

# Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	6LHX
$\operatorname{Title}$	:	Crystal structure of ThsA
Authors	:	Bae, E.; Ka, D.; Oh, H.
Deposited on	:	2019-12-10
Resolution	:	2.50  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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\operatorname{CCP4}$	:	7.0.044  (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	$4661 \ (2.50-2.50)$
Clashscore	141614	$5346\ (2.50-2.50)$
Ramachandran outliers	138981	5231(2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559(2.50-2.50)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	А	476	83%	13%	•			
1	В	476	76% 9%	15%	_			
1	С	476	5%	12%	·			
1	D	476	6%           72%           12%	16%	_			



#### 6LHX

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13332 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.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	Δ	461	Total	С	Ν	Ο	$\mathbf{S}$	$\mathbf{Se}$	0	0	0
	Л	401	3556	2273	597	677	2	7	0		0
1	В	406	Total	С	Ν	Ο	$\mathbf{S}$	Se	0	0	0
	D	400	3170	2034	531	596	1	8			U
1	C	459	Total	С	Ν	Ο	S	Se	0	0	0
	400	3535	2262	587	677	2	7	0	0	0	
1	D 401	401	Total	С	Ν	Ο	S	Se	0	0	0
	401	3035	1944	514	569	1	7	U	0	0	

• Molecule 1 is a protein called ThsA.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	GLY	-	expression tag	UNP J8G6Z1
А	2	HIS	-	expression tag	UNP J8G6Z1
В	1	GLY	-	expression tag	UNP J8G6Z1
В	2	HIS	-	expression tag	UNP J8G6Z1
С	1	GLY	-	expression tag	UNP J8G6Z1
С	2	HIS	-	expression tag	UNP J8G6Z1
D	1	GLY	-	expression tag	UNP J8G6Z1
D	2	HIS	-	expression tag	UNP J8G6Z1

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	15	Total O 15 15	0	0
2	В	9	Total O 9 9	0	0
2	С	7	Total O 7 7	0	0
2	D	5	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 5 & 5 \end{array}$	0	0



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

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: ThsA



# 1376 R336 1385 R331 7385 R331 7385 R331 7385 R331 7414 P232 7415 P235 7416 P235 7416 P235 7436 P366 744 P366 7436 P366 744 P366 744 P346 745 P347 746<





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	180.42Å $168.58$ Å $93.61$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $106.71^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{B}_{\mathrm{ascolution}}(\mathbf{\hat{A}})$	31.64 - 2.50	Depositor
Resolution (A)	47.81 - 2.50	EDS
% Data completeness	99.2(31.64-2.50)	Depositor
(in resolution range)	88.5(47.81-2.50)	EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.43 (at 2.51 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
D D.	0.242 , $0.273$	Depositor
$n, n_{free}$	0.244 , $0.272$	DCC
$R_{free}$ test set	1996 reflections $(2.18\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	49.5	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.31 , $60.4$	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13332	wwPDB-VP
Average B, all atoms $(Å^2)$	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 11.56% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.24	0/3610	0.44	0/4874	
1	В	0.26	0/3219	0.48	1/4339~(0.0%)	
1	С	0.24	0/3594	0.44	0/4867	
1	D	0.25	0/3083	0.45	0/4172	
All	All	0.25	0/13506	0.45	1/18252~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms Z		$Observed(^{o})$	$Ideal(^{o})$
1	В	230	ARG	NE-CZ-NH1	5.66	123.13	120.30

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	А	3556	0	3330	42	0
1	В	3170	0	3017	34	0
1	С	3535	0	3298	36	0
1	D	3035	0	2793	31	0
2	А	15	0	0	0	0
2	В	9	0	0	0	0
2	С	7	0	0	0	0
2	D	5	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13332	0	12438	135	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 (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:C:142:VAL:HG12	1:C:143:LYS:HG2	1.65	0.77
1:A:76:ARG:NH2	1:A:167:ASP:OD1	2.20	0.74
1:A:69:CYS:SG	1:A:170:LYS:NZ	2.63	0.72
1:B:283:LYS:NZ	1:B:317:ASP:O	2.23	0.71
1:A:228:GLU:HG2	1:A:242:ARG:HB3	1.72	0.71
1:C:230:ARG:NH1	1:C:236:GLU:OE2	2.23	0.71
1:C:385:TYR:HA	1:C:421:GLY:HA2	1.73	0.71
1:D:99:ILE:HG21	1:D:273:LEU:HB3	1.75	0.69
1:C:69:CYS:SG	1:C:170:LYS:NZ	2.65	0.69
1:C:186:LEU:O	1:C:211:ARG:NH2	2.26	0.68
1:A:230:ARG:NE	1:A:236:GLU:OE2	2.25	0.68
1:A:414:VAL:HG12	1:A:416:PRO:HD3	1.74	0.67
1:D:284:THR:HG22	1:D:378:THR:HG22	1.80	0.63
1:D:11:ILE:HD13	1:D:275:ARG:HG2	1.80	0.63
1:C:348:ASP:HB3	1:C:351:ARG:HG2	1.81	0.62
1:B:312:GLU:HG2	1:B:468:ILE:HD13	1.82	0.61
1:B:284:THR:HG22	1:B:378:THR:HG22	1.82	0.61
1:A:380:VAL:HG22	1:A:413:TYR:HB2	1.83	0.60
1:A:284:THR:HG22	1:A:378:THR:HG22	1.84	0.60
1:B:228:GLU:HG3	1:B:242:ARG:HH21	1.67	0.60
1:A:428:TRP:HZ2	1:A:451:GLY:HA2	1.68	0.59
1:D:380:VAL:HG22	1:D:413:TYR:HB2	1.83	0.59
1:C:433:GLU:N	1:C:433:GLU:OE1	2.36	0.58
1:A:475:SER:O	1:A:475:SER:OG	2.21	0.58
1:A:377:ARG:NH2	1:B:349:ASP:OD2	2.36	0.58
1:B:286:PHE:HB2	1:B:378:THR:HG21	1.86	0.57
1:C:421:GLY:HA3	1:C:424:ALA:HB3	1.85	0.57
1:A:404:PHE:HE2	1:A:414:VAL:HG11	1.68	0.57
1:A:405:ASN:O	1:A:409:GLU:HG3	2.04	0.57
1:C:211:ARG:HH21	1:C:221:HIS:HE2	1.53	0.57
1:A:404:PHE:CE2	1:A:414:VAL:HG11	2.40	0.56
1:A:439:TYR:HE2	1:A:474:LEU:HD21	1.70	0.56
1:A:371:ARG:HA	1:A:374:MSE:HE3	1.86	0.56



Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlan (Å)		
1:D:286:PHE:HB2	1:D:378:THR:HG21	1.88	0.56		
1:C:283:LYS:NZ	1:C:316:LYS:O	2.38	0.56		
1:A:141:LYS:NZ	1:C:156:GLU:OE2	2.33	0.55		
1:A:286:PHE:HB2	1:A:378:THR:HG21	1.88	0.55		
1:A:361:LYS:O	1:A:365:GLU:HG3	2.07	0.55		
1:A:294:TYR:O	1:A:296:HIS:N	2.40	0.54		
1:B:182:LEU:HD23	1:B:210:VAL:HG11	1.88	0.54		
1:B:433:GLU:OE1	1:B:433:GLU:N	2.41	0.54		
1:B:446:MSE:HG3	1:B:473:ILE:HG21	1.90	0.53		
1:D:443:ASP:HA	1:D:446:MSE:HB3	1.91	0.53		
1:C:151:MSE:HE1	1:C:206:ILE:HD13	1.89	0.53		
1:D:428:TRP:HZ2	1:D:451:GLY:HA2	1.74	0.53		
1:C:211:ARG:NH2	1:C:221:HIS:HE2	2.08	0.52		
1:B:19:MSE:SE	1:B:283:LYS:HE2	2.59	0.52		
1:C:250:ILE:HG12	1:C:260:THR:HG21	1.91	0.51		
1:B:230:ARG:HH11	1:B:230:ARG:CG	2.24	0.51		
1:C:414:VAL:O	1:C:439:TYR:OH	2.20	0.51		
1:B:268:GLU:HA	1:B:271:GLU:HG3	1.93	0.51		
1:B:293:GLU:O	1:B:387:ASN:ND2	2.40	0.51		
1:D:182:LEU:HD23	1:D:210:VAL:HG11	1.93	0.51		
1:D:439:TYR:HE1	1:D:474:LEU:HD21	1.75	0.51		
1:D:206:ILE:O	1:D:210:VAL:HG22	2.10	0.51		
1:B:206:ILE:O	1:B:210:VAL:HG22	2.11	0.50		
1:C:230:ARG:HG2	1:C:239:PHE:CG	2.47	0.50		
1:B:475:SER:OG	1:B:475:SER:O	2.24	0.50		
1:C:45:GLU:HA	1:C:48:ALA:HB3	1.95	0.49		
1:A:291:ALA:O	1:A:327:GLY:HA3	2.12	0.49		
1:B:26:PHE:HA	1:B:109:TRP:O	2.12	0.49		
1:C:73:GLN:HE21	1:C:76:ARG:HD2	1.78	0.48		
1:B:26:PHE:HZ	1:B:111:THR:HG23	1.78	0.48		
1:A:349:ASP:OD1	1:B:377:ARG:NH1	2.46	0.48		
1:D:286:PHE:CE2	1:D:288:SER:HB2	2.48	0.48		
1:D:333:ILE:O	1:D:337:LEU:HD12	2.13	0.48		
1:A:348:ASP:HB3	1:A:351:ARG:HG2	1.95	0.48		
1:A:349:ASP:OD1	1:B:377:ARG:NH2	2.46	0.48		
1:D:314:ILE:O	1:D:351:ARG:NH2	2.45	0.48		
1:A:286:PHE:CE2	1:A:288:SER:HB2	2.48	0.47		
1:A:135:LYS:HG2	1:B:217:ASP:HB3	1.95	0.47		
1:A:192:LEU:HD11	1:A:224:LEU:HG	1.96	0.47		
1:B:307:HIS:CE1	1:B:335:GLY:HA2	2.50	0.47		
1:B:313:LEU:O	1:B:318:PHE:HB2	2.15	0.47		



Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlap(Å)		
1:C:284:THR:HG22	1:C:378:THR:HG22	1.95	0.47		
1:A:421:GLY:O	1:A:423:ILE:N	2.47	0.47		
1:C:337:LEU:HD22	1:C:341:TYR:CE2	2.50	0.47		
1:B:230:ARG:HH11	1:B:230:ARG:HG3	1.80	0.46		
1:B:286:PHE:CE2	1:B:288:SER:HB2	2.50	0.46		
1:C:368:ASP:O	1:C:372:ARG:HG3	2.14	0.46		
1:B:337:LEU:HD21	1:B:347:ILE:HD11	1.96	0.46		
1:C:134:VAL:HG21	1:C:174:LYS:HA	1.98	0.46		
1:D:372:ARG:O	1:D:376:THR:OG1	2.27	0.46		
1:D:211:ARG:NH1	1:D:256:PHE:O	2.45	0.46		
1:D:374:MSE:HB3	1:D:374:MSE:HE2	1.92	0.46		
1:C:286:PHE:CE2	1:C:288:SER:HB2	2.51	0.46		
1:A:265:ASN:ND2	1:A:267:ASN:HB2	2.31	0.46		
1:B:314:ILE:HG23	1:B:351:ARG:HH21	1.80	0.46		
1:B:26:PHE:CZ	1:B:111:THR:HG23	2.51	0.45		
1:C:50:GLU:HG2	1:C:51:ILE:H	1.81	0.45		
1:C:286:PHE:HB2	1:C:378:THR:HG21	1.98	0.45		
1:C:43:LEU:O	1:C:46:PRO:HD2	2.17	0.45		
1:A:250:ILE:HG12	1:A:260:THR:HG21	1.99	0.45		
1:B:405:ASN:O	1:B:409:GLU:HG3	2.17	0.45		
1:A:385:TYR:CD1	1:A:420:THR:HB	2.52	0.44		
1:A:337:LEU:HD22	1:A:341:TYR:CE2	2.53	0.44		
1:B:348:ASP:HB3	1:B:351:ARG:HG2	1.99	0.44		
1:A:206:ILE:O	1:A:210:VAL:HG22	2.18	0.44		
1:D:376:THR:HA	1:D:410:GLN:NE2	2.32	0.44		
1:D:364:GLU:HA	1:D:367:TRP:CG	2.53	0.43		
1:D:114:ASP:O	1:D:150:LYS:NZ	2.48	0.43		
1:A:293:GLU:O	1:A:387:ASN:ND2	2.40	0.43		
1:C:383:PHE:HB2	1:C:416:PRO:HA	2.01	0.43		
1:A:373:ASP:OD2	1:B:347:ILE:HG13	2.19	0.43		
1:D:464:ILE:HG13	1:D:465:ASN:N	2.33	0.43		
1:B:337:LEU:HD22	1:B:341:TYR:CZ	2.54	0.43		
1:C:370:TYR:O	1:C:374:MSE:HG3	2.18	0.43		
1:D:313:LEU:O	1:D:318:PHE:HB2	2.18	0.42		
1:D:140:THR:HG23	1:D:144:ARG:CZ	2.50	0.42		
1:C:140:THR:HG23	1:C:144:ARG:CZ	2.50	0.42		
1:C:323:GLY:N	1:C:374:MSE:HE1	2.34	0.42		
1:A:347:ILE:HG13	1:B:373:ASP:OD2	2.20	0.42		
1:D:156:GLU:O	1:D:157:HIS:CG	2.72	0.42		
1:D:471:VAL:O	1:D:474:LEU:HB2	2.20	0.42		
1:A:299:THR:O	1:A:303:GLU:HG3	2.20	0.42		



Atom 1		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:C:374:MSE:HB3	1:C:374:MSE:HE2	1.81	0.42
1:A:224:LEU:HD23	1:A:261:ILE:HB	2.03	0.41
1:A:313:LEU:O	1:A:318:PHE:HB2	2.19	0.41
1:D:307:HIS:NE2	1:D:338:GLU:OE2	2.34	0.41
1:A:20:GLU:OE1	1:B:142:VAL:HG13	2.19	0.41
1:C:192:LEU:HD11	1:C:224:LEU:HG	2.02	0.41
1:A:385:TYR:CE1	1:A:420:THR:HB	2.55	0.41
1:C:314:ILE:HG23	1:C:351:ARG:NH2	2.35	0.41
1:A:401:GLN:O	1:A:404:PHE:HB3	2.20	0.41
1:B:300:GLU:O	1:B:303:GLU:HB2	2.19	0.41
1:D:93:LEU:HD11	1:D:120:ALA:HB2	2.03	0.41
1:D:176:ASP:HB3	1:D:177:PRO:HD3	2.02	0.41
1:C:314:ILE:HG21	1:C:340:LEU:CD1	2.50	0.41
1:C:118:GLU:HG2	1:C:130:VAL:CG2	2.50	0.41
1:D:99:ILE:O	1:D:103:LEU:HG	2.21	0.40
1:C:298:GLU:HG3	1:C:301:HIS:HB2	2.02	0.40
1:D:131:LYS:NZ	1:D:139:THR:O	2.53	0.40
1:D:211:ARG:NH2	1:D:218:GLN:HB3	2.36	0.40
1:A:337:LEU:HD21	1:A:347:ILE:HD11	2.03	0.40
1:D:471:VAL:HA	1:D:474:LEU:HD12	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	Perce	entiles
1	А	443/476~(93%)	430 (97%)	13 (3%)	0	100	100
1	В	392/476~(82%)	377~(96%)	15~(4%)	0	100	100
1	С	448/476~(94%)	431 (96%)	17 (4%)	0	100	100
1	D	385/476~(81%)	371~(96%)	13 (3%)	1 (0%)	41	61
All	All	1668/1904~(88%)	1609 (96%)	58 (4%)	1 (0%)	51	73



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	419	ALA

#### 5.3.2 Protein sidechains (i)

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	Perce	ntiles
1	А	356/417~(85%)	355~(100%)	1 (0%)	92	97
1	В	323/417~(78%)	321~(99%)	2(1%)	86	95
1	С	355/417~(85%)	354 (100%)	1 (0%)	92	97
1	D	293/417~(70%)	289~(99%)	4 (1%)	67	86
All	All	1327/1668~(80%)	1319 (99%)	8 (1%)	86	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	26	PHE
1	В	26	PHE
1	В	230	ARG
1	С	314	ILE
1	D	26	PHE
1	D	312	GLU
1	D	337	LEU
1	D	423	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	157	HIS
1	В	304	GLN
1	В	359	GLN
1	С	73	GLN
1	D	2	HIS
1	D	267	ASN



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$\mathbf{Mol}$	Chain	$\mathbf{Res}$	Type
1	D	411	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 monosaccharides in this entry.

# 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 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 (i)

# 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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	$OWAB(Å^2)$	$Q{<}0.9$
1	А	453/476~(95%)	0.29	15 (3%) 46 50	45, 77, 119, 138	0
1	В	398/476~(83%)	0.21	10 (2%) 57 61	44, 78, 114, 135	0
1	С	450/476~(94%)	0.34	22 (4%) 29 31	44, 82, 121, 145	0
1	D	394/476~(82%)	0.42	28 (7%) 16 16	51, 88, 128, 160	0
All	All	1695/1904~(89%)	0.32	75 (4%) 34 37	44, 81, 121, 160	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	155	VAL	6.0
1	D	297	TRP	5.7
1	С	420	THR	5.5
1	D	395	VAL	5.0
1	А	292	VAL	4.4
1	С	61	LEU	4.3
1	С	294	TYR	4.0
1	D	290	SER	3.8
1	С	47	ILE	3.7
1	В	159	SER	3.7
1	С	436	GLU	3.7
1	А	427	LEU	3.6
1	D	394	VAL	3.6
1	D	158	PRO	3.5
1	D	154	ASP	3.5
1	А	61	LEU	3.4
1	А	431	VAL	3.4
1	С	431	VAL	3.3
1	С	292	VAL	3.2
1	В	158	PRO	3.2
1	А	296	HIS	3.2



Mol	Chain	Res	Type	RSRZ
1	D	91	VAL	3.2
1	D	87	PHE	3.1
1	С	434	GLU	3.1
1	С	360	GLY	3.0
1	D	113	TYR	3.0
1	А	439	TYR	2.9
1	С	437	THR	2.9
1	D	384	LEU	2.8
1	D	299	THR	2.8
1	А	299	THR	2.8
1	С	428	TRP	2.8
1	В	113	TYR	2.8
1	В	408	PHE	2.8
1	С	234	GLU	2.6
1	А	301	HIS	2.6
1	А	87	PHE	2.6
1	D	422	TYR	2.5
1	С	448	LYS	2.5
1	В	91	VAL	2.5
1	D	385	TYR	2.4
1	D	298	GLU	2.4
1	С	439	TYR	2.4
1	D	408	PHE	2.4
1	D	2	HIS	2.4
1	D	289	GLY	2.4
1	В	90	LYS	2.3
1	D	388	LYS	2.3
1	С	417	VAL	2.3
1	В	132	TYR	2.3
1	D	438	TYR	2.3
1	А	232	PRO	2.2
1	С	432	ASN	2.2
1	D	153	GLY	2.2
1	D	390	ASP	2.2
1	А	66	GLN	2.2
1	D	86	GLU	2.2
1	А	428	TRP	2.2
1	А	291	ALA	2.2
1	С	48	ALA	2.2
1	D	383	PHE	2.1
1	В	154	ASP	2.1
1	С	233	ASP	2.1



Mol	Chain	Res	Type	RSRZ
1	С	459	SER	2.1
1	В	89	ARG	2.1
1	D	216	ARG	2.1
1	В	294	TYR	2.1
1	С	341	TYR	2.1
1	D	301	HIS	2.1
1	D	429	ASN	2.1
1	А	426	ASP	2.0
1	А	346	THR	2.0
1	D	427	LEU	2.0
1	С	413	TYR	2.0
1	С	232	PRO	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 monosaccharides in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.

