wwPDB X-ray Structure Validation Summary Report (i)

Oct 30, 2023 – 05:44 PM JST

PDB ID	:	4XBT
Title	:	Crystal Structure of the L74F/M78F/L103V/L114V/I116V/F139V/L147V mutant of LEH complexed with (S,S)-cyclohexanediol
Authors	:	Kong, X.D.; Sun, Z.; Lonsdale, R.; Xu, J.H.; Reetz, M.T.; Zhou, J.
Deposited on	:	2014-12-17
Resolution	:	1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

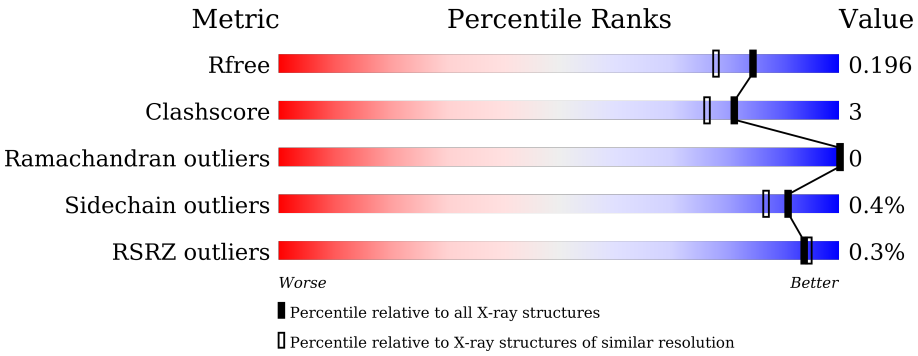
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 of 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	A	155	90% 6%
1	B	155	91% 7%
1	C	155	92%
1	D	155	90% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5578 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 Limonene-1,2-epoxide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	4	0
			1183	757	192	231	3			
1	B	144	Total	C	N	O	S	0	3	0
			1137	728	182	224	3			
1	C	149	Total	C	N	O	S	0	3	0
			1179	753	192	231	3			
1	D	145	Total	C	N	O	S	0	3	0
			1146	734	184	225	3			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP Q9ZAG3
A	-4	HIS	-	expression tag	UNP Q9ZAG3
A	-3	HIS	-	expression tag	UNP Q9ZAG3
A	-2	HIS	-	expression tag	UNP Q9ZAG3
A	-1	HIS	-	expression tag	UNP Q9ZAG3
A	0	HIS	-	expression tag	UNP Q9ZAG3
A	1	HIS	-	expression tag	UNP Q9ZAG3
A	74	PHE	LEU	engineered mutation	UNP Q9ZAG3
A	78	PHE	MET	engineered mutation	UNP Q9ZAG3
A	103	VAL	LEU	engineered mutation	UNP Q9ZAG3
A	114	VAL	LEU	engineered mutation	UNP Q9ZAG3
A	116	VAL	ILE	engineered mutation	UNP Q9ZAG3
A	139	VAL	PHE	engineered mutation	UNP Q9ZAG3
A	147	VAL	LEU	engineered mutation	UNP Q9ZAG3
B	-5	MET	-	initiating methionine	UNP Q9ZAG3
B	-4	HIS	-	expression tag	UNP Q9ZAG3
B	-3	HIS	-	expression tag	UNP Q9ZAG3
B	-2	HIS	-	expression tag	UNP Q9ZAG3
B	-1	HIS	-	expression tag	UNP Q9ZAG3
B	0	HIS	-	expression tag	UNP Q9ZAG3
B	1	HIS	-	expression tag	UNP Q9ZAG3

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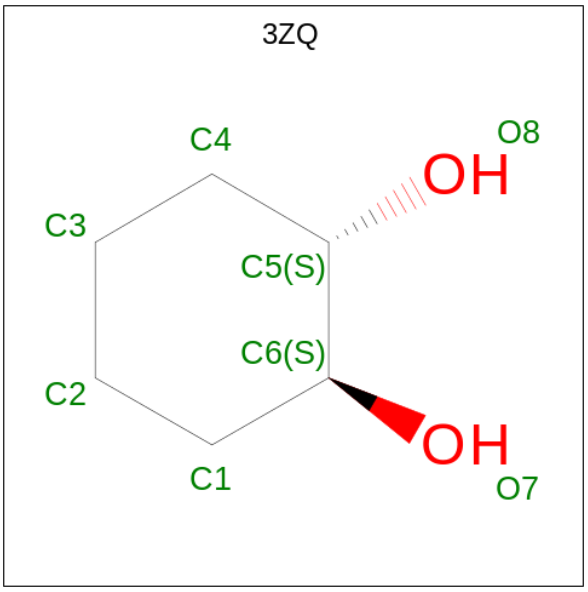
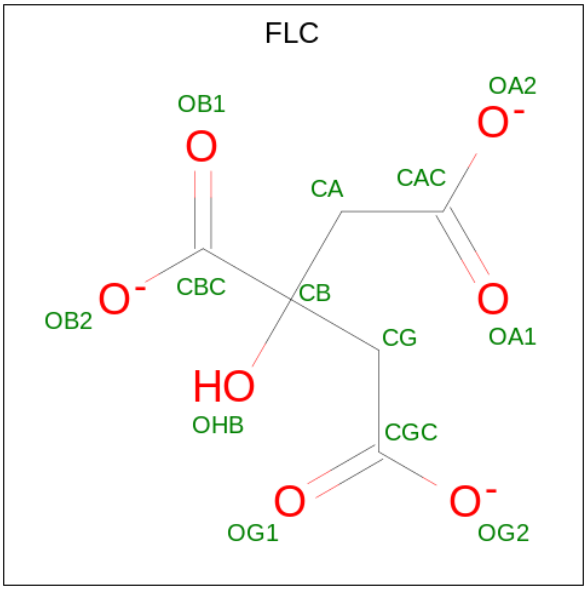
Chain	Residue	Modelled	Actual	Comment	Reference
B	74	PHE	LEU	engineered mutation	UNP Q9ZAG3
B	78	PHE	MET	engineered mutation	UNP Q9ZAG3
B	103	VAL	LEU	engineered mutation	UNP Q9ZAG3
B	114	VAL	LEU	engineered mutation	UNP Q9ZAG3
B	116	VAL	ILE	engineered mutation	UNP Q9ZAG3
B	139	VAL	PHE	engineered mutation	UNP Q9ZAG3
B	147	VAL	LEU	engineered mutation	UNP Q9ZAG3
C	-5	MET	-	initiating methionine	UNP Q9ZAG3
C	-4	HIS	-	expression tag	UNP Q9ZAG3
C	-3	HIS	-	expression tag	UNP Q9ZAG3
C	-2	HIS	-	expression tag	UNP Q9ZAG3
C	-1	HIS	-	expression tag	UNP Q9ZAG3
C	0	HIS	-	expression tag	UNP Q9ZAG3
C	1	HIS	-	expression tag	UNP Q9ZAG3
C	74	PHE	LEU	engineered mutation	UNP Q9ZAG3
C	78	PHE	MET	engineered mutation	UNP Q9ZAG3
C	103	VAL	LEU	engineered mutation	UNP Q9ZAG3
C	114	VAL	LEU	engineered mutation	UNP Q9ZAG3
C	116	VAL	ILE	engineered mutation	UNP Q9ZAG3
C	139	VAL	PHE	engineered mutation	UNP Q9ZAG3
C	147	VAL	LEU	engineered mutation	UNP Q9ZAG3
D	-5	MET	-	initiating methionine	UNP Q9ZAG3
D	-4	HIS	-	expression tag	UNP Q9ZAG3
D	-3	HIS	-	expression tag	UNP Q9ZAG3
D	-2	HIS	-	expression tag	UNP Q9ZAG3
D	-1	HIS	-	expression tag	UNP Q9ZAG3
D	0	HIS	-	expression tag	UNP Q9ZAG3
D	1	HIS	-	expression tag	UNP Q9ZAG3
D	74	PHE	LEU	engineered mutation	UNP Q9ZAG3
D	78	PHE	MET	engineered mutation	UNP Q9ZAG3
D	103	VAL	LEU	engineered mutation	UNP Q9ZAG3
D	114	VAL	LEU	engineered mutation	UNP Q9ZAG3
D	116	VAL	ILE	engineered mutation	UNP Q9ZAG3
D	139	VAL	PHE	engineered mutation	UNP Q9ZAG3
D	147	VAL	LEU	engineered mutation	UNP Q9ZAG3

- Molecule 2 is (1S,2S)-cyclohexane-1,2-diol (three-letter code: 3ZQ) (formula: $C_6H_{12}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 13 6 7	0	0
3	D	1	Total C O 13 6 7	0	0

- Molecule 4 is water.

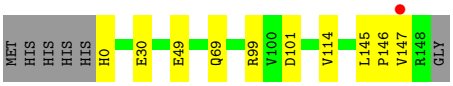
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	243	Total O 243 243	0	0
4	B	197	Total O 197 197	0	0
4	C	248	Total O 248 248	0	0
4	D	203	Total O 203 203	0	0

3 Residue-property plots (i)

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.

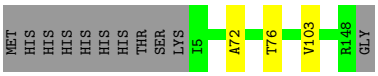
• Molecule 1: Limonene-1,2-epoxide hydrolase

Chain A:



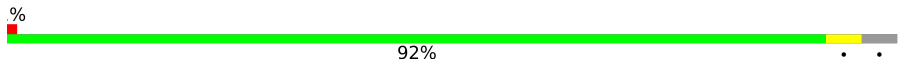
• Molecule 1: Limonene-1,2-epoxide hydrolase

Chain B:



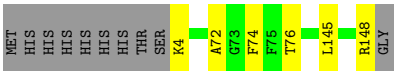
• Molecule 1: Limonene-1,2-epoxide hydrolase

Chain C:



• Molecule 1: Limonene-1,2-epoxide hydrolase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.74Å 66.45Å 91.55Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	33.68 – 1.70 33.68 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (33.68-1.70) 97.2 (33.68-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 1.70Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.156 , 0.195 0.156 , 0.196	Depositor DCC
R_{free} test set	3251 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.487 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5578	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 3ZQ, FLC

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	0.35	0/1222	0.53	0/1664
1	B	0.34	0/1171	0.53	0/1595
1	C	0.33	0/1215	0.53	0/1654
1	D	0.33	0/1180	0.51	0/1606
All	All	0.34	0/4788	0.52	0/6519

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1183	0	1160	7	0
1	B	1137	0	1109	3	0
1	C	1179	0	1151	6	0
1	D	1146	0	1122	6	0
2	A	8	0	12	0	0
2	C	8	0	12	2	0
3	B	13	0	5	3	0
3	D	13	0	5	2	0
4	A	243	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	197	0	0	1	0
4	C	248	0	0	4	0
4	D	203	0	0	2	0
All	All	5578	0	4576	24	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 3.

The worst 5 of 24 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:B:103[A]:VAL:HG11	3:B:201:FLC:HA2	1.70	0.74
3:B:201:FLC:OA2	4:B:399:HOH:O	2.05	0.74
1:A:49:GLU:OE1	4:A:301:HOH:O	2.08	0.71
1:A:30:GLU:OE1	4:A:424:HOH:O	2.13	0.66
3:D:201:FLC:OHB	3:D:201:FLC:OA2	2.13	0.65

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	151/155 (97%)	150 (99%)	1 (1%)	0	100	100
1	B	145/155 (94%)	145 (100%)	0	0	100	100
1	C	150/155 (97%)	150 (100%)	0	0	100	100
1	D	146/155 (94%)	146 (100%)	0	0	100	100
All	All	592/620 (96%)	591 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	129/130 (99%)	128 (99%)	1 (1%)	81 74
1	B	123/130 (95%)	123 (100%)	0	100 100
1	C	128/130 (98%)	127 (99%)	1 (1%)	81 74
1	D	124/130 (95%)	124 (100%)	0	100 100
All	All	504/520 (97%)	502 (100%)	2 (0%)	91 87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	C	99	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\| > 2$
3	FLC	D	201	-	12,12,12	1.36	1 (8%)	17,17,17	1.08	1 (5%)
2	3ZQ	A	201	-	8,8,8	0.60	0	10,10,10	3.03	2 (20%)
2	3ZQ	C	201	-	8,8,8	0.33	0	10,10,10	1.63	2 (20%)
3	FLC	B	201	-	12,12,12	1.49	2 (16%)	17,17,17	1.45	2 (11%)

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
3	FLC	D	201	-	-	9/16/16/16	-
2	3ZQ	A	201	-	-	-	0/1/1/1
2	3ZQ	C	201	-	-	-	0/1/1/1
3	FLC	B	201	-	-	11/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	FLC	CB-CBC	-2.71	1.50	1.53
3	B	201	FLC	CA-CB	-2.18	1.51	1.53
3	D	201	FLC	CB-CBC	-2.04	1.51	1.53

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	3ZQ	C4-C5-C6	-7.48	105.15	111.12
2	A	201	3ZQ	C1-C6-C5	-5.71	106.57	111.12
3	B	201	FLC	OB1-CBC-CB	-3.36	117.50	122.25
3	B	201	FLC	OB2-CBC-CB	3.28	118.75	113.05
2	C	201	3ZQ	C3-C4-C5	3.26	117.43	111.47

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	FLC	CA-CB-CG-CGC
3	B	201	FLC	CBC-CB-CG-CGC
3	B	201	FLC	OHB-CB-CG-CGC
3	D	201	FLC	CAC-CA-CB-CBC
3	D	201	FLC	CAC-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	201	FLC	2	0
2	C	201	3ZQ	2	0
3	B	201	FLC	3	0

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^{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	A	149/155 (96%)	-0.67	1 (0%) 87 90	14, 18, 30, 41	0
1	B	144/155 (92%)	-0.74	0 100 100	13, 19, 29, 48	0
1	C	149/155 (96%)	-0.68	1 (0%) 87 90	14, 18, 32, 43	0
1	D	145/155 (93%)	-0.74	0 100 100	13, 19, 29, 50	0
All	All	587/620 (94%)	-0.71	2 (0%) 94 94	13, 18, 30, 50	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	147	VAL	2.8
1	A	147	VAL	2.5

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	3ZQ	C	201	8/8	0.70	0.18	29,33,35,35	8
2	3ZQ	A	201	8/8	0.81	0.20	30,32,35,36	8
3	FLC	D	201	13/13	0.82	0.30	17,28,32,36	13
3	FLC	B	201	13/13	0.83	0.28	20,27,34,36	13

6.5 Other polymers (i)

There are no such residues in this entry.