



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:56 AM GMT

PDB ID : 4F4B  
Title : Structure of OSH4 with a cholesterol analog  
Authors : Koag, M.C.; Monzingo, A.F.; Cheun, Y.; Lee, S.  
Deposited on : 2012-05-10  
Resolution : 1.87 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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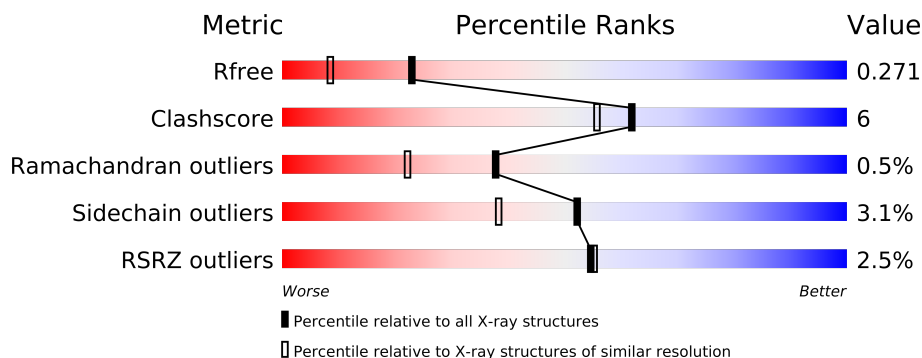
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.87 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	5260 (1.90-1.86)
Clashscore	79885	6268 (1.90-1.86)
Ramachandran outliers	78287	6195 (1.90-1.86)
Sidechain outliers	78261	6196 (1.90-1.86)
RSRZ outliers	66119	5262 (1.90-1.86)

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	436	
1	B	436	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7052 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.

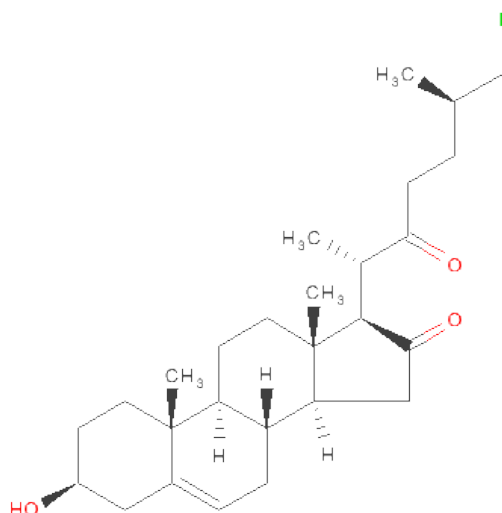
- Molecule 1 is a protein called Protein KES1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3348	2148	546	647	7			
1	B	425	Total	C	N	O	S	0	0	0
			3364	2159	554	644	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P35844
A	0	ASP	-	EXPRESSION TAG	UNP P35844
A	1	PRO	-	EXPRESSION TAG	UNP P35844
B	-1	MET	-	EXPRESSION TAG	UNP P35844
B	0	ASP	-	EXPRESSION TAG	UNP P35844
B	1	PRO	-	EXPRESSION TAG	UNP P35844

- Molecule 2 is (3BETA,9BETA,25R)-3-HYDROXY-26-iodocholest-5-ene-16,22-dione (three-letter code: L39) (formula: C<sub>27</sub>H<sub>41</sub>IO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 31	C 27	I 1	O 3	0	0
2	B	1	Total 31	C 27	I 1	O 3	0	0

- Molecule 3 is water.

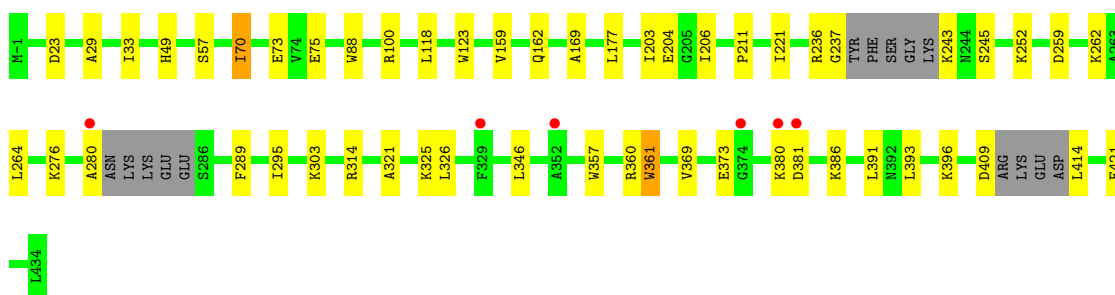
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	143	Total 143	O 143	0	0
3	B	135	Total 135	O 135	0	0

### 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.

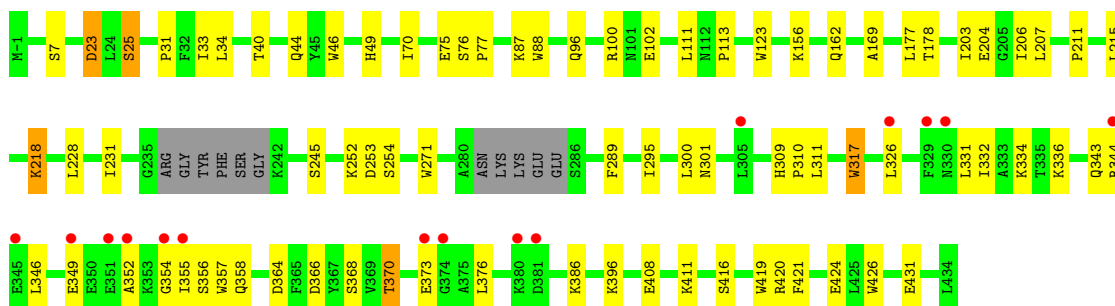
#### • Molecule 1: Protein KES1

Chain A: 



#### • Molecule 1: Protein KES1

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.12Å 65.40Å 82.31Å 96.56° 100.28° 95.91°	Depositor
Resolution (Å)	20.00 – 1.87 18.46 – 1.87	Depositor EDS
% Data completeness (in resolution range)	87.2 (20.00-1.87) 87.4 (18.46-1.87)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.214 , 0.271 0.214 , 0.271	Depositor DCC
$R_{free}$ test set	3700 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.5	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 43.8	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 81133 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7052	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: L39

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	1.01	5/3432 (0.1%)	0.98	6/4647 (0.1%)
1	B	1.03	8/3449 (0.2%)	0.96	4/4672 (0.1%)
All	All	1.02	13/6881 (0.2%)	0.97	10/9319 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	TRP	CD2-CE2	8.19	1.51	1.41
1	A	88	TRP	CD2-CE2	7.43	1.50	1.41
1	B	419	TRP	CD2-CE2	6.72	1.49	1.41
1	A	357	TRP	CD2-CE2	6.42	1.49	1.41
1	B	123	TRP	CD2-CE2	5.95	1.48	1.41
1	A	123	TRP	CD2-CE2	5.89	1.48	1.41
1	A	361	TRP	CD2-CE2	5.57	1.48	1.41
1	A	236	ARG	N-CA	5.54	1.57	1.46
1	B	426	TRP	CD2-CE2	5.37	1.47	1.41
1	B	7	SER	CB-OG	5.36	1.49	1.42
1	B	75	GLU	CD-OE2	5.21	1.31	1.25
1	B	317	TRP	CD2-CE2	5.03	1.47	1.41
1	B	46	TRP	CD2-CE2	5.02	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ARG	N-CA-C	7.74	131.89	111.00
1	A	409	ASP	CB-CG-OD1	6.59	124.23	118.30
1	B	23	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	360	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	156	LYS	CD-CE-NZ	-5.92	98.08	111.70
1	A	221	ILE	CG1-CB-CG2	-5.88	98.47	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	364	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	314	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	218	LYS	CD-CE-NZ	-5.12	99.92	111.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 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	3348	0	3250	26	0
1	B	3364	0	3269	49	0
2	A	31	0	41	4	0
2	B	31	0	41	3	0
3	A	143	0	0	5	0
3	B	135	0	0	7	0
All	All	7052	0	6601	76	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 6.

All (76) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:206:ILE:HD12	2:B:1001:L39:I1	2.35	0.96
1:B:206:ILE:CD1	2:B:1001:L39:I1	2.83	0.96
1:A:206:ILE:CD1	2:A:1001:L39:I1	2.91	0.88
1:B:206:ILE:HD11	2:B:1001:L39:I1	2.47	0.85
1:A:49:HIS:HE1	3:A:1207:HOH:O	1.62	0.82
1:A:206:ILE:HD12	2:A:1001:L39:I1	2.50	0.81
1:A:206:ILE:HD11	2:A:1001:L39:I1	2.53	0.79
1:B:252:LYS:HG3	3:B:1113:HOH:O	1.85	0.76
1:B:162:GLN:NE2	1:B:421:PHE:H	1.87	0.73
1:A:380:LYS:CB	3:A:1212:HOH:O	2.35	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:49:HIS:HE1	3:B:1153:HOH:O	1.73	0.72
1:A:381:ASP:N	1:A:381:ASP:OD2	2.18	0.72
1:B:76:SER:HB2	1:B:77:PRO:HD2	1.72	0.72
1:A:162:GLN:NE2	1:A:421:PHE:H	1.90	0.70
1:A:162:GLN:HE22	1:A:421:PHE:H	1.44	0.65
1:A:259:ASP:HB3	1:A:262:LYS:HD2	1.80	0.63
1:A:243:LYS:HB3	3:A:1218:HOH:O	1.99	0.63
1:A:280:ALA:O	3:A:1216:HOH:O	2.16	0.61
1:B:206:ILE:HG12	3:B:1147:HOH:O	1.99	0.61
1:B:253:ASP:HB2	3:B:1197:HOH:O	2.00	0.61
1:B:370:THR:HG22	1:B:370:THR:O	2.01	0.60
1:B:87:LYS:HE3	1:B:289:PHE:O	2.02	0.60
1:A:369:VAL:O	1:A:369:VAL:HG12	2.02	0.60
1:A:237:GLY:C	3:A:1228:HOH:O	2.40	0.58
1:B:111:LEU:O	1:B:113:PRO:HD3	2.04	0.58
1:B:162:GLN:HE22	1:B:420:ARG:HA	1.70	0.56
1:B:346:LEU:HD13	1:B:346:LEU:O	2.04	0.56
1:A:70:ILE:HD12	1:A:289:PHE:HD1	1.70	0.56
1:B:370:THR:O	1:B:370:THR:CG2	2.54	0.55
1:B:162:GLN:HE22	1:B:421:PHE:H	1.53	0.55
1:B:177:LEU:HD23	1:B:203:ILE:HD13	1.89	0.55
1:B:332:ILE:O	1:B:336:LYS:HB2	2.07	0.54
1:B:356:SER:C	1:B:358:GLN:H	2.11	0.54
1:A:396:LYS:HD3	1:A:414:LEU:HD23	1.90	0.54
1:B:44:GLN:NE2	1:B:300:LEU:HD22	2.24	0.53
1:B:23:ASP:OD1	1:B:25:SER:HB2	2.08	0.53
2:A:1001:L39:H30	2:A:1001:L39:H5	1.91	0.52
1:B:102:GLU:HG3	3:B:1183:HOH:O	2.11	0.51
1:B:349:GLU:O	1:B:352:ALA:HB3	2.11	0.51
1:B:178:THR:HG22	3:B:1115:HOH:O	2.10	0.51
1:B:49:HIS:CD2	1:B:295:ILE:HG22	2.45	0.50
1:A:252:LYS:HG2	1:A:264:LEU:HD21	1.93	0.50
1:B:31:PRO:HA	1:B:34:LEU:HG	1.94	0.49
1:B:40:THR:HG23	1:B:113:PRO:HB3	1.95	0.49
1:B:356:SER:O	1:B:358:GLN:N	2.45	0.49
1:A:321:ALA:O	1:A:325:LYS:HG3	2.13	0.48
1:B:424:GLU:CD	1:B:424:GLU:H	2.17	0.48
1:B:366:ASP:OD1	1:B:368:SER:HB2	2.13	0.48
1:B:331:LEU:HD12	1:B:334:LYS:HD3	1.97	0.47
1:A:169:ALA:HB1	1:A:177:LEU:HD11	1.96	0.47
1:B:311:LEU:HD23	1:B:343:GLN:HE22	1.80	0.47
1:A:118:LEU:HD22	1:A:361:TRP:CZ3	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:111:LEU:HD13	1:B:317:TRP:CD2	2.51	0.45
1:B:207:LEU:HD23	1:B:207:LEU:HA	1.75	0.45
1:B:49:HIS:HD2	3:B:1116:HOH:O	1.99	0.45
1:B:162:GLN:NE2	1:B:420:ARG:HA	2.30	0.44
1:B:44:GLN:NE2	1:B:300:LEU:CD2	2.80	0.44
1:A:204:GLU:O	1:A:211:PRO:HA	2.17	0.44
1:B:396:LYS:HA	1:B:416:SER:OG	2.17	0.44
1:B:311:LEU:CD2	1:B:343:GLN:HE22	2.30	0.44
1:A:369:VAL:O	1:A:369:VAL:CG1	2.66	0.43
1:A:57:SER:HB3	1:A:159:VAL:CG2	2.49	0.43
1:B:206:ILE:HD13	1:B:211:PRO:HB3	1.99	0.43
1:B:169:ALA:HB1	1:B:177:LEU:HD11	2.00	0.43
1:B:111:LEU:HD13	1:B:317:TRP:CE3	2.54	0.43
1:A:391:LEU:HD23	1:A:393:LEU:HB2	2.00	0.43
1:A:177:LEU:HD23	1:A:203:ILE:HD13	2.01	0.42
1:B:408:GLU:O	1:B:411:LYS:HG3	2.19	0.42
1:B:228:LEU:HD22	1:B:254:SER:HB2	2.00	0.42
1:B:355:ILE:HD13	1:B:431:GLU:OE2	2.20	0.42
1:B:218:LYS:HA	1:B:231:ILE:O	2.21	0.41
1:B:215:LEU:HD12	1:B:271:TRP:CE2	2.56	0.41
1:A:49:HIS:CD2	1:A:295:ILE:HG22	2.56	0.41
1:A:29:ALA:HB1	1:A:33:ILE:CG2	2.51	0.41
1:B:309:HIS:ND1	1:B:310:PRO:HD2	2.36	0.40
1:B:356:SER:C	1:B:358:GLN:N	2.73	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	414/436 (95%)	401 (97%)	12 (3%)	1 (0%)	56	43
1	B	419/436 (96%)	398 (95%)	18 (4%)	3 (1%)	30	14
All	All	833/872 (96%)	799 (96%)	30 (4%)	4 (0%)	38	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	357	TRP
1	B	373	GLU
1	B	354	GLY
1	A	373	GLU

### 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	367/391 (94%)	357 (97%)	10 (3%)	57	45
1	B	367/391 (94%)	354 (96%)	13 (4%)	48	32
All	All	734/782 (94%)	711 (97%)	23 (3%)	52	38

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ILE
1	A	73	GLU
1	A	75	GLU
1	A	100	ARG
1	A	245	SER
1	A	276	LYS
1	A	303	LYS
1	A	326	LEU
1	A	346	LEU
1	A	386	LYS
1	B	25	SER
1	B	33	ILE
1	B	70	ILE
1	B	96	GLN
1	B	100	ARG
1	B	204	GLU
1	B	245	SER
1	B	301	ASN
1	B	326	LEU
1	B	344	ARG

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Mol	Chain	Res	Type
1	B	370	THR
1	B	376	LEU
1	B	386	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	96	GLN
1	A	112	ASN
1	A	162	GLN
1	A	166	GLN
1	A	343	GLN
1	B	44	GLN
1	B	49	HIS
1	B	96	GLN
1	B	162	GLN
1	B	166	GLN
1	B	244	ASN
1	B	343	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 ⓘ

2 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	L39	A	1001	-	34,34,34	2.46	12 (35%)	53,53,53	1.98	13 (24%)
2	L39	B	1001	-	34,34,34	2.47	16 (47%)	53,53,53	1.77	14 (26%)

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	L39	A	1001	-	-	1/15/76/76	0/0/4/4
2	L39	B	1001	-	-	0/15/76/76	0/0/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	L39	C15-C16	7.55	1.63	1.51
2	B	1001	L39	O16-C16	6.94	1.33	1.21
2	B	1001	L39	C7-C8	5.01	1.63	1.53
2	A	1001	L39	O22-C22	4.61	1.29	1.21
2	A	1001	L39	C7-C6	-4.24	1.40	1.50
2	A	1001	L39	C11-C9	4.04	1.61	1.53
2	B	1001	L39	O22-C22	3.70	1.28	1.21
2	B	1001	L39	C7-C6	-3.68	1.42	1.50
2	A	1001	L39	O16-C16	3.67	1.28	1.21
2	B	1001	L39	C26-I1	3.53	2.22	2.15
2	A	1001	L39	C4-C5	-3.15	1.43	1.51
2	B	1001	L39	C8-C14	3.09	1.59	1.53
2	B	1001	L39	C18-C13	3.05	1.60	1.54
2	A	1001	L39	C13-C17	2.97	1.61	1.56
2	B	1001	L39	C11-C9	2.74	1.58	1.53
2	B	1001	L39	C1-C10	2.71	1.59	1.54
2	A	1001	L39	C6-C5	2.65	1.40	1.33
2	A	1001	L39	C8-C14	2.62	1.59	1.53
2	A	1001	L39	C1-C10	2.55	1.59	1.54
2	B	1001	L39	C4-C5	-2.48	1.45	1.51
2	B	1001	L39	C15-C16	2.40	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	L39	C13-C14	2.40	1.60	1.55
2	B	1001	L39	C17-C16	2.31	1.56	1.51
2	B	1001	L39	C13-C17	2.23	1.60	1.56
2	A	1001	L39	C10-C5	-2.22	1.47	1.52
2	B	1001	L39	C6-C5	2.17	1.38	1.33
2	B	1001	L39	C12-C11	2.12	1.58	1.53
2	B	1001	L39	C8-C9	-2.10	1.49	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	L39	C4-C5-C10	5.67	125.13	116.42
2	B	1001	L39	C11-C12-C13	-5.23	103.33	112.83
2	A	1001	L39	O16-C16-C15	-4.66	120.24	125.86
2	B	1001	L39	O16-C16-C15	-4.65	120.26	125.86
2	A	1001	L39	C4-C5-C6	-4.32	113.23	120.59
2	A	1001	L39	C21-C20-C22	-4.13	97.74	109.68
2	A	1001	L39	C1-C10-C9	-3.69	103.69	108.60
2	B	1001	L39	C24-C23-C22	-3.56	106.95	114.09
2	A	1001	L39	C23-C24-C25	-3.47	108.07	115.42
2	A	1001	L39	C15-C14-C13	3.42	105.89	104.25
2	A	1001	L39	C24-C23-C22	-3.31	107.45	114.09
2	B	1001	L39	C15-C14-C8	-3.29	112.18	119.93
2	B	1001	L39	C17-C13-C14	-2.68	95.43	100.03
2	B	1001	L39	C11-C9-C8	-2.67	107.87	111.73
2	B	1001	L39	C4-C5-C10	2.61	120.43	116.42
2	A	1001	L39	C23-C22-C20	-2.54	113.15	117.15
2	B	1001	L39	C4-C5-C6	-2.53	116.28	120.59
2	B	1001	L39	C21-C20-C22	-2.53	102.37	109.68
2	B	1001	L39	C2-C3-C4	2.48	114.97	110.31
2	A	1001	L39	C19-C10-C5	2.47	112.35	108.39
2	A	1001	L39	C13-C17-C20	-2.37	114.02	119.33
2	B	1001	L39	O16-C16-C17	2.35	128.98	125.15
2	A	1001	L39	O1-C3-C4	2.35	115.91	109.33
2	B	1001	L39	C15-C14-C13	2.34	105.37	104.25
2	B	1001	L39	O22-C22-C20	-2.13	116.46	120.43
2	A	1001	L39	C18-C13-C14	2.10	115.96	111.76
2	B	1001	L39	C12-C13-C14	-2.01	103.92	107.28

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	L39	C27-C25-C26-I1

There are no ring outliers.

## 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	422/436 (96%)	-0.06	6 (1%) 72 73	11, 20, 36, 46	0
1	B	425/436 (97%)	0.09	15 (3%) 42 42	9, 20, 45, 63	0
All	All	847/872 (97%)	0.01	21 (2%) 54 55	9, 20, 39, 63	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	ALA	4.3
1	B	355	ILE	4.3
1	A	329	PHE	3.9
1	B	354	GLY	3.8
1	B	380	LYS	3.4
1	B	345	GLU	3.2
1	B	326	LEU	3.1
1	B	349	GLU	3.1
1	B	329	PHE	2.9
1	A	381	ASP	2.7
1	A	380	LYS	2.5
1	B	330	ASN	2.4
1	B	374	GLY	2.4
1	B	351	GLU	2.4
1	B	373	GLU	2.4
1	A	352	ALA	2.3
1	B	344	ARG	2.3
1	B	305	LEU	2.2
1	A	374	GLY	2.2
1	A	280	ALA	2.1
1	B	381	ASP	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

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	L39	A	1001	31/31	0.15	1.56	11,16,67,214	0
2	L39	B	1001	31/31	0.12	0.58	11,14,44,96	0

## 6.5 Other polymers

There are no such residues in this entry.