.08
2	B	347	OLC	C8-C9-C10	-2.47	108.17	125.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	346	OLC	C8-C9-C10	-2.44	110.56	127.08
2	A	349	OLC	O20-C1-O19	-2.43	117.21	123.49
2	E	341	OLC	O20-C1-O19	-2.42	117.23	123.49
2	A	355	OLC	C8-C9-C10	-2.38	110.94	127.08
2	E	346	OLC	C8-C9-C10	-2.38	110.99	127.08
2	B	348	OLC	C11-C10-C9	-2.37	108.81	125.34
2	A	344	OLC	C8-C9-C10	-2.37	111.06	127.08
2	C	355	OLC	C8-C9-C10	-2.35	111.16	127.08
2	C	353	OLC	C8-C9-C10	-2.34	111.24	127.08
2	F	342	OLC	C8-C9-C10	-2.33	109.13	125.34
2	F	344	OLC	C8-C9-C10	-2.32	111.35	127.08
2	A	348	OLC	C8-C9-C10	-2.32	111.35	127.08
2	B	352	OLC	C11-C10-C9	-2.32	109.20	125.34
2	C	354	OLC	C8-C9-C10	-2.29	111.55	127.08
2	B	352	OLC	C8-C9-C10	-2.28	109.47	125.34
2	C	347	OLC	C8-C9-C10	-2.28	111.66	127.08
2	A	357	OLC	C8-C9-C10	-2.27	111.70	127.08
2	B	344	OLC	C8-C9-C10	-2.27	111.72	127.08
2	A	352	OLC	C8-C9-C10	-2.25	111.87	127.08
2	C	341	OLC	C8-C9-C10	-2.23	111.97	127.08
2	A	358	OLC	O20-C1-O19	-2.21	117.78	123.49
2	C	350	OLC	C11-C10-C9	-2.20	110.00	125.34
2	E	343	OLC	C8-C9-C10	-2.20	110.00	125.34
2	A	346	OLC	O20-C1-O19	-2.19	117.84	123.49
2	C	364	OLC	C8-C9-C10	-2.18	110.17	125.34
2	E	344	OLC	C8-C9-C10	-2.16	110.31	125.34
2	F	347	OLC	C11-C10-C9	-2.15	110.38	125.34
2	A	359	OLC	O20-C1-O19	-2.13	118.00	123.49
2	C	363	OLC	C21-O20-C1	-2.10	110.97	116.85
2	E	345	OLC	C11-C10-C9	-2.10	110.71	125.34
2	A	351	OLC	C8-C9-C10	-2.09	110.78	125.34
2	B	342	OLC	C11-C10-C9	-2.07	110.91	125.34
2	A	350	OLC	C11-C10-C9	-2.07	110.94	125.34
2	B	342	OLC	C8-C9-C10	-2.06	111.01	125.34
2	D	346	OLC	C8-C9-C10	-2.04	111.14	125.34
2	E	347	OLC	O20-C1-O19	-2.04	118.23	123.49
2	D	342	OLC	C7-C8-C9	2.02	123.02	112.45
2	E	347	OLC	C12-C11-C10	2.05	123.21	112.45
2	E	347	OLC	C21-O20-C1	2.09	122.69	116.85
2	B	350	OLC	O20-C1-C2	2.17	118.50	111.90
2	D	349	OLC	C12-C11-C10	2.49	125.51	112.45
2	C	358	OLC	O20-C1-C2	2.71	120.14	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	351	OLC	O20-C1-C2	2.78	120.37	111.90
2	D	342	OLC	O20-C1-C2	3.02	121.11	111.90
2	C	360	OLC	O20-C1-C2	3.04	121.16	111.90
2	A	359	OLC	O20-C1-C2	3.05	121.19	111.90
2	A	349	OLC	O20-C1-C2	3.12	121.41	111.90
2	C	359	OLC	C21-O20-C1	3.18	125.73	116.85
2	B	345	OLC	O20-C1-C2	3.25	121.80	111.90
2	A	346	OLC	O20-C1-C2	3.36	122.13	111.90
2	E	347	OLC	O20-C1-C2	3.64	122.99	111.90
2	D	349	OLC	O20-C1-C2	3.64	123.00	111.90
2	C	359	OLC	O20-C1-C2	3.64	123.00	111.90
2	A	358	OLC	O20-C1-C2	3.67	123.07	111.90
2	A	356	OLC	O20-C1-C2	3.91	123.83	111.90
2	C	363	OLC	O20-C1-C2	3.92	123.85	111.90
2	B	346	OLC	O20-C1-C2	4.11	124.42	111.90
2	E	341	OLC	O20-C1-C2	4.20	124.68	111.90
2	C	362	OLC	O20-C1-C2	4.22	124.75	111.90
2	A	361	OLC	O20-C1-C2	4.74	126.35	111.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

44 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	341	OLC	2	0
2	A	343	OLC	1	0
2	A	344	OLC	1	0
2	A	345	OLC	1	0
2	A	349	OLC	3	0
2	A	353	OLC	1	0
2	A	356	OLC	2	0
2	A	359	OLC	3	0
2	A	360	OLC	4	0
2	A	361	OLC	8	0
2	A	362	OLC	1	0
2	A	365	OLC	5	0
2	B	344	OLC	1	0
2	B	345	OLC	2	0
2	B	350	OLC	1	0
2	B	351	OLC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	347	OLC	2	0
2	C	348	OLC	2	0
2	C	349	OLC	3	0
2	C	352	OLC	3	0
2	C	353	OLC	1	0
2	C	358	OLC	2	0
2	C	359	OLC	3	0
2	C	360	OLC	2	0
2	C	362	OLC	2	0
2	C	363	OLC	4	0
2	D	342	OLC	4	0
2	D	345	OLC	1	0
2	D	346	OLC	1	0
2	D	348	OLC	1	0
2	D	349	OLC	1	0
2	E	341	OLC	1	0
2	E	342	OLC	1	0
2	E	343	OLC	1	0
2	E	344	OLC	3	0
2	E	346	OLC	2	0
2	E	347	OLC	11	0
2	E	348	OLC	6	0
2	F	341	OLC	1	0
2	F	342	OLC	3	0
2	F	343	OLC	1	0
2	F	344	OLC	1	0
2	F	345	OLC	1	0
2	F	347	OLC	3	0

## 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	340/340 (100%)	-0.44	3 (0%) 85 86	11, 19, 38, 53	0
1	B	340/340 (100%)	-0.26	9 (2%) 59 60	14, 25, 46, 59	0
1	C	340/340 (100%)	-0.31	8 (2%) 62 63	13, 22, 40, 53	0
1	D	340/340 (100%)	-0.35	7 (2%) 67 67	12, 21, 42, 56	0
1	E	340/340 (100%)	-0.44	2 (0%) 90 90	11, 20, 38, 51	0
1	F	340/340 (100%)	-0.13	12 (3%) 48 49	13, 27, 49, 65	0
All	All	2040/2040 (100%)	-0.32	41 (2%) 68 69	11, 22, 44, 65	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	147	LEU	3.8
1	B	246	ASN	3.6
1	F	182	TYR	3.5
1	F	246	ASN	3.4
1	F	7	ASP	3.3
1	C	147	LEU	3.2
1	C	7	ASP	3.1
1	B	7	ASP	3.0
1	C	6	LYS	3.0
1	A	29	GLU	2.9
1	F	285	GLY	2.9
1	D	7	ASP	2.9
1	B	25	LYS	2.9
1	C	91	ALA	2.9
1	D	246	ASN	2.8
1	D	147	LEU	2.8
1	E	29	GLU	2.8
1	F	25	LYS	2.6
1	F	27	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	182	TYR	2.6
1	F	209	LYS	2.6
1	C	182	TYR	2.6
1	A	53	SER	2.5
1	B	209	LYS	2.5
1	C	246	ASN	2.4
1	A	7	ASP	2.4
1	F	53	SER	2.4
1	B	53	SER	2.3
1	B	267	PHE	2.3
1	F	91	ALA	2.3
1	C	29	GLU	2.3
1	B	147	LEU	2.3
1	F	244	PHE	2.2
1	B	266	ASP	2.2
1	C	149	ASP	2.2
1	D	29	GLU	2.2
1	D	26	GLY	2.1
1	D	243	LYS	2.1
1	B	91	ALA	2.0
1	E	7	ASP	2.0
1	F	29	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OLC	B	342	14/25	0.70	0.28	8.48	51,56,62,64	0
2	OLC	A	344	10/25	0.77	0.19	8.17	29,42,49,49	0
2	OLC	B	353	8/25	0.82	0.21	7.99	35,41,49,50	0
2	OLC	F	341	8/25	0.75	0.25	7.84	40,44,48,52	0
2	OLC	C	352	12/25	0.72	0.25	7.54	51,56,59,59	0
2	OLC	A	343	8/25	0.92	0.16	6.15	32,36,42,43	0
2	OLC	D	349	25/25	0.68	0.18	5.65	39,49,54,55	0
2	OLC	B	351	25/25	0.68	0.21	5.28	37,46,61,68	0
2	OLC	C	348	12/25	0.75	0.25	5.28	50,55,59,59	0
2	OLC	D	348	8/25	0.87	0.17	5.24	37,43,44,46	0
2	OLC	C	362	25/25	0.75	0.22	5.24	27,41,58,60	0
2	OLC	E	342	8/25	0.85	0.17	5.18	40,41,43,45	0
2	OLC	E	341	25/25	0.82	0.17	5.14	21,39,49,53	0
2	OLC	A	350	14/25	0.78	0.18	5.02	31,35,46,47	0
2	OLC	C	349	10/25	0.87	0.21	4.85	36,44,52,56	0
2	OLC	F	342	14/25	0.63	0.23	4.79	50,52,58,59	0
2	OLC	D	344	8/25	0.94	0.11	4.70	27,31,47,51	0
2	OLC	D	346	12/25	0.79	0.15	4.63	32,36,41,43	0
2	OLC	C	363	25/25	0.73	0.22	4.59	38,46,56,66	0
2	OLC	D	342	25/25	0.65	0.23	4.35	45,51,70,75	0
2	OLC	A	356	25/25	0.89	0.16	4.28	22,36,53,65	0
2	OLC	A	358	25/25	0.67	0.24	4.26	49,55,61,64	0
2	OLC	C	342	8/25	0.92	0.11	4.00	26,35,46,48	0
2	OLC	A	347	8/25	0.88	0.13	3.78	25,29,36,39	0
2	OLC	A	359	25/25	0.83	0.18	3.78	28,40,54,54	0
2	OLC	C	360	25/25	0.79	0.17	3.63	23,40,72,74	0
2	OLC	C	345	12/25	0.77	0.17	3.60	37,43,49,49	0
2	OLC	A	361	25/25	0.74	0.23	3.40	40,53,64,67	0
2	OLC	C	357	14/25	0.74	0.18	3.25	28,46,50,51	0
4	SCN	E	352	3/3	0.95	0.11	3.19	20,20,21,35	0
2	OLC	F	345	12/25	0.79	0.19	3.18	37,46,57,57	0
2	OLC	F	343	8/25	0.83	0.20	3.07	48,55,61,61	0
2	OLC	A	363	12/25	0.80	0.15	3.04	31,39,47,48	0
2	OLC	E	347	25/25	0.83	0.17	2.96	26,45,53,57	0
2	OLC	C	361	12/25	0.82	0.16	2.93	24,32,37,37	0
2	OLC	E	348	12/25	0.83	0.13	2.88	42,49,52,52	0
2	OLC	C	350	14/25	0.76	0.19	2.77	37,49,53,55	0
2	OLC	E	345	14/25	0.62	0.20	2.72	32,50,57,59	0
2	OLC	B	345	25/25	0.85	0.17	2.69	33,43,52,60	0
2	OLC	B	350	25/25	0.71	0.21	2.63	34,49,60,71	0
2	OLC	F	346	8/25	0.81	0.15	2.58	40,45,50,51	0
2	OLC	B	346	25/25	0.87	0.16	2.51	29,39,54,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OLC	A	346	25/25	0.81	0.17	2.26	35,44,57,61	0
2	OLC	C	359	25/25	0.86	0.15	2.18	30,38,57,63	0
2	OLC	A	357	10/25	0.84	0.18	2.13	26,37,44,46	0
2	OLC	A	354	8/25	0.91	0.16	2.08	28,35,39,44	0
2	OLC	E	343	12/25	0.83	0.14	2.07	40,48,52,54	0
2	OLC	A	349	25/25	0.82	0.19	2.07	36,42,56,63	0
2	OLC	C	358	25/25	0.83	0.18	2.04	31,39,63,66	0
2	OLC	B	352	16/25	0.86	0.15	2.02	32,41,46,47	0
2	OLC	B	347	14/25	0.86	0.12	1.58	30,38,47,49	0
3	K	D	352	1/1	1.00	0.09	1.43	38,38,38,38	0
3	K	F	350	1/1	0.95	0.18	1.41	42,42,42,42	0
2	OLC	A	348	10/25	0.81	0.15	1.28	40,44,49,50	0
2	OLC	D	347	8/25	0.84	0.15	1.25	28,36,41,41	0
2	OLC	A	362	14/25	0.81	0.15	1.22	38,44,49,49	0
2	OLC	C	364	12/25	0.88	0.14	1.00	37,44,47,47	0
2	OLC	B	344	10/25	0.87	0.12	0.64	42,44,53,54	0
3	K	B	356	1/1	0.97	0.14	0.62	38,38,38,38	0
2	OLC	F	348	14/25	0.82	0.15	0.59	36,43,50,50	0
4	SCN	B	358	3/3	0.95	0.08	0.49	25,25,26,37	0
4	SCN	F	352	3/3	0.97	0.08	0.39	21,21,23,34	0
4	SCN	E	353	3/3	0.96	0.13	0.28	40,40,44,49	0
4	SCN	A	369	3/3	0.95	0.07	-0.16	23,23,25,32	0
3	K	F	349	1/1	0.99	0.08	-0.97	30,30,30,30	0
3	K	B	355	1/1	0.98	0.08	-0.98	34,34,34,34	0
3	K	C	367	1/1	0.95	0.06	-1.45	38,38,38,38	0
4	SCN	D	354	3/3	0.96	0.06	-1.56	25,25,25,36	0
3	K	A	367	1/1	0.99	0.05	-1.90	27,27,27,27	0
3	K	C	365	1/1	0.99	0.04	-2.14	25,25,25,25	0
3	K	C	366	1/1	0.99	0.05	-2.18	28,28,28,28	0
3	K	E	350	1/1	0.99	0.04	-2.19	26,26,26,26	0
3	K	A	366	1/1	1.00	0.05	-2.75	25,25,25,25	0
3	K	D	351	1/1	0.99	0.04	-3.12	29,29,29,29	0
2	OLC	C	356	8/25	0.74	0.26	-	35,50,58,59	0
2	OLC	C	343	8/25	0.86	0.44	-	56,62,66,66	0
2	OLC	B	354	8/25	0.78	0.15	-	36,48,60,64	0
2	OLC	F	344	10/25	0.74	0.21	-	49,57,62,63	0
2	OLC	A	345	8/25	0.79	0.14	-	35,44,47,49	0
2	OLC	A	351	14/25	0.80	0.16	-	42,50,56,56	0
2	OLC	D	345	10/25	0.76	0.18	-	39,45,49,51	0
2	OLC	B	348	14/25	0.63	0.27	-	50,58,61,61	0
2	OLC	C	346	10/25	0.89	0.12	-	34,44,54,57	0
2	OLC	C	355	10/25	0.89	0.13	-	33,41,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OLC	D	343	8/25	0.91	0.20	-	39,44,48,53	0
2	OLC	C	354	10/25	0.73	0.36	-	60,64,67,67	0
2	OLC	A	365	8/25	0.72	0.27	-	44,48,60,60	0
3	K	C	368	1/1	0.99	0.10	-	36,36,36,36	0
2	OLC	A	355	10/25	0.79	0.23	-	40,51,66,66	0
2	OLC	A	353	8/25	0.94	0.08	-	32,34,43,44	0
2	OLC	B	343	8/25	0.94	0.14	-	30,37,44,48	0
2	OLC	C	344	8/25	0.80	0.18	-	40,44,53,55	0
2	OLC	A	342	8/25	0.87	0.12	-	48,50,58,60	0
2	OLC	A	364	12/25	0.86	0.33	-	48,54,56,56	0
2	OLC	A	360	12/25	0.70	0.31	-	49,54,68,68	0
2	OLC	B	349	8/25	0.83	0.14	-	43,45,49,50	0
3	K	A	368	1/1	0.99	0.06	-	32,32,32,32	0
2	OLC	E	346	10/25	0.76	0.19	-	58,60,62,62	0
2	OLC	C	341	10/25	0.82	0.13	-	36,40,55,59	0
3	K	E	349	1/1	1.00	0.02	-	23,23,23,23	0
2	OLC	F	347	14/25	0.78	0.35	-	49,60,63,64	0
2	OLC	A	352	10/25	0.86	0.17	-	38,47,51,51	0
3	K	B	357	1/1	0.99	0.15	-	41,41,41,41	0
2	OLC	B	341	5/25	0.70	0.17	-	42,44,47,47	0
3	K	E	351	1/1	0.97	0.12	-	33,33,33,33	0
2	OLC	D	341	5/25	0.94	0.10	-	36,39,44,45	0
3	K	F	351	1/1	0.99	0.22	-	44,44,44,44	0
2	OLC	C	347	10/25	0.77	0.22	-	49,50,62,63	0
2	OLC	E	344	12/25	0.72	0.29	-	29,54,59,59	0
3	K	D	350	1/1	1.00	0.04	-	23,23,23,23	0
2	OLC	C	353	10/25	0.80	0.28	-	54,56,62,63	0
3	K	D	353	1/1	0.98	0.08	-	38,38,38,38	0
2	OLC	C	351	8/25	0.72	0.26	-	53,56,60,60	0
2	OLC	A	341	8/25	0.94	0.10	-	28,32,41,43	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.