



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:23 PM GMT

PDB ID : 1OSM  
Title : OSMOPORIN (OMPK36) FROM KLEBSIELLA PNEUMONIAE  
Authors : Dutzler, R.; Schirmer, T.  
Deposited on : 1999-01-08  
Resolution : 3.20 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

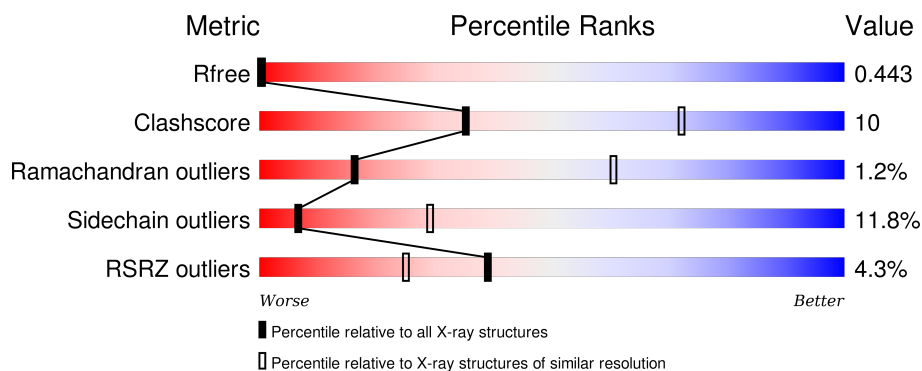
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	342	<div> <div>4%</div> <div>79%</div> <div>17%</div> <div>.</div> </div>
1	B	342	<div> <div>6%</div> <div>79%</div> <div>16%</div> <div>.</div> </div>
1	C	342	<div> <div>4%</div> <div>80%</div> <div>16%</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	D12	A	342	-	-	X	-
2	D12	A	344	-	-	-	X
2	D12	A	345	-	-	X	X
2	D12	A	346	-	-	-	X
2	D12	A	347	-	-	-	X
2	D12	A	348	-	-	X	X
2	D12	A	349	-	-	X	X

## 2 Entry composition [i](#)

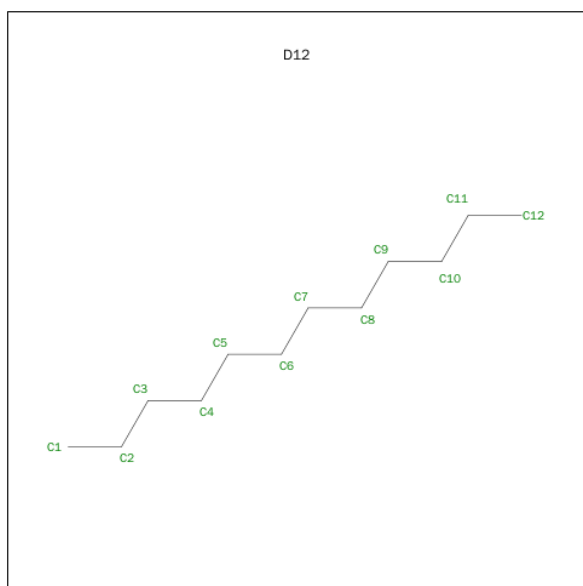
There are 2 unique types of molecules in this entry. The entry contains 8100 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OMPK36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2664	1670	442	550	2			
1	B	342	Total	C	N	O	S	0	0	0
			2664	1670	442	550	2			
1	C	342	Total	C	N	O	S	0	0	0
			2664	1670	442	550	2			

- Molecule 2 is DODECANE (three-letter code: D12) (formula:  $C_{12}H_{26}$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			12	12		
2	A	1	Total	C	0	0
			12	12		
2	A	1	Total	C	0	0
			12	12		

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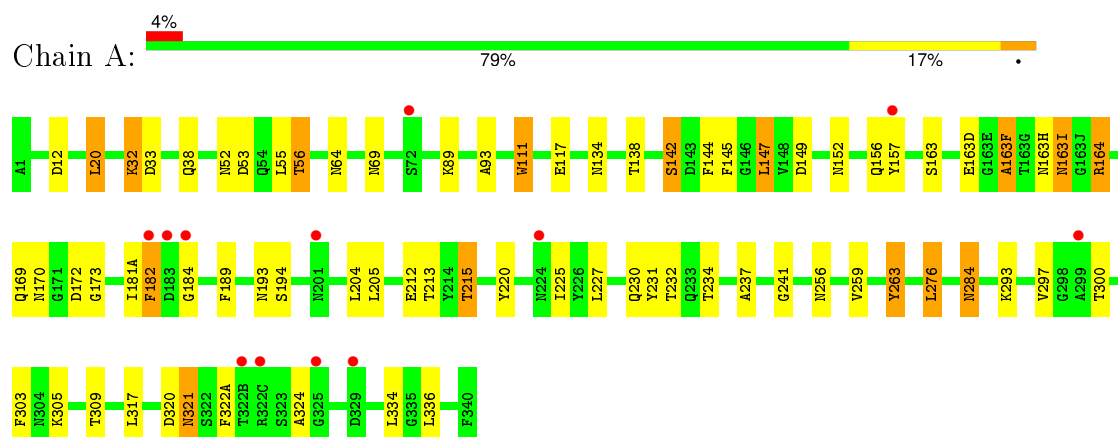
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 12 12	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 12 12	0	0

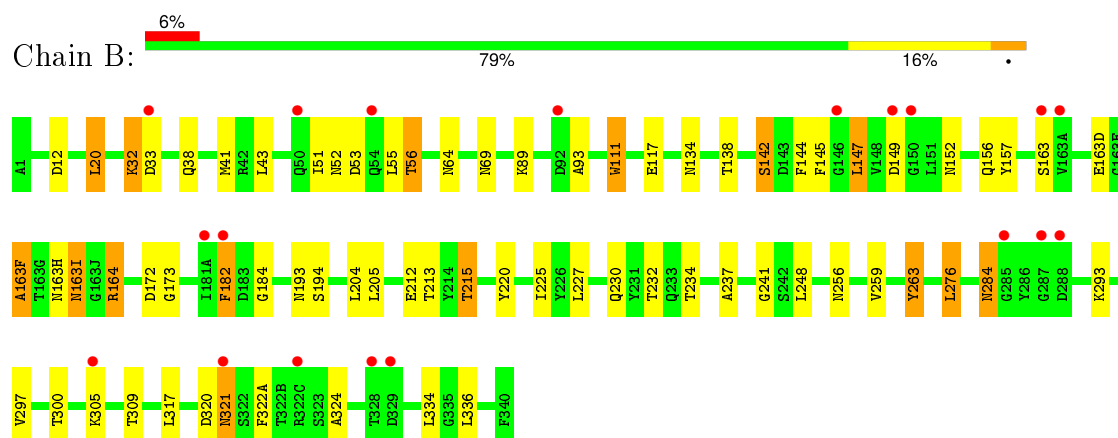
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

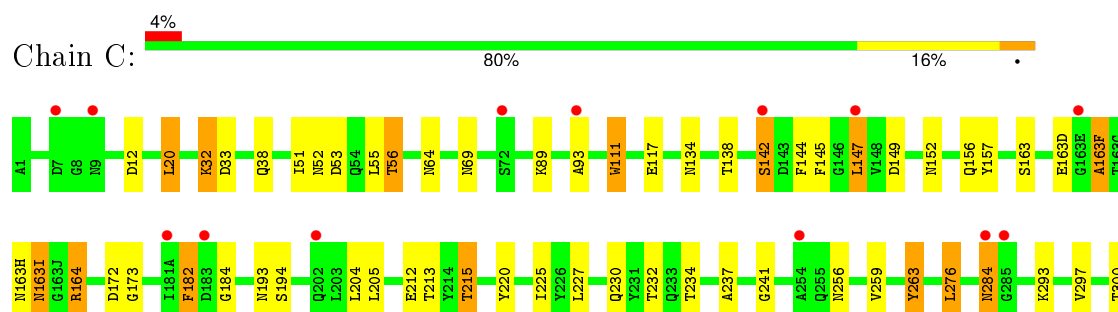
#### • Molecule 1: OMPK36

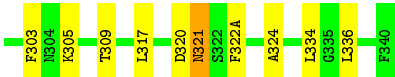


#### • Molecule 1: OMPK36



#### • Molecule 1: OMPK36





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.80 Å   76.80 Å   223.40 Å 90.00°   113.30°   90.00°	Depositor
Resolution (Å)	15.00 – 3.20 14.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (15.00-3.20) 96.1 (14.99-3.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 3.19 Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.208 , 0.223 0.441 , 0.443	Depositor DCC
$R_{free}$ test set	4430 reflections (9.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.3	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 68.3	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 47404 reflections	Xtriage
$F_o, F_c$ correlation	0.58	EDS
Total number of atoms	8100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D12

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	0.71	2/2720 (0.1%)	0.80	3/3682 (0.1%)
1	B	0.71	2/2720 (0.1%)	0.80	3/3682 (0.1%)
1	C	0.71	2/2720 (0.1%)	0.80	3/3682 (0.1%)
All	All	0.71	6/8160 (0.1%)	0.80	9/11046 (0.1%)

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	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	TRP	CB-CG	6.16	1.61	1.50
1	A	111	TRP	CB-CG	6.13	1.61	1.50
1	B	111	TRP	CB-CG	6.13	1.61	1.50
1	B	163(D)	GLU	CG-CD	5.31	1.59	1.51
1	C	163(D)	GLU	CG-CD	5.31	1.59	1.51
1	A	163(D)	GLU	CG-CD	5.29	1.59	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	SER	N-CA-C	5.62	126.16	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	SER	N-CA-C	5.61	126.14	111.00
1	C	142	SER	N-CA-C	5.60	126.11	111.00
1	B	111	TRP	CA-CB-CG	5.35	123.86	113.70
1	A	111	TRP	CA-CB-CG	5.34	123.84	113.70
1	C	111	TRP	CA-CB-CG	5.33	123.83	113.70
1	B	259	VAL	CB-CA-C	-5.03	101.85	111.40
1	A	259	VAL	CB-CA-C	-5.01	101.88	111.40
1	C	259	VAL	CB-CA-C	-5.00	101.90	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	TYR	Sidechain
1	B	263	TYR	Sidechain
1	C	263	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2664	0	2452	45	0
1	B	2664	0	2452	43	0
1	C	2664	0	2452	42	0
2	A	108	0	234	33	0
All	All	8100	0	7590	153	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 10.

All (153) 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:A:189:PHE:HB3	2:A:349:D12:H13	1.45	0.98
2:A:345:D12:H102	2:A:348:D12:H112	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:348:D12:H62	2:A:349:D12:H41	1.55	0.88
2:A:345:D12:H123	2:A:348:D12:C11	2.04	0.86
2:A:348:D12:H71	2:A:349:D12:H61	1.60	0.83
1:B:173:GLY:HA3	1:B:194:SER:HB3	1.60	0.83
1:C:173:GLY:HA3	1:C:194:SER:HB3	1.60	0.83
1:A:173:GLY:HA3	1:A:194:SER:HB3	1.60	0.82
1:B:215:THR:HB	1:B:232:THR:OG1	1.83	0.79
1:A:215:THR:HB	1:A:232:THR:OG1	1.83	0.78
1:C:215:THR:HB	1:C:232:THR:OG1	1.83	0.78
2:A:345:D12:H102	2:A:348:D12:C11	2.16	0.76
1:A:163(I):ASN:O	1:A:164:ARG:NH1	2.20	0.74
1:B:163(I):ASN:O	1:B:164:ARG:NH1	2.20	0.74
1:C:163(I):ASN:O	1:C:164:ARG:NH1	2.21	0.74
2:A:342:D12:H42	2:A:349:D12:H112	1.73	0.69
2:A:345:D12:H123	2:A:348:D12:H111	1.74	0.68
1:A:181(A):ILE:HD13	2:A:348:D12:H123	1.76	0.68
1:C:163(I):ASN:HD22	1:C:163(I):ASN:H	1.43	0.67
1:A:147:LEU:HD12	1:A:147:LEU:N	2.10	0.66
1:A:163(F):ALA:O	1:B:32:LYS:HD2	1.95	0.66
1:C:147:LEU:HD12	1:C:147:LEU:N	2.10	0.66
1:B:147:LEU:N	1:B:147:LEU:HD12	2.10	0.66
1:B:145:PHE:HB2	1:B:147:LEU:HD13	1.78	0.66
1:A:145:PHE:HB2	1:A:147:LEU:HD13	1.78	0.65
1:C:145:PHE:HB2	1:C:147:LEU:HD13	1.78	0.65
1:A:163(I):ASN:H	1:A:163(I):ASN:HD22	1.43	0.64
1:B:157:TYR:OH	1:B:172:ASP:HB3	1.98	0.64
1:C:134:ASN:ND2	1:C:164:ARG:NH2	2.46	0.64
1:A:157:TYR:OH	1:A:172:ASP:HB3	1.98	0.64
1:B:163(I):ASN:H	1:B:163(I):ASN:HD22	1.43	0.63
1:B:134:ASN:ND2	1:B:164:ARG:NH2	2.46	0.63
2:A:345:D12:H123	2:A:348:D12:C12	2.28	0.63
1:C:157:TYR:OH	1:C:172:ASP:HB3	1.98	0.63
2:A:345:D12:H123	2:A:348:D12:H121	1.80	0.63
1:A:134:ASN:ND2	1:A:164:ARG:NH2	2.46	0.62
2:A:342:D12:C12	2:A:347:D12:H112	2.30	0.62
2:A:345:D12:C10	2:A:348:D12:H112	2.28	0.61
1:B:163(F):ALA:O	1:C:32:LYS:HD2	2.01	0.61
1:B:321:ASN:ND2	1:B:322(A):PHE:H	2.00	0.60
2:A:345:D12:H82	2:A:348:D12:H92	1.84	0.59
2:A:346:D12:H112	2:A:349:D12:H21	1.85	0.59
1:C:321:ASN:ND2	1:C:322(A):PHE:H	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ASN:ND2	1:A:322(A):PHE:H	2.00	0.58
1:B:293:LYS:HG2	1:B:317:LEU:HB2	1.86	0.58
2:A:345:D12:H62	2:A:348:D12:H52	1.86	0.58
1:A:32:LYS:HD2	1:C:163(F):ALA:O	2.04	0.58
1:C:284:ASN:N	1:C:284:ASN:HD22	2.02	0.57
1:C:293:LYS:HG2	1:C:317:LEU:HB2	1.86	0.57
2:A:345:D12:H82	2:A:348:D12:H72	1.87	0.57
1:A:293:LYS:HG2	1:A:317:LEU:HB2	1.86	0.57
1:A:241:GLY:HA3	1:A:324:ALA:HB1	1.87	0.57
1:B:284:ASN:N	1:B:284:ASN:HD22	2.02	0.57
1:A:284:ASN:N	1:A:284:ASN:HD22	2.02	0.56
1:C:241:GLY:HA3	1:C:324:ALA:HB1	1.87	0.56
1:C:134:ASN:HD22	1:C:164:ARG:NH2	2.04	0.56
1:B:241:GLY:HA3	1:B:324:ALA:HB1	1.87	0.56
1:A:134:ASN:HD22	1:A:164:ARG:HH21	1.53	0.55
1:B:134:ASN:HD22	1:B:164:ARG:HH21	1.53	0.55
1:B:134:ASN:HD22	1:B:164:ARG:NH2	2.04	0.55
1:B:215:THR:HB	1:B:232:THR:CB	2.37	0.55
1:A:134:ASN:HD22	1:A:164:ARG:NH2	2.04	0.54
1:C:134:ASN:HD22	1:C:164:ARG:HH21	1.53	0.54
1:C:215:THR:HB	1:C:232:THR:CB	2.37	0.54
2:A:345:D12:H62	2:A:348:D12:C5	2.37	0.54
1:B:20:LEU:HB3	1:B:38:GLN:HB2	1.88	0.54
2:A:342:D12:H122	2:A:347:D12:H112	1.90	0.54
1:A:215:THR:HB	1:A:232:THR:CB	2.37	0.53
1:C:20:LEU:HB3	1:C:38:GLN:HB2	1.89	0.53
1:A:20:LEU:HB3	1:A:38:GLN:HB2	1.89	0.53
2:A:342:D12:H123	2:A:347:D12:H112	1.92	0.52
1:B:147:LEU:N	1:B:147:LEU:CD1	2.73	0.52
1:C:147:LEU:CD1	1:C:147:LEU:N	2.73	0.52
2:A:348:D12:H62	2:A:349:D12:C4	2.34	0.51
2:A:345:D12:H112	2:A:347:D12:H111	1.92	0.51
1:A:147:LEU:N	1:A:147:LEU:CD1	2.73	0.50
1:C:52:ASN:HB2	1:C:55:LEU:H	1.77	0.50
1:B:51:ILE:HD13	1:C:303:PHE:HB3	1.94	0.50
1:A:303:PHE:HB3	1:C:51:ILE:HD13	1.92	0.49
1:A:52:ASN:HB2	1:A:55:LEU:H	1.77	0.49
1:B:225:ILE:HD13	1:B:263:TYR:HD1	1.78	0.49
1:C:225:ILE:HD13	1:C:263:TYR:HD1	1.78	0.49
2:A:341:D12:H82	2:A:342:D12:H72	1.94	0.49
2:A:345:D12:H62	2:A:348:D12:H72	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:TYR:OH	1:C:172:ASP:CB	2.61	0.49
1:B:52:ASN:HB2	1:B:55:LEU:H	1.77	0.49
1:B:157:TYR:OH	1:B:172:ASP:CB	2.61	0.48
1:B:184:GLY:O	1:B:220:TYR:HA	2.14	0.48
1:C:184:GLY:O	1:C:220:TYR:HA	2.14	0.48
1:A:184:GLY:O	1:A:220:TYR:HA	2.14	0.48
2:A:345:D12:H102	2:A:348:D12:H92	1.95	0.47
1:A:225:ILE:HD13	1:A:263:TYR:HD1	1.78	0.47
1:A:157:TYR:OH	1:A:172:ASP:CB	2.61	0.47
2:A:345:D12:H112	2:A:347:D12:C12	2.44	0.47
2:A:342:D12:C4	2:A:349:D12:H112	2.43	0.47
2:A:346:D12:C11	2:A:349:D12:H21	2.44	0.46
1:A:52:ASN:HB3	1:A:53:ASP:H	1.54	0.46
1:A:147:LEU:H	1:A:147:LEU:HD12	1.81	0.46
1:C:147:LEU:CD1	1:C:147:LEU:H	2.29	0.46
1:B:147:LEU:H	1:B:147:LEU:HD12	1.81	0.46
1:A:189:PHE:HB2	2:A:349:D12:H31	1.98	0.46
1:A:276:LEU:HD23	1:A:276:LEU:N	2.31	0.46
1:A:215:THR:HB	1:A:232:THR:HG1	1.77	0.46
1:A:147:LEU:H	1:A:147:LEU:CD1	2.28	0.46
1:B:276:LEU:HD23	1:B:276:LEU:N	2.31	0.46
1:B:234:THR:HB	1:B:237:ALA:HB3	1.99	0.45
1:C:234:THR:HB	1:C:237:ALA:HB3	1.98	0.45
2:A:345:D12:C12	2:A:348:D12:C11	2.88	0.45
1:B:147:LEU:CD1	1:B:147:LEU:H	2.28	0.45
1:B:52:ASN:HB3	1:B:53:ASP:H	1.54	0.45
1:A:234:THR:HB	1:A:237:ALA:HB3	1.98	0.45
1:C:276:LEU:N	1:C:276:LEU:HD23	2.31	0.45
1:C:147:LEU:HD12	1:C:147:LEU:H	1.81	0.45
1:B:193:ASN:HD22	1:B:212:GLU:HG2	1.82	0.45
1:A:56:THR:HG23	1:A:89:LYS:HB3	1.99	0.45
1:C:56:THR:HG23	1:C:89:LYS:HB3	1.99	0.45
2:A:342:D12:H62	2:A:349:D12:H112	1.99	0.44
1:A:163:SER:O	1:A:163(F):ALA:HA	2.18	0.44
1:B:55:LEU:HA	1:B:55:LEU:HD12	1.78	0.44
1:C:193:ASN:HD22	1:C:212:GLU:HG2	1.82	0.44
1:B:56:THR:HG23	1:B:89:LYS:HB3	1.99	0.44
1:A:204:LEU:HG	1:A:205:LEU:HD12	1.99	0.44
1:C:157:TYR:OH	1:C:172:ASP:CG	2.56	0.44
1:B:204:LEU:HG	1:B:205:LEU:HD12	2.00	0.44
1:B:144:PHE:O	1:B:145:PHE:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:SER:O	1:C:163(F):ALA:HA	2.18	0.44
1:C:204:LEU:HG	1:C:205:LEU:HD12	2.00	0.44
1:A:157:TYR:OH	1:A:172:ASP:CG	2.56	0.44
2:A:342:D12:H62	2:A:349:D12:C11	2.48	0.43
1:B:157:TYR:OH	1:B:172:ASP:CG	2.56	0.43
1:C:32:LYS:HA	1:C:32:LYS:HD3	1.65	0.43
1:B:163:SER:O	1:B:163(F):ALA:HA	2.18	0.43
1:A:193:ASN:HD22	1:A:212:GLU:HG2	1.82	0.43
1:A:32:LYS:HA	1:A:32:LYS:HD3	1.65	0.43
1:C:205:LEU:HD12	1:C:205:LEU:N	2.34	0.43
1:A:205:LEU:N	1:A:205:LEU:HD12	2.34	0.43
1:C:134:ASN:ND2	1:C:164:ARG:HH21	2.13	0.43
1:B:134:ASN:ND2	1:B:164:ARG:HH21	2.13	0.43
1:C:144:PHE:O	1:C:145:PHE:HB2	2.18	0.43
1:C:52:ASN:HB3	1:C:53:ASP:H	1.54	0.43
1:B:205:LEU:HD12	1:B:205:LEU:N	2.34	0.42
1:A:231:TYR:HB3	2:A:349:D12:H111	2.01	0.42
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.77	0.42
1:A:144:PHE:O	1:A:145:PHE:HB2	2.18	0.42
1:B:163(F):ALA:O	1:C:32:LYS:HG3	2.19	0.42
1:A:134:ASN:ND2	1:A:164:ARG:HH21	2.13	0.41
1:B:41:MET:HE2	1:B:43:LEU:HB2	2.02	0.41
1:B:232:THR:HG22	1:B:256:ASN:HB2	2.03	0.41
1:A:169:GLN:O	1:A:170:ASN:HB3	2.21	0.41
1:B:20:LEU:HD23	1:B:20:LEU:HA	1.91	0.40
1:A:232:THR:HG22	1:A:256:ASN:HB2	2.03	0.40
1:C:232:THR:HG22	1:C:256:ASN:HB2	2.03	0.40
1:B:205:LEU:HD13	1:B:248:LEU:HB3	2.03	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	340/342 (99%)	313 (92%)	23 (7%)	4 (1%)	16	60
1	B	340/342 (99%)	313 (92%)	23 (7%)	4 (1%)	16	60
1	C	340/342 (99%)	313 (92%)	23 (7%)	4 (1%)	16	60
All	All	1020/1026 (99%)	939 (92%)	69 (7%)	12 (1%)	16	60

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163(F)	ALA
1	B	163(F)	ALA
1	C	163(F)	ALA
1	A	147	LEU
1	B	147	LEU
1	C	147	LEU
1	A	93	ALA
1	B	93	ALA
1	C	93	ALA
1	A	182	PHE
1	B	182	PHE
1	C	182	PHE

### 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	272/272 (100%)	240 (88%)	32 (12%)	6	29
1	B	272/272 (100%)	240 (88%)	32 (12%)	6	29
1	C	272/272 (100%)	240 (88%)	32 (12%)	6	29
All	All	816/816 (100%)	720 (88%)	96 (12%)	6	29

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP

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Mol	Chain	Res	Type
1	A	20	LEU
1	A	32	LYS
1	A	33	ASP
1	A	56	THR
1	A	64	ASN
1	A	69	ASN
1	A	111	TRP
1	A	117	GLU
1	A	138	THR
1	A	142	SER
1	A	149	ASP
1	A	152	ASN
1	A	156	GLN
1	A	163(H)	ASN
1	A	163(I)	ASN
1	A	164	ARG
1	A	182	PHE
1	A	213	THR
1	A	215	THR
1	A	227	LEU
1	A	230	GLN
1	A	276	LEU
1	A	284	ASN
1	A	297	VAL
1	A	300	THR
1	A	305	LYS
1	A	309	THR
1	A	320	ASP
1	A	321	ASN
1	A	334	LEU
1	A	336	LEU
1	B	12	ASP
1	B	20	LEU
1	B	32	LYS
1	B	33	ASP
1	B	56	THR
1	B	64	ASN
1	B	69	ASN
1	B	111	TRP
1	B	117	GLU
1	B	138	THR
1	B	142	SER

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Mol	Chain	Res	Type
1	B	149	ASP
1	B	152	ASN
1	B	156	GLN
1	B	163(H)	ASN
1	B	163(I)	ASN
1	B	164	ARG
1	B	182	PHE
1	B	213	THR
1	B	215	THR
1	B	227	LEU
1	B	230	GLN
1	B	276	LEU
1	B	284	ASN
1	B	297	VAL
1	B	300	THR
1	B	305	LYS
1	B	309	THR
1	B	320	ASP
1	B	321	ASN
1	B	334	LEU
1	B	336	LEU
1	C	12	ASP
1	C	20	LEU
1	C	32	LYS
1	C	33	ASP
1	C	56	THR
1	C	64	ASN
1	C	69	ASN
1	C	111	TRP
1	C	117	GLU
1	C	138	THR
1	C	142	SER
1	C	149	ASP
1	C	152	ASN
1	C	156	GLN
1	C	163(H)	ASN
1	C	163(I)	ASN
1	C	164	ARG
1	C	182	PHE
1	C	213	THR
1	C	215	THR
1	C	227	LEU

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Mol	Chain	Res	Type
1	C	230	GLN
1	C	276	LEU
1	C	284	ASN
1	C	297	VAL
1	C	300	THR
1	C	305	LYS
1	C	309	THR
1	C	320	ASP
1	C	321	ASN
1	C	334	LEU
1	C	336	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	60	GLN
1	A	134	ASN
1	A	163(I)	ASN
1	A	193	ASN
1	A	202	GLN
1	A	252	ASN
1	A	284	ASN
1	A	306	ASN
1	A	316	ASN
1	A	321	ASN
1	B	9	ASN
1	B	60	GLN
1	B	134	ASN
1	B	163(I)	ASN
1	B	193	ASN
1	B	202	GLN
1	B	252	ASN
1	B	284	ASN
1	B	306	ASN
1	B	316	ASN
1	B	321	ASN
1	C	9	ASN
1	C	60	GLN
1	C	134	ASN
1	C	163(I)	ASN
1	C	193	ASN

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Mol	Chain	Res	Type
1	C	202	GLN
1	C	252	ASN
1	C	277	GLN
1	C	284	ASN
1	C	306	ASN
1	C	316	ASN
1	C	321	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

9 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	D12	A	341	-	11,11,11	0.32	0	10,10,10	0.66	0
2	D12	A	342	-	11,11,11	0.39	0	10,10,10	0.61	0
2	D12	A	343	-	11,11,11	0.33	0	10,10,10	0.67	0
2	D12	A	344	-	11,11,11	0.45	0	10,10,10	0.58	0
2	D12	A	345	-	11,11,11	0.36	0	10,10,10	0.63	0
2	D12	A	346	-	11,11,11	0.37	0	10,10,10	0.63	0
2	D12	A	347	-	11,11,11	0.42	0	10,10,10	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	D12	A	348	-	11,11,11	0.29	0	10,10,10	0.70	0
2	D12	A	349	-	11,11,11	0.29	0	10,10,10	0.74	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	D12	A	341	-	-	0/9/9/9	0/0/0/0
2	D12	A	342	-	-	0/9/9/9	0/0/0/0
2	D12	A	343	-	-	0/9/9/9	0/0/0/0
2	D12	A	344	-	-	0/9/9/9	0/0/0/0
2	D12	A	345	-	-	0/9/9/9	0/0/0/0
2	D12	A	346	-	-	0/9/9/9	0/0/0/0
2	D12	A	347	-	-	0/9/9/9	0/0/0/0
2	D12	A	348	-	-	0/9/9/9	0/0/0/0
2	D12	A	349	-	-	0/9/9/9	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	341	D12	1	0
2	A	342	D12	8	0
2	A	345	D12	16	0
2	A	346	D12	2	0
2	A	347	D12	5	0
2	A	348	D12	18	0
2	A	349	D12	12	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	342/342 (100%)	0.40	12 (3%)	48	32	28, 51, 78, 97	0
1	B	342/342 (100%)	0.39	19 (5%)	28	16	28, 51, 78, 97	0
1	C	342/342 (100%)	0.33	13 (3%)	44	29	28, 51, 78, 97	0
All	All	1026/1026 (100%)	0.37	44 (4%)	39	25	28, 51, 78, 97	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	PHE	8.4
1	B	149	ASP	4.7
1	A	183	ASP	4.5
1	C	181(A)	ILE	4.2
1	B	287	GLY	3.7
1	B	92	ASP	3.6
1	A	322(C)	ARG	3.5
1	A	182	PHE	3.4
1	B	181(A)	ILE	3.2
1	A	322(B)	THR	3.1
1	C	163(E)	GLY	3.0
1	A	325	GLY	2.9
1	B	33	ASP	2.8
1	B	146	GLY	2.8
1	A	72	SER	2.7
1	C	72	SER	2.5
1	B	322(C)	ARG	2.5
1	B	328	THR	2.4
1	A	157	TYR	2.4
1	C	9	ASN	2.4
1	B	285	GLY	2.4
1	C	7	ASP	2.4
1	B	50	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	284	ASN	2.4
1	C	285	GLY	2.4
1	A	224	ASN	2.3
1	B	54	GLN	2.3
1	C	142	SER	2.3
1	B	305	LYS	2.3
1	C	183	ASP	2.3
1	A	299	ALA	2.2
1	A	184	GLY	2.2
1	C	202	GLN	2.2
1	B	150	GLY	2.2
1	B	288	ASP	2.2
1	B	329	ASP	2.2
1	B	163	SER	2.1
1	C	254	ALA	2.1
1	B	321	ASN	2.1
1	A	201	ASN	2.1
1	C	93	ALA	2.0
1	C	147	LEU	2.0
1	A	329	ASP	2.0
1	B	163(A)	VAL	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(Å <sup>2</sup> )	Q<0.9
2	D12	A	344	12/12	0.65	0.47	8.62	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	D12	A	349	12/12	0.52	0.66	7.43	94,94,94,94	0
2	D12	A	346	12/12	0.66	0.45	4.40	67,67,67,67	0
2	D12	A	348	12/12	0.58	0.54	4.39	92,92,92,92	0
2	D12	A	347	12/12	0.67	0.41	2.76	69,69,69,69	0
2	D12	A	345	12/12	0.58	0.45	2.61	87,87,87,87	0
2	D12	A	342	12/12	0.77	0.27	1.74	81,81,81,81	0
2	D12	A	343	12/12	0.79	0.34	1.03	79,79,79,79	0
2	D12	A	341	12/12	0.77	0.27	0.83	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.