



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:42 PM GMT

PDB ID : 3UPG  
Title : Loop deletion mutant of Salmonella typhi osmoporin (OmpC):an Outer Membrane Protein.  
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Deposited on : 2011-11-18  
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

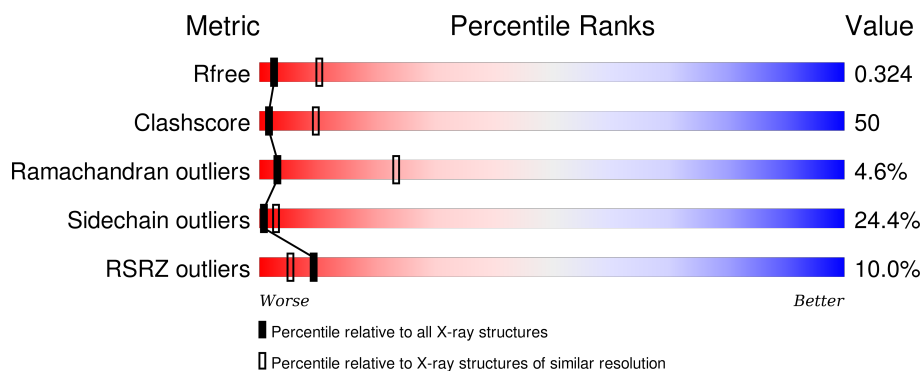
# 1 Overall quality at a glance

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	338	<div> <div>9%</div> <div>38%</div> <div>38%</div> <div>15%</div> <div>8%</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
3	CL	A	404	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2449 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 Outer membrane protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2406	1518	391	494	3			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	DELETION	UNP P0A263
A	?	-	SER	DELETION	UNP P0A263
A	?	-	GLY	DELETION	UNP P0A263
A	?	-	GLU	DELETION	UNP P0A263
A	?	-	ASN	DELETION	UNP P0A263
A	?	-	THR	DELETION	UNP P0A263
A	?	-	ASN	DELETION	UNP P0A263
A	?	-	GLY	DELETION	UNP P0A263
A	?	-	ARG	DELETION	UNP P0A263
A	?	-	SER	DELETION	UNP P0A263
A	?	-	ASN	DELETION	UNP P0A263
A	?	-	GLY	DELETION	UNP P0A263
A	?	-	SER	DELETION	UNP P0A263
A	?	-	ASN	DELETION	UNP P0A263
A	?	-	PRO	DELETION	UNP P0A263
A	?	-	SER	DELETION	UNP P0A263
A	?	-	THR	DELETION	UNP P0A263
A	?	-	SER	DELETION	UNP P0A263
A	?	-	TYR	DELETION	UNP P0A263

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Cl	0	0
			3	3		

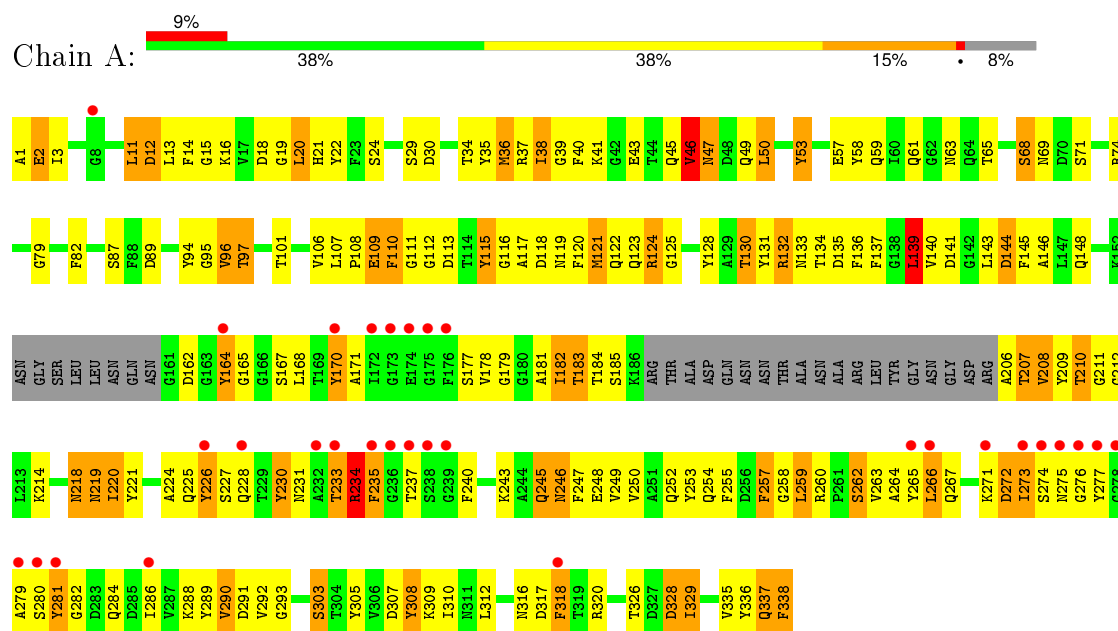
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		

### 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 ( $RSRZ > 2$ ). 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: Outer membrane protein C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.15Å 115.15Å 216.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 49.86 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.20) 99.2 (49.86-3.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.288 , 0.325 0.284 , 0.324	Depositor DCC
$R_{free}$ test set	731 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.8	Xtriage
Anisotropy	0.893	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	1 of 14582 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	2449	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.54% 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: CA, CL

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	0.78	1/2459 (0.0%)	0.84	4/3328 (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	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	VAL	CB-CG1	5.89	1.65	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASN	N-CA-C	-6.71	92.89	111.00
1	A	47	ASN	N-CA-CB	5.95	121.31	110.60
1	A	12	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	139	LEU	CA-CB-CG	5.48	127.91	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	GLN	Peptide
1	A	46	VAL	Mainchain,Peptide

## 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	2406	0	2174	230	0
2	A	2	0	0	0	0
3	A	3	0	0	2	0
4	A	38	0	0	15	0
All	All	2449	0	2174	230	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 50.

All (230) 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:24:SER:HB2	1:A:329:ILE:CG2	1.56	1.33
1:A:209:TYR:HA	4:A:610:HOH:O	1.38	1.24
1:A:24:SER:CB	1:A:329:ILE:HG23	1.68	1.22
1:A:143:LEU:HA	4:A:614:HOH:O	1.43	1.19
1:A:182:ILE:HA	4:A:610:HOH:O	1.45	1.15
1:A:209:TYR:O	1:A:227:SER:OG	1.61	1.13
1:A:135:ASP:HA	4:A:613:HOH:O	1.49	1.11
1:A:184:THR:HG22	1:A:207:THR:HB	1.33	1.11
1:A:220:ILE:HA	4:A:616:HOH:O	1.50	1.11
1:A:290:VAL:HG12	1:A:310:ILE:HB	1.37	1.03
1:A:24:SER:HB2	1:A:329:ILE:HG23	1.05	1.02
1:A:275:ASN:HB2	1:A:279:ALA:CB	1.88	1.02
1:A:228:GLN:HE21	1:A:245:GLN:HG3	1.32	0.95
1:A:271:LYS:O	1:A:273:ILE:HG12	1.66	0.94
1:A:24:SER:CB	1:A:329:ILE:CG2	2.35	0.93
1:A:53:TYR:HE1	1:A:79:GLY:HA3	1.33	0.93
1:A:24:SER:HB2	1:A:329:ILE:HG22	1.51	0.91
1:A:132:ARG:HD3	1:A:146:ALA:HB2	1.51	0.91
1:A:37:ARG:NH2	3:A:404:CL:CL	2.40	0.91
1:A:46:VAL:O	1:A:50:LEU:HD23	1.70	0.90
1:A:46:VAL:O	1:A:50:LEU:O	1.88	0.88
1:A:228:GLN:NE2	1:A:245:GLN:HG3	1.89	0.88
1:A:248:GLU:HB3	1:A:266:LEU:HB3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASN:HB2	1:A:279:ALA:HB3	1.57	0.86
1:A:170:TYR:HA	4:A:614:HOH:O	1.75	0.86
1:A:130:THR:HG23	1:A:148:GLN:HG3	1.58	0.84
1:A:218:ASN:O	1:A:220:ILE:HD13	1.76	0.84
1:A:125:GLY:HA3	1:A:128:TYR:CE2	2.13	0.84
1:A:280:SER:O	1:A:282:GLY:N	2.11	0.83
1:A:252:GLN:HG2	1:A:262:SER:HB2	1.63	0.81
1:A:309:LYS:HD3	1:A:329:ILE:HD11	1.63	0.81
1:A:275:ASN:HB2	1:A:279:ALA:HB2	1.64	0.80
1:A:119:ASN:HD22	1:A:234:ARG:HH21	1.29	0.79
1:A:284:GLN:HE22	1:A:316:ASN:HD21	1.31	0.76
1:A:309:LYS:HB3	1:A:329:ILE:HD12	1.69	0.75
1:A:53:TYR:CE1	1:A:79:GLY:HA3	2.22	0.75
1:A:308:TYR:CE2	1:A:310:ILE:HD13	2.23	0.74
1:A:210:THR:HG23	1:A:227:SER:HB2	1.69	0.73
1:A:36:MET:HG2	1:A:37:ARG:N	2.03	0.73
1:A:11:LEU:HD12	1:A:11:LEU:C	2.07	0.73
1:A:235:PHE:HD2	1:A:235:PHE:O	1.71	0.72
1:A:139:LEU:HD23	1:A:140:VAL:HG23	1.72	0.71
1:A:206:ALA:HA	1:A:230:TYR:HB3	1.71	0.71
1:A:253:TYR:HD2	1:A:255:PHE:CE2	2.09	0.70
1:A:128:TYR:HD1	1:A:148:GLN:NE2	1.89	0.70
1:A:24:SER:O	1:A:30:ASP:HB2	1.92	0.69
1:A:309:LYS:HD3	1:A:329:ILE:CD1	2.22	0.69
1:A:235:PHE:C	1:A:235:PHE:CD2	2.65	0.69
1:A:235:PHE:CE1	1:A:286:ILE:HG23	2.28	0.69
1:A:97:THR:OG1	1:A:183:THR:HG21	1.92	0.69
1:A:275:ASN:H	1:A:279:ALA:HB3	1.56	0.69
1:A:275:ASN:OD1	1:A:281:TYR:HE2	1.75	0.68
1:A:254:GLN:HG2	1:A:260:ARG:HH11	1.58	0.68
1:A:123:GLN:HE21	1:A:124:ARG:HH11	1.39	0.68
1:A:107:LEU:HB2	1:A:110:PHE:O	1.93	0.68
1:A:115:TYR:N	1:A:115:TYR:CD2	2.58	0.68
1:A:115:TYR:H	1:A:115:TYR:HD2	1.37	0.68
1:A:11:LEU:HD12	1:A:12:ASP:N	2.09	0.68
1:A:290:VAL:HG12	1:A:310:ILE:CB	2.22	0.67
1:A:337:GLN:O	1:A:338:PHE:HB3	1.94	0.67
1:A:181:ALA:O	4:A:610:HOH:O	2.13	0.66
1:A:308:TYR:HE2	1:A:310:ILE:HD13	1.60	0.66
1:A:184:THR:CG2	1:A:207:THR:HB	2.19	0.66
1:A:3:ILE:O	1:A:3:ILE:HG22	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:TYR:HB3	1:A:247:PHE:HD1	1.62	0.65
1:A:94:TYR:CE1	1:A:124:ARG:HD2	2.32	0.64
1:A:61:GLN:HB3	1:A:63:ASN:OD1	1.98	0.64
1:A:96:VAL:N	1:A:148:GLN:OE1	2.24	0.64
1:A:13:LEU:HG	1:A:13:LEU:O	1.96	0.64
1:A:107:LEU:HD23	1:A:291:ASP:OD1	1.98	0.64
1:A:74:ARG:CZ	1:A:94:TYR:OH	2.46	0.64
1:A:74:ARG:HG3	3:A:404:CL:CL	2.36	0.63
1:A:184:THR:HA	1:A:207:THR:HA	1.80	0.63
1:A:177:SER:HB2	1:A:214:LYS:HG2	1.81	0.62
1:A:224:ALA:HB2	1:A:249:VAL:HG23	1.80	0.62
1:A:164:TYR:O	4:A:605:HOH:O	2.16	0.62
1:A:235:PHE:HE1	1:A:286:ILE:HG12	1.66	0.61
1:A:308:TYR:CE2	1:A:310:ILE:CD1	2.84	0.60
1:A:170:TYR:HB3	1:A:178:VAL:HG12	1.83	0.60
1:A:289:TYR:CD2	1:A:309:LYS:HG3	2.36	0.60
1:A:253:TYR:HA	4:A:616:HOH:O	2.01	0.60
1:A:121:MET:HG2	1:A:183:THR:HB	1.84	0.60
1:A:131:TYR:HE2	1:A:133:ASN:HB2	1.67	0.60
1:A:120:PHE:O	1:A:121:MET:CB	2.50	0.59
1:A:97:THR:OG1	1:A:121:MET:HG3	2.02	0.59
1:A:116:GLY:H	1:A:119:ASN:HB2	1.67	0.59
1:A:131:TYR:CE2	1:A:133:ASN:HB2	2.38	0.58
1:A:254:GLN:HE21	1:A:260:ARG:HD2	1.68	0.58
1:A:338:PHE:HD2	1:A:338:PHE:OXT	1.86	0.58
1:A:235:PHE:O	1:A:235:PHE:CD2	2.56	0.58
1:A:235:PHE:CE1	1:A:286:ILE:HG12	2.39	0.57
1:A:171:ALA:HA	1:A:177:SER:HA	1.86	0.57
1:A:53:TYR:HE1	1:A:79:GLY:CA	2.12	0.57
1:A:1:ALA:N	1:A:338:PHE:OXT	2.36	0.57
1:A:2:GLU:HA	1:A:12:ASP:HA	1.87	0.57
1:A:40:PHE:CD2	1:A:40:PHE:O	2.57	0.57
1:A:183:THR:O	1:A:208:VAL:N	2.30	0.57
1:A:167:SER:O	1:A:168:LEU:HD22	2.05	0.57
1:A:271:LYS:O	1:A:272:ASP:C	2.42	0.57
1:A:338:PHE:CD2	1:A:338:PHE:OXT	2.58	0.57
1:A:310:ILE:HA	1:A:328:ASP:OD2	2.06	0.56
1:A:255:PHE:HD1	1:A:257:PHE:CE1	2.23	0.56
1:A:255:PHE:HD1	1:A:257:PHE:HE1	1.52	0.56
1:A:246:ASN:OD1	1:A:246:ASN:N	2.37	0.56
1:A:96:VAL:HG12	1:A:121:MET:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:MET:HG2	1:A:183:THR:CB	2.36	0.56
1:A:336:TYR:CE1	1:A:337:GLN:O	2.59	0.55
1:A:274:SER:HB3	4:A:615:HOH:O	2.06	0.55
1:A:292:VAL:HG12	1:A:308:TYR:HB3	1.89	0.55
1:A:184:THR:HG22	1:A:207:THR:CB	2.23	0.55
1:A:266:LEU:HD12	1:A:266:LEU:N	2.21	0.55
1:A:226:TYR:HB2	1:A:247:PHE:HA	1.88	0.55
1:A:284:GLN:NE2	1:A:316:ASN:HD21	2.03	0.54
1:A:94:TYR:HA	1:A:124:ARG:HA	1.89	0.53
1:A:248:GLU:CB	1:A:266:LEU:HB3	2.36	0.53
1:A:115:TYR:N	1:A:115:TYR:HD2	2.01	0.53
1:A:289:TYR:HB2	1:A:310:ILE:O	2.08	0.53
1:A:253:TYR:CD2	1:A:255:PHE:CE2	2.93	0.53
1:A:177:SER:HB2	1:A:214:LYS:CG	2.38	0.53
1:A:235:PHE:CE1	1:A:286:ILE:CG2	2.92	0.53
1:A:336:TYR:C	1:A:336:TYR:CD1	2.80	0.53
1:A:59:GLN:NE2	1:A:61:GLN:OE1	2.38	0.53
1:A:96:VAL:HG22	1:A:167:SER:HB3	1.91	0.52
1:A:226:TYR:HB2	1:A:246:ASN:O	2.09	0.52
1:A:284:GLN:HB2	1:A:318:PHE:CD1	2.44	0.52
1:A:117:ALA:O	1:A:118:ASP:HB2	2.10	0.52
1:A:38:ILE:CG2	1:A:38:ILE:O	2.57	0.52
1:A:292:VAL:CG1	1:A:308:TYR:HB3	2.40	0.52
1:A:14:PHE:CE2	1:A:41:LYS:HG3	2.46	0.52
1:A:19:GLY:HA2	1:A:34:THR:HG23	1.92	0.52
1:A:40:PHE:CD2	1:A:40:PHE:C	2.82	0.51
1:A:53:TYR:CE1	1:A:79:GLY:CA	2.90	0.51
1:A:275:ASN:OD1	1:A:281:TYR:CE2	2.62	0.51
1:A:96:VAL:HB	1:A:148:GLN:OE1	2.11	0.51
1:A:262:SER:N	1:A:293:GLY:O	2.38	0.50
1:A:210:THR:HG23	1:A:225:GLN:HE21	1.75	0.50
1:A:258:GLY:O	1:A:259:LEU:HB2	2.10	0.50
1:A:95:GLY:HA2	1:A:128:TYR:HE1	1.76	0.50
1:A:284:GLN:HE22	1:A:316:ASN:ND2	2.06	0.50
1:A:233:THR:HA	1:A:240:PHE:CB	2.42	0.49
1:A:233:THR:O	1:A:234:ARG:C	2.50	0.49
1:A:116:GLY:H	1:A:119:ASN:CB	2.24	0.49
1:A:235:PHE:HE1	1:A:286:ILE:CG2	2.26	0.49
1:A:95:GLY:HA2	1:A:128:TYR:CE1	2.47	0.49
1:A:206:ALA:N	4:A:620:HOH:O	2.46	0.49
1:A:183:THR:HG23	4:A:630:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:HA	1:A:291:ASP:O	2.13	0.48
1:A:218:ASN:O	1:A:220:ILE:N	2.47	0.48
1:A:120:PHE:O	1:A:121:MET:HB3	2.14	0.48
1:A:179:GLY:O	1:A:211:GLY:HA2	2.13	0.47
1:A:220:ILE:HD12	1:A:253:TYR:CD1	2.48	0.47
1:A:253:TYR:CD2	1:A:255:PHE:CD2	3.02	0.47
1:A:183:THR:OG1	1:A:208:VAL:HG13	2.13	0.47
1:A:226:TYR:HB3	1:A:247:PHE:CD1	2.45	0.47
1:A:49:GLN:HB3	1:A:82:PHE:CZ	2.49	0.47
1:A:288:LYS:HG3	1:A:312:LEU:HB2	1.96	0.47
1:A:220:ILE:HD12	1:A:253:TYR:HD1	1.78	0.47
1:A:65:THR:O	1:A:68:SER:HB3	2.14	0.47
1:A:125:GLY:CA	1:A:128:TYR:CE2	2.92	0.47
1:A:318:PHE:C	1:A:318:PHE:CD2	2.89	0.47
1:A:250:VAL:HG23	1:A:264:ALA:HB2	1.97	0.47
1:A:234:ARG:NE	1:A:234:ARG:O	2.49	0.46
1:A:243:LYS:O	1:A:271:LYS:HB3	2.16	0.46
1:A:115:TYR:HB2	1:A:122:GLN:HB2	1.97	0.46
1:A:87:SER:O	1:A:131:TYR:HA	2.15	0.46
1:A:18:ASP:HB3	1:A:35:TYR:CE1	2.51	0.46
1:A:252:GLN:HG2	1:A:262:SER:CB	2.42	0.46
1:A:115:TYR:HB3	1:A:122:GLN:OE1	2.16	0.46
1:A:318:PHE:C	1:A:318:PHE:HD2	2.19	0.45
1:A:132:ARG:HB2	1:A:132:ARG:HE	1.49	0.45
1:A:29:SER:O	1:A:30:ASP:C	2.55	0.45
1:A:144:ASP:OD2	1:A:144:ASP:N	2.49	0.45
1:A:136:PHE:CD2	1:A:137:PHE:HD2	2.35	0.45
1:A:107:LEU:HD21	1:A:264:ALA:HB3	1.99	0.44
1:A:58:TYR:CE2	1:A:71:SER:HB2	2.51	0.44
1:A:221:TYR:HB3	1:A:252:GLN:HB2	1.99	0.44
1:A:15:GLY:HA3	1:A:338:PHE:CZ	2.52	0.44
1:A:184:THR:N	4:A:605:HOH:O	2.39	0.44
1:A:265:TYR:OH	1:A:267:GLN:CD	2.56	0.44
1:A:128:TYR:HD1	1:A:148:GLN:HE22	1.61	0.44
1:A:253:TYR:HD2	1:A:255:PHE:HE2	1.62	0.44
1:A:14:PHE:CD2	1:A:14:PHE:N	2.85	0.44
1:A:145:PHE:CB	1:A:168:LEU:HD13	2.48	0.44
1:A:13:LEU:O	1:A:338:PHE:HE2	2.01	0.44
1:A:218:ASN:C	1:A:220:ILE:H	2.21	0.43
1:A:253:TYR:HD2	1:A:255:PHE:CD2	2.36	0.43
1:A:303:SER:OG	1:A:335:VAL:CG2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:CD1	1:A:35:TYR:N	2.85	0.43
1:A:3:ILE:O	1:A:3:ILE:CG2	2.64	0.43
1:A:233:THR:O	1:A:235:PHE:HB3	2.18	0.43
1:A:97:THR:HG1	1:A:121:MET:HG3	1.82	0.43
1:A:24:SER:HB3	1:A:329:ILE:CG2	2.37	0.43
1:A:253:TYR:O	1:A:260:ARG:HA	2.18	0.43
1:A:316:ASN:C	1:A:316:ASN:OD1	2.57	0.43
1:A:21:HIS:HD2	1:A:22:TYR:O	2.01	0.43
1:A:37:ARG:NH2	1:A:74:ARG:HD2	2.34	0.43
1:A:20:LEU:HD11	1:A:109:GLU:OE2	2.18	0.42
1:A:11:LEU:C	1:A:11:LEU:CD1	2.79	0.42
1:A:139:LEU:CD2	1:A:140:VAL:HG23	2.44	0.42
1:A:252:GLN:CG	1:A:262:SER:HB2	2.41	0.42
1:A:115:TYR:CB	1:A:122:GLN:HB2	2.49	0.42
1:A:123:GLN:HE21	1:A:124:ARG:NH1	2.12	0.42
1:A:107:LEU:HD13	1:A:111:GLY:HA3	2.02	0.42
1:A:15:GLY:HA3	1:A:338:PHE:CE1	2.55	0.42
1:A:14:PHE:CE1	1:A:39:GLY:HA3	2.55	0.42
1:A:254:GLN:NE2	1:A:260:ARG:HD2	2.33	0.42
1:A:108:PRO:HD2	1:A:307:ASP:OD2	2.20	0.42
1:A:206:ALA:HA	1:A:230:TYR:CB	2.43	0.42
1:A:143:LEU:N	4:A:613:HOH:O	2.52	0.42
1:A:255:PHE:HB3	1:A:257:PHE:CE1	2.55	0.42
1:A:235:PHE:HE1	1:A:286:ILE:CG1	2.32	0.41
1:A:39:GLY:HA2	1:A:57:GLU:HA	2.02	0.41
1:A:226:TYR:CB	1:A:247:PHE:HA	2.50	0.41
1:A:240:PHE:C	1:A:273:ILE:HG23	2.41	0.41
1:A:145:PHE:HB3	1:A:168:LEU:HD13	2.02	0.41
1:A:14:PHE:HE2	1:A:41:LYS:HG3	1.85	0.41
1:A:254:GLN:CG	1:A:260:ARG:HH11	2.31	0.41
1:A:125:GLY:HA3	1:A:128:TYR:HE2	1.79	0.41
1:A:275:ASN:O	1:A:277:TYR:N	2.54	0.41
1:A:262:SER:O	1:A:293:GLY:N	2.54	0.41
1:A:264:ALA:O	1:A:291:ASP:N	2.53	0.41
1:A:164:TYR:CD1	1:A:165:GLY:N	2.88	0.41
1:A:182:ILE:CA	4:A:610:HOH:O	2.30	0.40
1:A:170:TYR:O	1:A:178:VAL:N	2.45	0.40
1:A:167:SER:C	1:A:168:LEU:HD22	2.41	0.40
1:A:212:GLY:HA2	1:A:225:GLN:HA	2.02	0.40
1:A:210:THR:CG2	1:A:225:GLN:HE21	2.35	0.40
1:A:185:SER:O	1:A:206:ALA:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TYR:C	1:A:131:TYR:CD2	2.95	0.40
1:A:337:GLN:HB2	1:A:338:PHE:H	1.69	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	305/338 (90%)	256 (84%)	35 (12%)	14 (5%)	3	23

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	ASP
1	A	219	ASN
1	A	234	ARG
1	A	281	TYR
1	A	121	MET
1	A	218	ASN
1	A	233	THR
1	A	259	LEU
1	A	272	ASP
1	A	276	GLY
1	A	320	ARG
1	A	47	ASN
1	A	112	GLY
1	A	106	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	238 / 266 (90%)	180 (76%)	58 (24%)	<b>1</b> <b>3</b>

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	11	LEU
1	A	16	LYS
1	A	20	LEU
1	A	36	MET
1	A	38	ILE
1	A	43	GLU
1	A	50	LEU
1	A	53	TYR
1	A	68	SER
1	A	69	ASN
1	A	89	ASP
1	A	96	VAL
1	A	97	THR
1	A	101	THR
1	A	109	GLU
1	A	110	PHE
1	A	115	TYR
1	A	124	ARG
1	A	130	THR
1	A	132	ARG
1	A	134	THR
1	A	139	LEU
1	A	141	ASP
1	A	144	ASP
1	A	162	ASP
1	A	164	TYR
1	A	170	TYR
1	A	182	ILE
1	A	183	THR

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Mol	Chain	Res	Type
1	A	207	THR
1	A	208	VAL
1	A	210	THR
1	A	219	ASN
1	A	220	ILE
1	A	226	TYR
1	A	230	TYR
1	A	231	ASN
1	A	234	ARG
1	A	235	PHE
1	A	237	THR
1	A	245	GLN
1	A	246	ASN
1	A	257	PHE
1	A	262	SER
1	A	266	LEU
1	A	273	ILE
1	A	290	VAL
1	A	303	SER
1	A	305	TYR
1	A	308	TYR
1	A	317	ASP
1	A	318	PHE
1	A	326	THR
1	A	328	ASP
1	A	329	ILE
1	A	337	GLN
1	A	338	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	69	ASN
1	A	119	ASN
1	A	123	GLN
1	A	228	GLN
1	A	245	GLN
1	A	284	GLN
1	A	325	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](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

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	311/338 (92%)	0.43	31 (9%) <b>9</b> <b>5</b>	47, 95, 130, 143	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	SER	11.4
1	A	237	THR	9.6
1	A	236	GLY	9.3
1	A	235	PHE	8.5
1	A	239	GLY	6.5
1	A	274	SER	4.9
1	A	278	GLY	4.6
1	A	172	ILE	4.0
1	A	279	ALA	3.9
1	A	232	ALA	3.8
1	A	174	GLU	3.8
1	A	173	GLY	3.2
1	A	281	TYR	3.1
1	A	265	TYR	3.0
1	A	228	GLN	3.0
1	A	8	GLY	3.0
1	A	273	ILE	2.9
1	A	275	ASN	2.9
1	A	276	GLY	2.9
1	A	226	TYR	2.8
1	A	280	SER	2.8
1	A	233	THR	2.7
1	A	164	TYR	2.6
1	A	277	TYR	2.5
1	A	286	ILE	2.5
1	A	266	LEU	2.4
1	A	176	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	318	PHE	2.2
1	A	175	GLY	2.2
1	A	170	TYR	2.0
1	A	271	LYS	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
3	CL	A	403	1/1	0.90	0.21	-0.64	111,111,111,111	0
2	CA	A	402	1/1	0.77	0.09	-1.33	132,132,132,132	0
3	CL	A	405	1/1	0.90	0.30	-	91,91,91,91	1
2	CA	A	401	1/1	0.84	0.14	-	142,142,142,142	0
3	CL	A	404	1/1	0.83	0.26	-	104,104,104,104	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.