



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:23 PM GMT

PDB ID : 3HSI  
Title : Crystal structure of phosphatidylserine synthase Haemophilus influenzae Rd KW20  
Authors : Chang, C.; Li, H.; Buck, K.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2009-06-10  
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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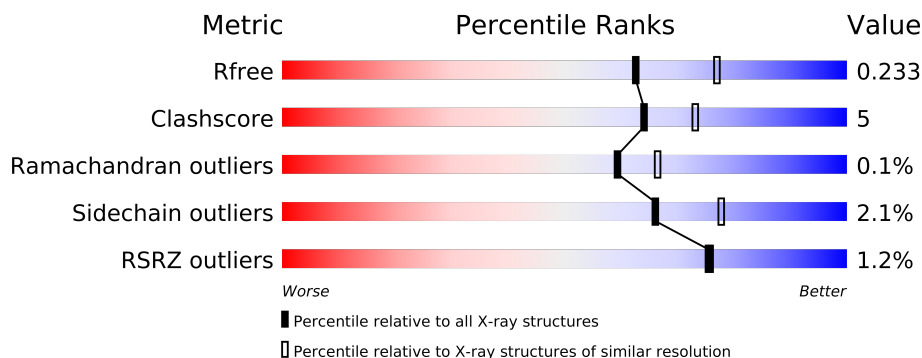
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	458	
1	B	458	
1	C	458	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11690 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Phosphatidylserine synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	Se	0	5	0
			3678	2365	636	669	3	5			
1	B	451	Total	C	N	O	S	Se	0	5	0
			3693	2371	639	676	3	4			
1	C	448	Total	C	N	O	S	Se	0	4	0
			3670	2359	638	665	3	5			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP P44704
A	-1	ASN	-	EXPRESSION TAG	UNP P44704
A	0	ALA	-	EXPRESSION TAG	UNP P44704
B	-2	SER	-	EXPRESSION TAG	UNP P44704
B	-1	ASN	-	EXPRESSION TAG	UNP P44704
B	0	ALA	-	EXPRESSION TAG	UNP P44704
C	-2	SER	-	EXPRESSION TAG	UNP P44704
C	-1	ASN	-	EXPRESSION TAG	UNP P44704
C	0	ALA	-	EXPRESSION TAG	UNP P44704

- Molecule 2 is water.

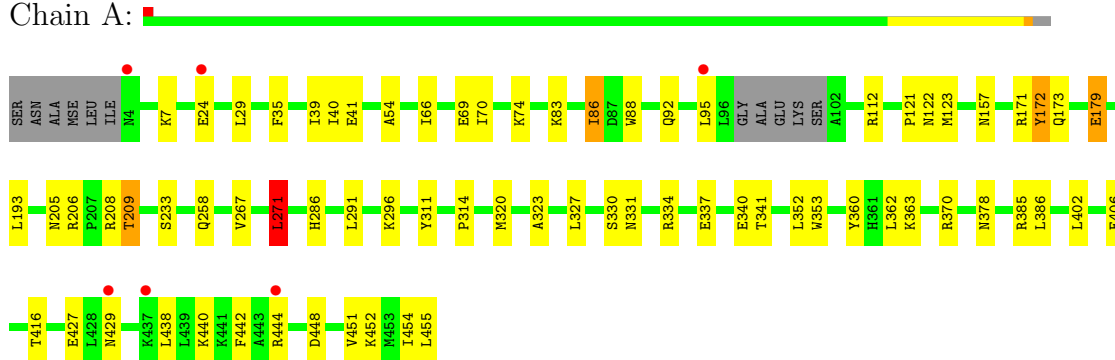
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	220	Total	O	0	0
			220	220		
2	B	217	Total	O	0	0
			217	217		
2	C	212	Total	O	0	0
			212	212		

### 3 Residue-property plots

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.

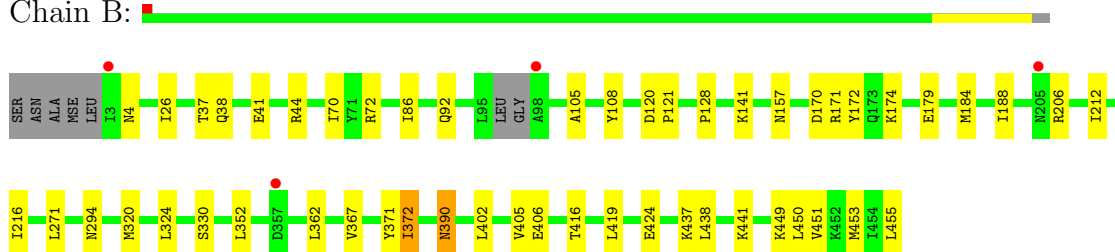
- Molecule 1: Phosphatidylserine synthase

Chain A:



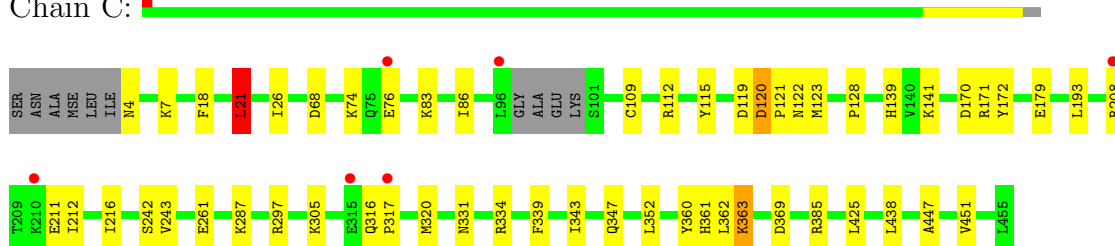
- Molecule 1: Phosphatidylserine synthase

Chain B:



- Molecule 1: Phosphatidylserine synthase

Chain C:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.56Å 154.24Å 214.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 47.45 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-2.20) 98.0 (47.45-2.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, $R_{free}$	0.190 , 0.236 0.187 , 0.233	Depositor DCC
$R_{free}$ test set	4233 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 84362 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11690	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

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	0.64	0/3755	0.71	1/5089 (0.0%)
1	B	0.64	0/3771	0.70	0/5111
1	C	0.69	1/3747 (0.0%)	0.71	1/5079 (0.0%)
All	All	0.66	1/11273 (0.0%)	0.70	2/15279 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109	CYS	CB-SG	-5.14	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	LEU	CA-CB-CG	5.22	127.30	115.30
1	C	21	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3678	0	3630	44	0
1	B	3693	0	3620	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3670	0	3616	39	0
2	A	220	0	0	8	0
2	B	217	0	0	3	0
2	C	212	0	0	2	0
All	All	11690	0	10866	119	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (119) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:128:PRO:HG2	1:C:216:ILE:HD12	1.54	0.89
1:A:205:ASN:HB3	2:A:574:HOH:O	1.75	0.86
1:A:112:ARG:NH1	1:A:122:ASN:OD1	2.08	0.85
1:B:128:PRO:HG2	1:B:216:ILE:HD12	1.61	0.82
1:C:74:LYS:HD3	1:C:123[A]:MSE:HE1	1.60	0.81
1:A:429:ASN:HB3	2:A:529:HOH:O	1.83	0.79
1:B:212:ILE:HD12	1:B:216:ILE:HD11	1.68	0.76
1:C:74:LYS:CD	1:C:123[A]:MSE:HE1	2.16	0.75
1:B:44:ARG:NE	1:B:72:ARG:HH22	1.85	0.74
1:A:171:ARG:HG3	1:A:362:LEU:HD22	1.71	0.73
1:C:128:PRO:CG	1:C:216:ILE:HD12	2.23	0.68
1:C:171:ARG:HG3	1:C:362:LEU:HD22	1.76	0.68
1:C:68:ASP:OD1	1:C:115:TYR:OH	2.12	0.65
1:A:83:LYS:HD3	1:A:193:LEU:HD11	1.80	0.64
1:C:297:ARG:HH11	1:C:347:GLN:HG3	1.62	0.64
1:C:74:LYS:HG2	1:C:123[A]:MSE:HE1	1.82	0.62
1:A:451:VAL:HG13	1:A:455:LEU:HD12	1.80	0.62
1:B:179:GLU:HG3	2:B:581:HOH:O	1.99	0.62
1:C:385:ARG:NH1	2:C:614:HOH:O	2.31	0.62
1:B:450:LEU:HA	1:B:453:MSE:HE3	1.82	0.61
1:C:74:LYS:CG	1:C:123[A]:MSE:HE1	2.31	0.60
1:A:95:LEU:HD21	2:A:648:HOH:O	2.01	0.60
1:C:352:LEU:HD11	1:C:425:LEU:HD21	1.84	0.59
1:B:44:ARG:HE	1:B:72:ARG:HH22	1.49	0.59
1:A:208:ARG:NH1	2:A:552:HOH:O	2.35	0.59
1:B:320:MSE:HB2	1:B:438:LEU:HD21	1.86	0.58
1:B:92:GLN:HE21	1:B:206:ARG:HH21	1.50	0.58
1:C:76[B]:GLU:HG3	1:C:76[B]:GLU:O	2.04	0.57
1:C:74:LYS:HD3	1:C:123[A]:MSE:CE	2.35	0.56
1:A:327:LEU:HD11	1:A:448:ASP:HB2	1.88	0.55
1:A:40[A]:ILE:HD12	1:A:69:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:44:ARG:HE	1:B:72:ARG:NH2	2.05	0.55
1:A:74:LYS:HE2	1:A:121:PRO:HG3	1.88	0.55
1:A:29:LEU:HB2	1:A:172:TYR:HB2	1.88	0.54
1:B:184:MSE:O	1:B:188[B]:ILE:HG12	2.08	0.54
1:C:208:ARG:O	1:C:211:GLU:HB3	2.08	0.53
1:A:291:LEU:HD22	1:A:296:LYS:HG3	1.88	0.53
1:A:92:GLN:HE21	1:A:206:ARG:HE	1.57	0.52
1:B:402:LEU:O	1:B:406:GLU:HG3	2.09	0.52
1:B:128:PRO:CG	1:B:216:ILE:HD12	2.37	0.52
1:B:372:ILE:CD1	1:B:405:VAL:HG21	2.40	0.52
1:B:450:LEU:HA	1:B:453:MSE:CE	2.39	0.51
1:B:372:ILE:HD12	1:B:405:VAL:HG21	1.92	0.51
1:C:212:ILE:HD12	1:C:216:ILE:HD11	1.91	0.51
1:C:320:MSE:HG2	1:C:438:LEU:HD21	1.93	0.51
1:A:267:VAL:HG21	1:A:271:LEU:HG	1.93	0.50
1:A:35:PHE:O	1:A:39:ILE:HG13	2.12	0.50
1:B:171:ARG:HG3	1:B:362:LEU:HD22	1.93	0.50
1:A:402:LEU:O	1:A:406:GLU:HG3	2.11	0.50
1:A:92:GLN:NE2	1:A:206:ARG:HE	2.10	0.50
1:C:18:PHE:HB3	1:C:242:SER:HB3	1.94	0.49
1:C:297:ARG:NH1	1:C:347:GLN:HG3	2.26	0.49
1:C:119:ASP:O	1:C:120:ASP:HB3	2.12	0.49
1:B:141:LYS:H	1:B:390:ASN:ND2	2.12	0.48
1:A:88:TRP:HE1	1:A:209:THR:HG22	1.78	0.48
1:B:324:LEU:HD21	1:B:451:VAL:HG11	1.95	0.48
1:A:320:MSE:CE	1:A:442:PHE:HZ	2.27	0.48
1:C:21:LEU:HD12	1:C:243:VAL:HB	1.94	0.48
1:B:141:LYS:H	1:B:390:ASN:HD21	1.61	0.48
1:B:437:LYS:O	1:B:441:LYS:HG3	2.14	0.48
1:C:360:TYR:CE1	1:C:362:LEU:HD12	2.48	0.48
1:C:361:HIS:CE1	1:C:363:LYS:CE	2.97	0.48
1:B:324:LEU:HD11	1:B:455:LEU:HD12	1.97	0.47
1:B:419:LEU:HD22	1:B:424:GLU:HB2	1.96	0.47
1:C:361:HIS:CE1	1:C:363:LYS:HE3	2.49	0.47
1:C:122:ASN:ND2	2:C:633:HOH:O	2.47	0.47
1:A:179:GLU:OE1	1:A:233:SER:OG	2.18	0.47
1:A:171:ARG:HG3	1:A:362:LEU:CD2	2.44	0.47
1:C:76[B]:GLU:CG	1:C:76[B]:GLU:O	2.62	0.47
1:C:316:GLN:HB3	1:C:317:PRO:HD2	1.97	0.47
1:A:70:ILE:HG21	1:A:123[A]:MSE:SE	2.65	0.47
1:C:170:ASP:HA	1:C:362:LEU:HD23	1.98	0.46
1:A:440:LYS:O	1:A:444:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:385:ARG:HG3	1:A:386:LEU:HG	1.98	0.45
1:A:363:LYS:HD3	1:A:378:ASN:OD1	2.17	0.45
1:C:112:ARG:NH1	1:C:122:ASN:OD1	2.24	0.45
1:A:88:TRP:HE1	1:A:209:THR:CG2	2.30	0.45
1:B:294:ASN:ND2	2:B:502:HOH:O	2.48	0.45
1:C:120:ASP:N	1:C:121:PRO:CD	2.80	0.44
1:A:327:LEU:HD21	1:A:452:LYS:HE3	2.00	0.44
1:C:261:GLU:HB3	1:C:287:LYS:HE2	1.99	0.44
1:A:337:GLU:O	1:A:340:GLU:HB2	2.17	0.44
1:C:447:ALA:O	1:C:451:VAL:HG23	2.17	0.44
1:C:4:ASN:HB3	1:C:7:LYS:HB2	2.00	0.44
1:B:4:ASN:HB2	2:B:629:HOH:O	2.17	0.44
1:B:120:ASP:HB3	1:B:121:PRO:HD2	2.00	0.44
1:A:54:ALA:O	1:A:86:ILE:HA	2.18	0.44
1:A:205:ASN:CB	2:A:574:HOH:O	2.50	0.43
1:C:21:LEU:HD22	1:C:26:ILE:HD11	2.00	0.43
1:B:372:ILE:HD12	1:B:405:VAL:CG2	2.49	0.43
1:C:83:LYS:HD2	1:C:193:LEU:HD11	2.00	0.43
1:B:44:ARG:NE	1:B:72:ARG:NH2	2.60	0.43
1:A:171:ARG:HB3	1:A:173:GLN:HE22	1.84	0.42
1:A:454:ILE:HG13	1:A:455:LEU:HG	2.01	0.42
1:C:331:ASN:OD1	1:C:334:ARG:NH1	2.47	0.42
1:B:449:LYS:HG2	1:B:453:MSE:HE2	2.01	0.42
1:A:41:GLU:HG3	2:A:626:HOH:O	2.19	0.42
1:B:37:THR:O	1:B:41[B]:GLU:HG3	2.20	0.42
1:A:286:HIS:HB2	2:A:509:HOH:O	2.18	0.42
1:C:120:ASP:N	1:C:121:PRO:HD3	2.34	0.42
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.86	0.42
1:B:367:VAL:HB	1:B:371:TYR:HB2	2.02	0.41
1:B:170:ASP:HA	1:B:362:LEU:HD23	2.01	0.41
1:C:339:PHE:O	1:C:343:ILE:HG12	2.21	0.41
1:A:323:ALA:CB	1:A:438:LEU:HD23	2.50	0.41
1:A:157:ASN:C	1:A:157:ASN:OD1	2.58	0.41
1:A:7:LYS:HA	2:A:537:HOH:O	2.20	0.41
1:B:38:GLN:NE2	1:B:41[B]:GLU:OE1	2.54	0.41
1:A:331:ASN:OD1	1:A:334:ARG:NH2	2.54	0.41
1:B:105:ALA:HA	1:B:108:TYR:CD2	2.56	0.41
1:C:369:ASP:OD1	1:C:369:ASP:N	2.53	0.41
1:A:40[A]:ILE:HD11	1:A:66:ILE:CD1	2.50	0.40
1:A:24[B]:GLU:HG3	1:A:24[B]:GLU:O	2.21	0.40
1:A:311:TYR:OH	1:A:314:PRO:HD3	2.20	0.40
1:C:139:HIS:O	1:C:141:LYS:HE2	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:157:ASN:OD1	1:B:157:ASN:C	2.60	0.40
1:A:352:LEU:O	1:A:416:THR:HA	2.22	0.40
1:B:352:LEU:O	1:B:416:THR:HA	2.22	0.40
1:A:353:TRP:CE3	1:A:360:TYR:HB2	2.57	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	448/458 (98%)	431 (96%)	17 (4%)	0	100	100
1	B	452/458 (99%)	436 (96%)	16 (4%)	0	100	100
1	C	448/458 (98%)	430 (96%)	16 (4%)	2 (0%)	43	45
All	All	1348/1374 (98%)	1297 (96%)	49 (4%)	2 (0%)	59	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	305	LYS
1	C	120	ASP

### 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	391/404 (97%)	381 (97%)	10 (3%)	59	70
1	B	390/404 (96%)	381 (98%)	9 (2%)	63	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	388/404 (96%)	383 (99%)	5 (1%)	80	89
All	All	1169/1212 (96%)	1145 (98%)	24 (2%)	66	78

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ILE
1	A	172	TYR
1	A	179	GLU
1	A	209	THR
1	A	258	GLN
1	A	271	LEU
1	A	330	SER
1	A	341	THR
1	A	370	ARG
1	A	427	GLU
1	B	26	ILE
1	B	70	ILE
1	B	86	ILE
1	B	172	TYR
1	B	174	LYS
1	B	271	LEU
1	B	330	SER
1	B	372	ILE
1	B	390	ASN
1	C	21	LEU
1	C	86	ILE
1	C	172	TYR
1	C	179	GLU
1	C	363	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	92	GLN
1	A	258	GLN
1	A	436	GLN
1	B	11	GLN
1	B	38	GLN
1	B	92	GLN

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Mol	Chain	Res	Type
1	B	285	GLN
1	B	331	ASN
1	B	390	ASN
1	B	415	HIS
1	B	436	GLN
1	C	92	GLN
1	C	415	HIS
1	C	436	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

### 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	447/458 (97%)	-0.06	6 (1%) 74 74	18, 27, 40, 55	0
1	B	451/458 (98%)	-0.21	4 (0%) 81 82	19, 27, 39, 53	0
1	C	448/458 (97%)	-0.11	6 (1%) 74 74	18, 26, 38, 50	0
All	All	1346/1374 (97%)	-0.12	16 (1%) 75 76	18, 27, 39, 55	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	96	LEU	4.1
1	A	4	ASN	3.6
1	B	98	ALA	3.2
1	A	24[A]	GLU	3.1
1	C	76[A]	GLU	3.0
1	A	429	ASN	2.9
1	A	95	LEU	2.9
1	C	317	PRO	2.7
1	B	205	ASN	2.7
1	C	315	GLU	2.7
1	C	210	LYS	2.5
1	B	357	ASP	2.4
1	A	444	ARG	2.2
1	A	437	LYS	2.1
1	B	3	ILE	2.1
1	C	208	ARG	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 ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.