



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2017 – 11:17 PM EST

PDB ID : 5OGE  
Title : Crystal structure of a nucleotide sugar transporter  
Authors : Newstead, S.; Parker, J.L.  
Deposited on : unknown  
Resolution : 3.22 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

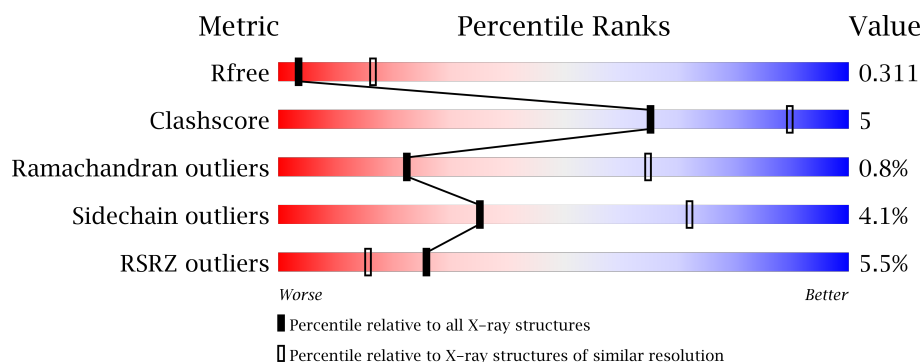
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.22 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.



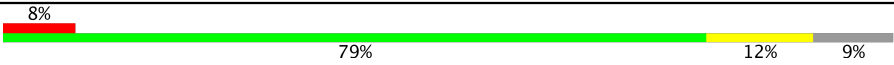


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1036 (3.24-3.20)
Clashscore	112137	1161 (3.24-3.20)
Ramachandran outliers	110173	1140 (3.24-3.20)
Sidechain outliers	110143	1139 (3.24-3.20)
RSRZ outliers	101464	1040 (3.24-3.20)

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	337	<div> <div>4%</div> <div>77%</div> <div>11%</div> <div>11%</div> </div>
1	B	337	<div> <div>4%</div> <div>74%</div> <div>14%</div> <div>11%</div> </div>
1	C	337	<div> <div>4%</div> <div>77%</div> <div>11%</div> <div>10%</div> </div>
1	D	337	<div> <div>3%</div> <div>78%</div> <div>12%</div> <div>10%</div> </div>
1	E	337	<div> <div>6%</div> <div>77%</div> <div>12%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	337	
1	G	337	
1	H	337	

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	401	-	-	-	X
2	OLC	A	402	-	-	-	X
2	OLC	A	403	-	-	-	X
2	OLC	A	404	-	-	-	X
2	OLC	B	402	-	-	-	X
2	OLC	D	401	-	-	-	X
2	OLC	D	402	-	-	-	X
2	OLC	D	404	-	-	-	X
2	OLC	D	405	-	-	-	X
2	OLC	E	401	-	-	-	X

## 2 Entry composition

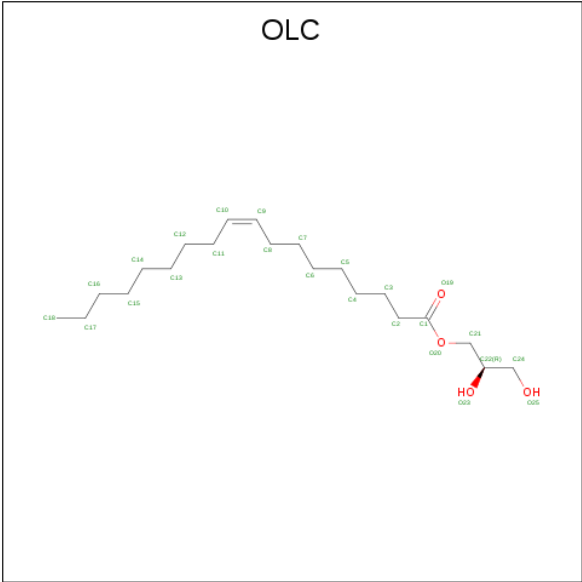
There are 2 unique types of molecules in this entry. The entry contains 19617 atoms, of which 480 are hydrogens and 0 are deuteriums.

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 GDP-mannose transporter 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2334	1545	361	411	17			
1	B	299	Total	C	N	O	S	0	0	0
			2337	1547	362	411	17			
1	C	302	Total	C	N	O	S	0	0	0
			2355	1558	365	415	17			
1	D	303	Total	C	N	O	S	0	0	0
			2360	1561	366	416	17			
1	E	304	Total	C	N	O	S	0	0	0
			2365	1564	367	417	17			
1	F	305	Total	C	N	O	S	0	0	0
			2369	1566	368	418	17			
1	G	306	Total	C	N	O	S	0	0	0
			2386	1578	372	419	17			
1	H	299	Total	C	N	O	S	0	0	0
			2331	1541	362	411	17			

- 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>).

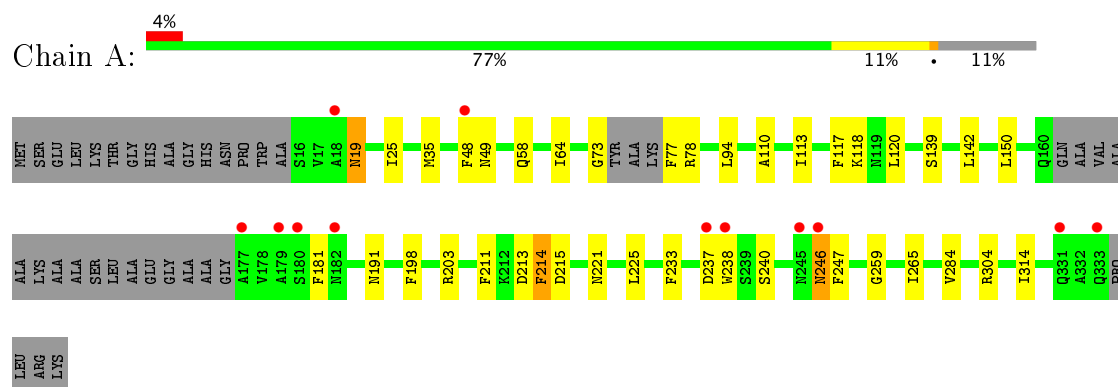


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			65	21	40	4		
2	A	1	Total	C	H	O	0	0
			65	21	40	4		
2	A	1	Total	C	H	O	0	0
			65	21	40	4		
2	A	1	Total	C	H	O	0	0
			65	21	40	4		
2	B	1	Total	C	H	O	0	0
			65	21	40	4		
2	B	1	Total	C	H	O	0	0
			65	21	40	4		
2	D	1	Total	C	H	O	0	0
			65	21	40	4		
2	D	1	Total	C	H	O	0	0
			65	21	40	4		
2	D	1	Total	C	H	O	0	0
			65	21	40	4		
2	D	1	Total	C	H	O	0	0
			65	21	40	4		
2	D	1	Total	C	H	O	0	0
			65	21	40	4		
2	E	1	Total	C	H	O	0	0
			65	21	40	4		

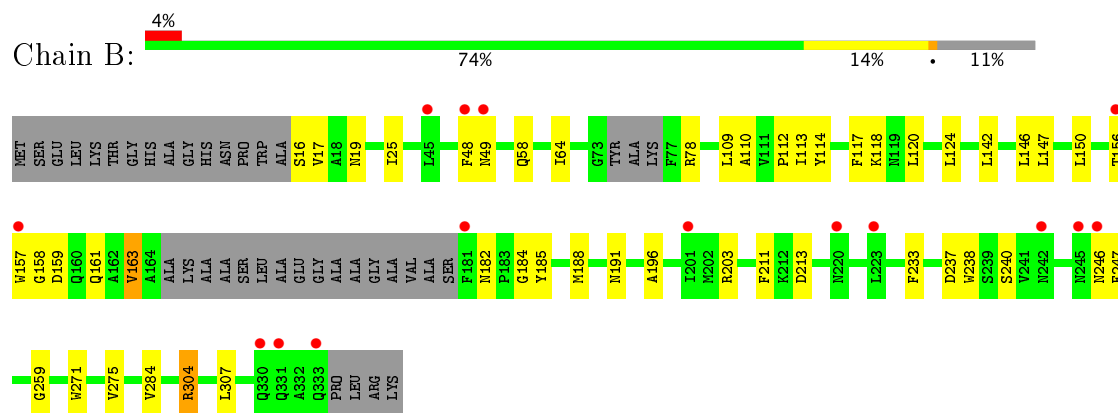
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

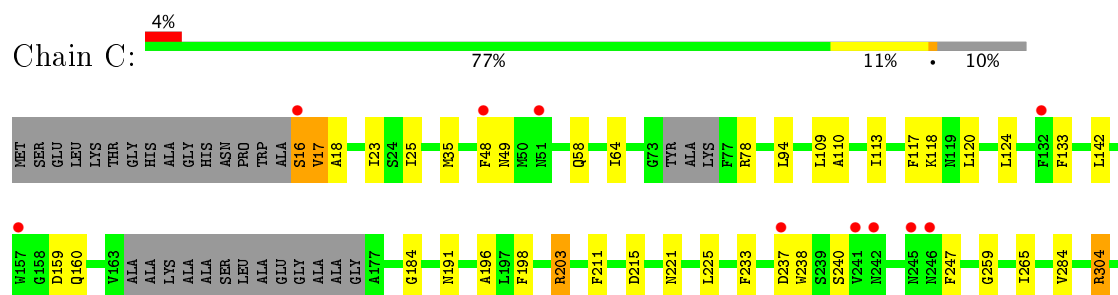
#### • Molecule 1: GDP-mannose transporter 1

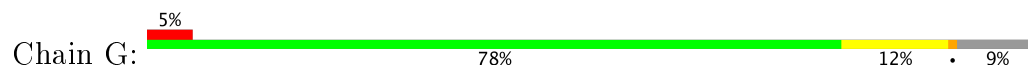


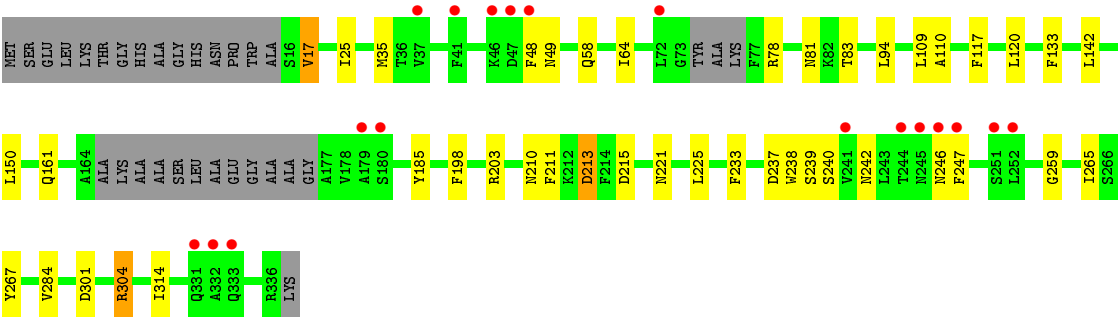
#### • Molecule 1: GDP-mannose transporter 1



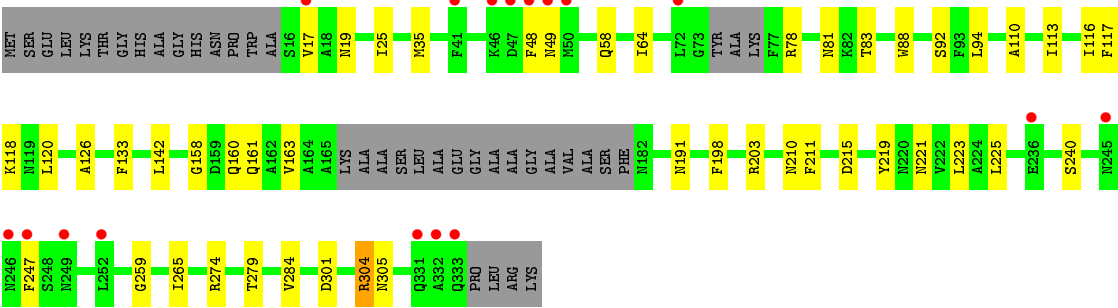
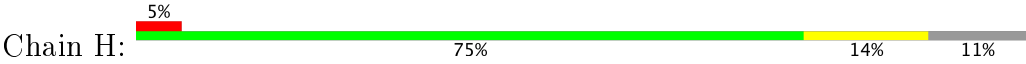
#### • Molecule 1: GDP-mannose transporter 1







• Molecule 1: GDP-mannose transporter 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.57Å 102.91Å 181.41Å 89.92° 90.12° 90.06°	Depositor
Resolution (Å)	45.35 – 3.22 44.78 – 3.22	Depositor EDS
% Data completeness (in resolution range)	90.3 (45.35-3.22) 89.9 (44.78-3.22)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.280 , 0.306 0.294 , 0.311	Depositor DCC
$R_{free}$ test set	2328 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	87.2	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.378 for h,-k,-l 0.368 for -h,k,-l 0.357 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	19617	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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: OLC

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	0.43	0/2384	0.61	0/3235
1	B	0.44	0/2387	0.62	0/3239
1	C	0.43	0/2405	0.60	0/3264
1	D	0.43	0/2410	0.61	0/3271
1	E	0.44	0/2415	0.60	0/3278
1	F	0.44	0/2419	0.61	0/3283
1	G	0.44	0/2437	0.60	0/3308
1	H	0.44	0/2380	0.60	0/3230
All	All	0.44	0/19237	0.61	0/26108

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	2334	0	2410	20	0
1	B	2337	0	2413	36	0
1	C	2355	0	2432	18	0
1	D	2360	0	2437	22	0
1	E	2365	0	2442	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2369	0	2445	21	0
1	G	2386	0	2468	27	0
1	H	2331	0	2409	25	0
2	A	100	160	160	0	0
2	B	50	80	80	0	0
2	D	125	200	200	0	0
2	E	25	40	40	0	0
All	All	19137	480	19936	183	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 5.

All (183) 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:E:150:LEU:HD22	1:E:314:ILE:HG21	1.41	1.02
1:G:150:LEU:HD22	1:G:314:ILE:HG21	1.44	1.00
1:D:49:ASN:ND2	1:D:246:ASN:HD21	1.61	0.99
1:A:150:LEU:HD22	1:A:314:ILE:HG21	1.48	0.96
1:B:112:PRO:HB2	1:B:156:THR:OG1	1.72	0.89
1:G:110:ALA:CB	1:G:161:GLN:HG2	2.05	0.85
1:G:110:ALA:HB1	1:G:161:GLN:HG2	1.61	0.82
1:E:150:LEU:CD2	1:E:314:ILE:HG21	2.10	0.82
1:B:124:LEU:HD11	1:B:196:ALA:HB2	1.61	0.81
1:B:157:TRP:CD1	1:B:307:LEU:HD22	2.16	0.81
1:G:150:LEU:CD2	1:G:314:ILE:HG21	2.12	0.79
1:A:150:LEU:CD2	1:A:314:ILE:HG21	2.12	0.78
1:D:49:ASN:ND2	1:D:246:ASN:ND2	2.31	0.77
1:B:157:TRP:HD1	1:B:307:LEU:HD22	1.49	0.77
1:E:150:LEU:CD2	1:E:314:ILE:HD13	2.14	0.77
1:D:49:ASN:HD21	1:D:246:ASN:HD21	1.30	0.76
1:G:150:LEU:CD2	1:G:314:ILE:HD13	2.15	0.76
1:A:150:LEU:CD2	1:A:314:ILE:HD13	2.16	0.75
1:B:124:LEU:CD1	1:B:196:ALA:HB2	2.17	0.75
1:B:146:LEU:O	1:B:150:LEU:HG	1.87	0.74
1:H:19:ASN:ND2	1:H:274:ARG:NH2	2.36	0.73
1:F:17:VAL:O	1:F:17:VAL:HG12	1.91	0.69
1:G:110:ALA:HB2	1:G:161:GLN:HG2	1.76	0.67
1:E:150:LEU:HD22	1:E:314:ILE:CG2	2.22	0.67
1:G:17:VAL:HG12	1:G:17:VAL:O	1.95	0.66
1:B:49:ASN:HD21	1:B:246:ASN:HD21	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:LEU:HD11	1:F:196:ALA:HB2	1.79	0.64
1:D:124:LEU:HD11	1:D:196:ALA:HB2	1.78	0.63
1:C:124:LEU:HD11	1:C:196:ALA:HB2	1.79	0.63
1:G:150:LEU:HD22	1:G:314:ILE:CG2	2.25	0.63
1:E:150:LEU:HD21	1:E:314:ILE:HD13	1.79	0.63
1:H:161:GLN:HG3	1:H:163:VAL:HG13	1.81	0.63
1:G:150:LEU:HD21	1:G:314:ILE:HD13	1.80	0.62
1:H:17:VAL:O	1:H:17:VAL:HG23	2.00	0.61
1:A:150:LEU:HD22	1:A:314:ILE:CG2	2.27	0.61
1:H:160:GLN:O	1:H:160:GLN:HG2	2.00	0.60
1:A:150:LEU:HD21	1:A:314:ILE:HD13	1.82	0.60
1:B:158:GLY:O	1:B:159:ASP:OD1	2.20	0.59
1:C:118:LYS:HE2	1:C:191:ASN:HD21	1.67	0.59
1:A:19:ASN:ND2	1:A:213:ASP:OD2	2.37	0.57
1:B:147:LEU:HA	1:B:150:LEU:HD12	1.86	0.57
1:C:124:LEU:CD1	1:C:196:ALA:HB2	2.36	0.56
1:F:124:LEU:CD1	1:F:196:ALA:HB2	2.36	0.56
1:D:124:LEU:CD1	1:D:196:ALA:HB2	2.36	0.56
1:H:126:ALA:HA	1:H:279:THR:HG21	1.86	0.56
1:B:124:LEU:CD1	1:B:196:ALA:CB	2.82	0.56
1:B:304:ARG:HH22	1:G:304:ARG:HH12	1.54	0.56
1:D:49:ASN:HD22	1:D:246:ASN:ND2	2.02	0.55
1:B:17:VAL:HG13	1:B:17:VAL:O	2.07	0.55
1:A:233:PHE:HA	1:A:238:TRP:HE1	1.72	0.55
1:B:49:ASN:ND2	1:B:246:ASN:HD21	2.05	0.55
1:F:163:VAL:O	1:F:163:VAL:HG22	2.07	0.54
1:F:233:PHE:HA	1:F:238:TRP:HE1	1.72	0.54
1:B:233:PHE:HA	1:B:238:TRP:HE1	1.73	0.54
1:B:118:LYS:HE2	1:B:191:ASN:HD21	1.74	0.53
1:C:233:PHE:HA	1:C:238:TRP:HE1	1.73	0.53
1:E:233:PHE:HA	1:E:238:TRP:HE1	1.73	0.53
1:D:233:PHE:HA	1:D:238:TRP:HE1	1.74	0.53
1:B:304:ARG:HH12	1:G:304:ARG:HH22	1.57	0.53
1:C:304:ARG:HH22	1:H:304:ARG:HH12	1.57	0.53
1:G:233:PHE:HA	1:G:238:TRP:HE1	1.73	0.53
1:B:19:ASN:O	1:B:275:VAL:HG11	2.09	0.52
1:H:221:ASN:O	1:H:225:LEU:HG	2.10	0.52
1:D:49:ASN:HD22	1:D:246:ASN:HD21	1.52	0.51
1:E:118:LYS:HE2	1:E:191:ASN:HD21	1.75	0.51
1:A:118:LYS:HE2	1:A:191:ASN:HD21	1.76	0.50
1:C:304:ARG:HH12	1:H:304:ARG:HH22	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASN:ND2	1:A:246:ASN:OD1	2.45	0.49
1:B:109:LEU:HG	1:B:184:GLY:HA3	1.94	0.49
1:B:112:PRO:HB2	1:B:156:THR:CB	2.41	0.49
1:C:18:ALA:HB1	1:C:23:ILE:HD13	1.95	0.49
1:F:17:VAL:CG1	1:F:17:VAL:O	2.58	0.49
1:F:163:VAL:O	1:F:163:VAL:HG13	2.13	0.48
1:H:88:TRP:CD1	1:H:219:TYR:HB3	2.48	0.48
1:H:58:GLN:HG2	1:H:259:GLY:HA2	1.96	0.48
1:B:49:ASN:ND2	1:B:246:ASN:ND2	2.61	0.48
1:D:114:TYR:CD1	1:D:188:MET:HE1	2.48	0.48
1:F:161:GLN:HG2	1:F:161:GLN:O	2.14	0.48
1:G:58:GLN:HG2	1:G:259:GLY:HA2	1.96	0.48
1:E:58:GLN:HG2	1:E:259:GLY:HA2	1.95	0.48
1:B:17:VAL:HG22	1:B:17:VAL:O	2.14	0.47
1:B:19:ASN:OD1	1:B:213:ASP:OD2	2.32	0.47
1:F:58:GLN:HG2	1:F:259:GLY:HA2	1.96	0.47
1:G:17:VAL:O	1:G:17:VAL:CG1	2.61	0.47
1:C:58:GLN:HG2	1:C:259:GLY:HA2	1.97	0.47
1:B:58:GLN:HG2	1:B:259:GLY:HA2	1.97	0.47
1:D:117:PHE:HA	1:D:120:LEU:HD12	1.97	0.47
1:E:35:MET:CE	1:E:265:ILE:HD13	2.45	0.47
1:D:109:LEU:CD1	1:D:188:MET:HE3	2.44	0.47
1:D:58:GLN:HG2	1:D:259:GLY:HA2	1.97	0.47
1:G:239:SER:HB2	1:G:242:ASN:HD22	1.79	0.47
1:D:19:ASN:HA	1:D:271:TRP:HZ2	1.79	0.47
1:F:155:ALA:O	1:F:159:ASP:HB2	2.15	0.47
1:E:25:ILE:HG12	1:E:284:VAL:HG21	1.97	0.47
1:F:118:LYS:HE2	1:F:191:ASN:HD21	1.79	0.46
1:G:94:LEU:HB3	1:G:198:PHE:HB2	1.97	0.46
1:G:25:ILE:HG12	1:G:284:VAL:HG21	1.97	0.46
1:A:117:PHE:HA	1:A:120:LEU:HD12	1.97	0.46
1:H:126:ALA:HA	1:H:279:THR:CG2	2.45	0.46
1:B:112:PRO:HG2	1:B:156:THR:HG23	1.98	0.46
1:F:239:SER:HB2	1:F:242:ASN:HD22	1.79	0.46
1:A:58:GLN:HG2	1:A:259:GLY:HA2	1.98	0.46
1:E:239:SER:HB2	1:E:242:ASN:HD22	1.79	0.46
1:F:117:PHE:HA	1:F:120:LEU:HD12	1.98	0.46
1:C:117:PHE:HA	1:C:120:LEU:HD12	1.98	0.46
1:H:117:PHE:HA	1:H:120:LEU:HD12	1.98	0.46
1:H:25:ILE:HG12	1:H:284:VAL:HG21	1.98	0.46
1:B:117:PHE:HA	1:B:120:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:PHE:HA	1:E:120:LEU:HD12	1.98	0.46
1:G:117:PHE:HA	1:G:120:LEU:HD12	1.98	0.46
1:F:133:PHE:CZ	1:F:203:ARG:HG3	2.51	0.45
1:H:94:LEU:HB3	1:H:198:PHE:HB2	1.98	0.45
1:G:213:ASP:HB2	1:G:267:TYR:CE1	2.51	0.45
1:F:35:MET:CE	1:F:265:ILE:HD13	2.47	0.45
1:C:133:PHE:CZ	1:C:203:ARG:HG3	2.52	0.45
1:C:35:MET:CE	1:C:265:ILE:HD13	2.46	0.45
1:H:35:MET:CE	1:H:265:ILE:HD13	2.45	0.45
1:B:19:ASN:OD1	1:B:271:TRP:NE1	2.49	0.45
1:F:25:ILE:HG12	1:F:284:VAL:HG21	1.98	0.45
1:B:114:TYR:HA	1:B:188:MET:HE3	1.98	0.45
1:D:114:TYR:HD1	1:D:188:MET:HE1	1.82	0.44
1:E:94:LEU:HB3	1:E:198:PHE:HB2	1.99	0.44
1:A:213:ASP:O	1:A:214:PHE:HB2	2.18	0.44
1:D:35:MET:CE	1:D:265:ILE:HD13	2.47	0.44
1:F:94:LEU:HB3	1:F:198:PHE:HB2	1.99	0.44
1:G:110:ALA:HB1	1:G:161:GLN:CG	2.42	0.44
1:G:109:LEU:HD21	1:G:185:TYR:CD1	2.52	0.44
1:H:158:GLY:O	1:H:305:ASN:ND2	2.50	0.44
1:H:19:ASN:ND2	1:H:274:ARG:HH21	2.14	0.44
1:A:35:MET:SD	1:A:265:ILE:HG21	2.58	0.44
1:B:182:ASN:HA	1:B:185:TYR:HD2	1.83	0.44
1:A:73:GLY:HA3	1:A:77:PHE:HE1	1.82	0.43
1:D:25:ILE:HG12	1:D:284:VAL:HG21	2.00	0.43
1:G:35:MET:SD	1:G:265:ILE:HG21	2.58	0.43
1:B:25:ILE:HG12	1:B:284:VAL:HG21	2.00	0.43
1:B:157:TRP:CD2	1:B:157:TRP:O	2.71	0.43
1:C:109:LEU:HD13	1:C:184:GLY:HA3	1.99	0.43
1:H:160:GLN:OE1	1:H:160:GLN:N	2.51	0.43
1:A:49:ASN:HB2	1:A:247:PHE:HZ	1.84	0.43
1:G:133:PHE:CZ	1:G:203:ARG:HG3	2.53	0.43
1:C:16:SER:HB2	1:C:17:VAL:H	1.60	0.43
1:H:133:PHE:CZ	1:H:203:ARG:HG3	2.54	0.43
1:C:25:ILE:HG12	1:C:284:VAL:HG21	2.01	0.43
1:G:81:ASN:HD22	1:G:83:THR:H	1.67	0.43
1:A:110:ALA:HB3	1:A:113:ILE:HD12	2.01	0.42
1:A:94:LEU:HB3	1:A:198:PHE:HB2	2.01	0.42
1:C:94:LEU:HB3	1:C:198:PHE:HB2	2.01	0.42
1:D:94:LEU:HB3	1:D:198:PHE:HB2	2.01	0.42
1:A:25:ILE:HG12	1:A:284:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ASN:HB2	1:C:247:PHE:HZ	1.84	0.42
1:D:110:ALA:HB3	1:D:113:ILE:HD12	2.01	0.42
1:D:109:LEU:HD13	1:D:188:MET:HE3	2.00	0.42
1:D:49:ASN:HB2	1:D:247:PHE:HZ	1.85	0.42
1:F:221:ASN:O	1:F:225:LEU:HG	2.19	0.42
1:H:81:ASN:HD22	1:H:83:THR:H	1.68	0.42
1:B:110:ALA:HB3	1:B:113:ILE:HD12	2.01	0.42
1:E:163:VAL:O	1:E:163:VAL:HG12	2.19	0.42
1:E:16:SER:HB3	1:E:19:ASN:ND2	2.34	0.42
1:B:158:GLY:C	1:B:159:ASP:OD1	2.58	0.41
1:A:139:SER:HB2	1:E:139:SER:HB2	2.01	0.41
1:E:81:ASN:HD22	1:E:83:THR:H	1.68	0.41
1:D:114:TYR:HA	1:D:188:MET:HE1	2.02	0.41
1:B:49:ASN:HB2	1:B:247:PHE:HZ	1.85	0.41
1:H:113:ILE:HA	1:H:116:ILE:HD12	2.01	0.41
1:A:221:ASN:O	1:A:225:LEU:HG	2.21	0.41
1:B:163:VAL:O	1:B:163:VAL:HG13	2.20	0.41
1:B:163:VAL:HG22	1:B:163:VAL:O	2.20	0.41
1:D:220:ASN:O	1:D:224:ALA:HB2	2.21	0.41
1:G:221:ASN:O	1:G:225:LEU:HG	2.21	0.41
1:H:49:ASN:HB2	1:H:247:PHE:HZ	1.86	0.41
1:H:118:LYS:HE2	1:H:191:ASN:HD21	1.86	0.41
1:E:221:ASN:O	1:E:225:LEU:HG	2.20	0.41
1:G:49:ASN:HB2	1:G:247:PHE:HZ	1.86	0.41
1:H:110:ALA:HB3	1:H:113:ILE:HD12	2.02	0.41
1:E:49:ASN:HB2	1:E:247:PHE:HZ	1.86	0.41
1:F:161:GLN:N	1:F:161:GLN:OE1	2.50	0.41
1:C:221:ASN:O	1:C:225:LEU:HG	2.21	0.40
1:E:110:ALA:HB3	1:E:113:ILE:HD12	2.02	0.40
1:F:176:GLY:HA3	1:F:179:ALA:HB3	2.03	0.40
1:F:81:ASN:HD22	1:F:83:THR:H	1.69	0.40
1:H:219:TYR:O	1:H:223:LEU:HB2	2.21	0.40
1:C:110:ALA:HB3	1:C:113:ILE:HD12	2.03	0.40
1:B:304:ARG:HH22	1:G:304:ARG:HH22	1.68	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/337 (87%)	275 (94%)	15 (5%)	3 (1%)	18	61
1	B	293/337 (87%)	273 (93%)	18 (6%)	2 (1%)	25	68
1	C	296/337 (88%)	278 (94%)	16 (5%)	2 (1%)	25	68
1	D	297/337 (88%)	274 (92%)	20 (7%)	3 (1%)	18	61
1	E	298/337 (88%)	278 (93%)	18 (6%)	2 (1%)	25	68
1	F	299/337 (89%)	280 (94%)	17 (6%)	2 (1%)	25	68
1	G	300/337 (89%)	279 (93%)	18 (6%)	3 (1%)	18	61
1	H	293/337 (87%)	272 (93%)	19 (6%)	2 (1%)	25	68
All	All	2369/2696 (88%)	2209 (93%)	141 (6%)	19 (1%)	22	65

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	SER
1	B	240	SER
1	C	240	SER
1	D	213	ASP
1	D	240	SER
1	E	240	SER
1	F	240	SER
1	G	240	SER
1	H	240	SER
1	A	214	PHE
1	E	182	ASN
1	G	210	ASN
1	A	181	PHE
1	B	161	GLN
1	C	17	VAL
1	F	17	VAL
1	D	212	LYS

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Mol	Chain	Res	Type
1	H	210	ASN
1	G	17	VAL

### 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	266/289 (92%)	255 (96%)	11 (4%)	35	72
1	B	266/289 (92%)	256 (96%)	10 (4%)	38	74
1	C	268/289 (93%)	256 (96%)	12 (4%)	32	70
1	D	268/289 (93%)	255 (95%)	13 (5%)	29	68
1	E	268/289 (93%)	255 (95%)	13 (5%)	29	68
1	F	268/289 (93%)	260 (97%)	8 (3%)	46	78
1	G	271/289 (94%)	260 (96%)	11 (4%)	35	72
1	H	265/289 (92%)	256 (97%)	9 (3%)	42	76
All	All	2140/2312 (93%)	2053 (96%)	87 (4%)	35	72

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	48	PHE
1	A	64	ILE
1	A	78	ARG
1	A	142	LEU
1	A	203	ARG
1	A	211	PHE
1	A	215	ASP
1	A	237	ASP
1	A	246	ASN
1	A	304	ARG
1	B	16	SER
1	B	48	PHE

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Mol	Chain	Res	Type
1	B	64	ILE
1	B	78	ARG
1	B	142	LEU
1	B	163	VAL
1	B	203	ARG
1	B	211	PHE
1	B	237	ASP
1	B	304	ARG
1	C	16	SER
1	C	48	PHE
1	C	64	ILE
1	C	78	ARG
1	C	142	LEU
1	C	159	ASP
1	C	160	GLN
1	C	203	ARG
1	C	211	PHE
1	C	215	ASP
1	C	237	ASP
1	C	304	ARG
1	D	16	SER
1	D	48	PHE
1	D	64	ILE
1	D	78	ARG
1	D	142	LEU
1	D	182	ASN
1	D	203	ARG
1	D	211	PHE
1	D	213	ASP
1	D	237	ASP
1	D	301	ASP
1	D	304	ARG
1	D	328	LYS
1	E	16	SER
1	E	19	ASN
1	E	20	SER
1	E	48	PHE
1	E	64	ILE
1	E	78	ARG
1	E	142	LEU
1	E	193	ILE
1	E	203	ARG

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Mol	Chain	Res	Type
1	E	211	PHE
1	E	237	ASP
1	E	301	ASP
1	E	304	ARG
1	F	48	PHE
1	F	64	ILE
1	F	78	ARG
1	F	142	LEU
1	F	211	PHE
1	F	237	ASP
1	F	301	ASP
1	F	304	ARG
1	G	48	PHE
1	G	64	ILE
1	G	78	ARG
1	G	142	LEU
1	G	211	PHE
1	G	213	ASP
1	G	215	ASP
1	G	237	ASP
1	G	246	ASN
1	G	301	ASP
1	G	304	ARG
1	H	48	PHE
1	H	64	ILE
1	H	78	ARG
1	H	92	SER
1	H	142	LEU
1	H	211	PHE
1	H	215	ASP
1	H	301	ASP
1	H	304	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	49	ASN
1	A	58	GLN
1	A	81	ASN
1	A	191	ASN
1	A	246	ASN

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Mol	Chain	Res	Type
1	B	49	ASN
1	B	81	ASN
1	B	191	ASN
1	C	58	GLN
1	C	81	ASN
1	C	191	ASN
1	D	49	ASN
1	D	81	ASN
1	E	81	ASN
1	E	191	ASN
1	E	242	ASN
1	F	81	ASN
1	F	191	ASN
1	F	242	ASN
1	G	81	ASN
1	G	160	GLN
1	G	191	ASN
1	G	242	ASN
1	H	19	ASN
1	H	81	ASN
1	H	161	GLN
1	H	191	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 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	OLC	A	401	-	24,24,24	0.75	0	25,25,25	0.70	0
2	OLC	A	402	-	24,24,24	0.74	0	25,25,25	0.72	0
2	OLC	A	403	-	24,24,24	0.83	1 (4%)	25,25,25	0.66	0
2	OLC	A	404	-	24,24,24	0.69	0	25,25,25	0.80	0
2	OLC	B	401	-	24,24,24	0.67	0	25,25,25	0.73	0
2	OLC	B	402	-	24,24,24	0.79	0	25,25,25	0.66	0
2	OLC	D	401	-	24,24,24	0.75	0	25,25,25	0.64	0
2	OLC	D	402	-	24,24,24	0.71	0	25,25,25	0.66	0
2	OLC	D	403	-	24,24,24	0.74	0	25,25,25	0.98	2 (8%)
2	OLC	D	404	-	24,24,24	0.71	0	25,25,25	0.61	0
2	OLC	D	405	-	24,24,24	0.81	0	25,25,25	0.58	0
2	OLC	E	401	-	24,24,24	0.74	0	25,25,25	0.74	1 (4%)

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	401	-	-	0/24/24/24	0/0/0/0
2	OLC	A	402	-	-	0/24/24/24	0/0/0/0
2	OLC	A	403	-	-	0/24/24/24	0/0/0/0
2	OLC	A	404	-	-	0/24/24/24	0/0/0/0
2	OLC	B	401	-	-	0/24/24/24	0/0/0/0
2	OLC	B	402	-	-	0/24/24/24	0/0/0/0
2	OLC	D	401	-	-	0/24/24/24	0/0/0/0
2	OLC	D	402	-	-	0/24/24/24	0/0/0/0
2	OLC	D	403	-	-	0/24/24/24	0/0/0/0
2	OLC	D	404	-	-	0/24/24/24	0/0/0/0
2	OLC	D	405	-	-	0/24/24/24	0/0/0/0
2	OLC	E	401	-	-	0/24/24/24	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	403	OLC	O20-C1	2.16	1.39	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	OLC	O20-C1-O19	-2.62	117.04	123.55
2	E	401	OLC	C21-O20-C1	2.15	123.59	117.13
2	D	403	OLC	C21-O20-C1	2.48	124.60	117.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	299/337 (88%)	0.23	12 (4%)	39	26	67, 90, 139, 170	0
1	B	299/337 (88%)	0.27	15 (5%)	30	17	30, 89, 124, 167	0
1	C	302/337 (89%)	0.23	13 (4%)	36	24	30, 90, 131, 169	0
1	D	303/337 (89%)	0.23	10 (3%)	47	32	70, 90, 130, 153	0
1	E	304/337 (90%)	0.41	20 (6%)	19	12	67, 91, 158, 177	0
1	F	305/337 (90%)	0.43	27 (8%)	10	6	66, 91, 156, 172	0
1	G	306/337 (90%)	0.36	18 (5%)	23	14	62, 89, 158, 174	0
1	H	299/337 (88%)	0.33	17 (5%)	24	15	66, 89, 156, 175	0
All	All	2417/2696 (89%)	0.31	132 (5%)	26	16	30, 90, 147, 177	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	47	ASP	14.3
1	H	47	ASP	13.5
1	A	245	ASN	13.4
1	E	47	ASP	12.6
1	F	48	PHE	11.8
1	B	245	ASN	10.9
1	G	47	ASP	8.9
1	E	48	PHE	7.8
1	G	48	PHE	7.8
1	A	333	GLN	7.7
1	G	245	ASN	7.6
1	D	246	ASN	7.5
1	H	48	PHE	7.4
1	D	245	ASN	7.3
1	C	245	ASN	7.0
1	A	246	ASN	7.0

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Mol	Chain	Res	Type	RSRZ
1	G	246	ASN	6.6
1	E	16	SER	6.6
1	B	246	ASN	6.4
1	F	245	ASN	6.3
1	C	333	GLN	5.9
1	C	246	ASN	5.9
1	F	16	SER	5.3
1	H	333	GLN	5.1
1	H	245	ASN	5.1
1	B	333	GLN	5.0
1	E	332	ALA	5.0
1	H	46	LYS	4.8
1	E	245	ASN	4.8
1	D	241	VAL	4.8
1	F	46	LYS	4.7
1	C	237	ASP	4.6
1	E	333	GLN	4.5
1	D	237	ASP	4.4
1	G	244	THR	4.4
1	B	49	ASN	4.3
1	E	180	SER	4.2
1	E	46	LYS	4.2
1	B	181	PHE	4.1
1	G	247	PHE	4.0
1	A	237	ASP	4.0
1	C	242	ASN	3.9
1	D	333	GLN	3.9
1	F	333	GLN	3.9
1	F	332	ALA	3.9
1	D	242	ASN	3.8
1	G	252	LEU	3.8
1	F	241	VAL	3.7
1	D	131	LEU	3.6
1	G	180	SER	3.6
1	E	246	ASN	3.5
1	F	49	ASN	3.5
1	H	50	MET	3.5
1	G	46	LYS	3.5
1	H	72	LEU	3.4
1	H	246	ASN	3.4
1	B	242	ASN	3.3
1	B	156	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	331	GLN	3.3
1	H	247	PHE	3.3
1	F	331	GLN	3.3
1	E	17	VAL	3.2
1	H	41	PHE	3.2
1	H	332	ALA	3.1
1	F	180	SER	3.1
1	F	41	PHE	3.1
1	F	246	ASN	3.1
1	B	48	PHE	3.1
1	E	41	PHE	3.0
1	F	17	VAL	3.0
1	C	331	GLN	3.0
1	B	45	LEU	3.0
1	E	73	GLY	2.9
1	H	249	ASN	2.9
1	D	132	PHE	2.9
1	H	17	VAL	2.9
1	H	236	GLU	2.8
1	E	241	VAL	2.8
1	H	331	GLN	2.8
1	E	177	ALA	2.8
1	E	244	THR	2.8
1	A	331	GLN	2.7
1	B	220	ASN	2.7
1	G	41	PHE	2.7
1	F	244	THR	2.7
1	C	132	PHE	2.7
1	A	238	TRP	2.7
1	A	179	ALA	2.7
1	A	182	ASN	2.7
1	F	182	ASN	2.7
1	E	134	GLY	2.7
1	G	241	VAL	2.6
1	A	18	ALA	2.6
1	C	241	VAL	2.6
1	E	275	VAL	2.6
1	C	157	TRP	2.6
1	G	37	VAL	2.5
1	E	66	LEU	2.5
1	G	331	GLN	2.5
1	B	201	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	179	ALA	2.5
1	G	251	SER	2.5
1	C	330	GLN	2.5
1	C	48	PHE	2.4
1	B	331	GLN	2.4
1	A	180	SER	2.4
1	G	333	GLN	2.4
1	F	242	ASN	2.4
1	H	49	ASN	2.3
1	F	88	TRP	2.2
1	H	252	LEU	2.2
1	G	72	LEU	2.2
1	F	179	ALA	2.2
1	F	44	ASN	2.2
1	F	156	THR	2.2
1	F	50	MET	2.2
1	F	45	LEU	2.2
1	D	48	PHE	2.1
1	F	236	GLU	2.1
1	F	73	GLY	2.1
1	C	51	ASN	2.1
1	E	51	ASN	2.1
1	F	106	LEU	2.1
1	G	332	ALA	2.1
1	D	18	ALA	2.1
1	B	223	LEU	2.1
1	A	48	PHE	2.1
1	F	81	ASN	2.1
1	B	330	GLN	2.1
1	C	16	SER	2.1
1	B	157	TRP	2.1
1	A	177	ALA	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no 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(Å <sup>2</sup> )	Q<0.9
2	OLC	A	402	25/25	0.74	0.56	5.67	99,107,133,134	0
2	OLC	A	403	25/25	0.68	0.43	5.60	66,109,141,143	0
2	OLC	D	401	25/25	0.72	0.47	5.17	99,113,132,134	0
2	OLC	E	401	25/25	0.70	0.54	5.05	79,85,108,111	0
2	OLC	D	404	25/25	0.67	0.52	4.71	157,162,167,169	0
2	OLC	D	402	25/25	0.61	0.47	4.60	138,143,149,150	0
2	OLC	A	404	25/25	0.75	0.47	4.55	94,115,149,151	0
2	OLC	D	405	25/25	0.68	0.50	4.30	87,101,120,122	0
2	OLC	B	402	25/25	0.58	0.47	2.79	116,127,132,133	0
2	OLC	A	401	25/25	0.59	0.39	2.77	147,156,161,163	0
2	OLC	B	401	25/25	0.76	0.28	0.41	84,101,126,127	0
2	OLC	D	403	25/25	0.54	0.38	-	140,151,158,159	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.