



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 02:27 AM UTC

PDB ID : 3HPS / pdb_00003hps
Title : Crystal structure of Mycobacterium tuberculosis LeuA complexed with ke-toisocaproate (KIC)
Authors : Koon, N.; Squire, C.J.; Baker, E.N.
Deposited on : 2009-06-04
Resolution : 1.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

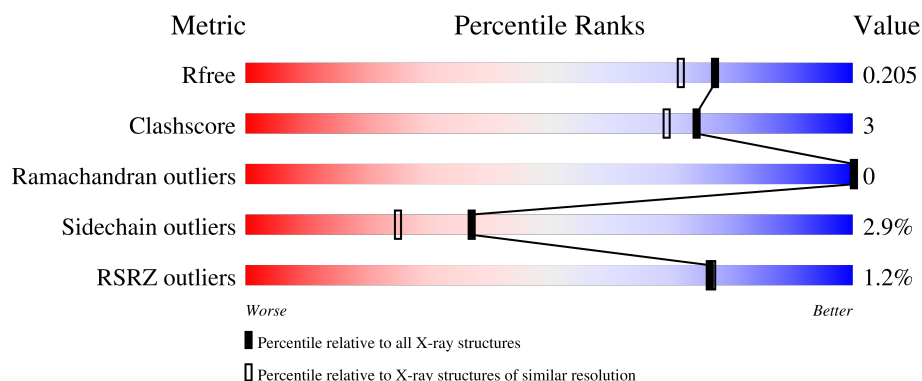
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

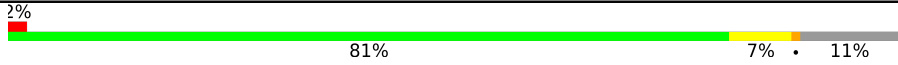
The reported resolution of this entry is 1.80 Å.

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	644	
1	B	644	

2 Entry composition [i](#)

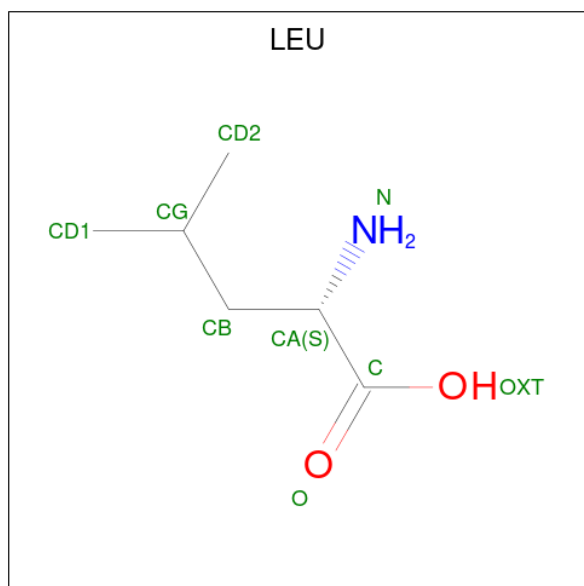
There are 6 unique types of molecules in this entry. The entry contains 9868 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-isopropylmalate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	4	0
			4369	2746	759	844	20			
1	B	577	Total	C	N	O	S	0	6	0
			4398	2765	769	844	20			

- Molecule 2 is LEUCINE (CCD ID: LEU) (formula: $C_6H_{13}NO_2$).

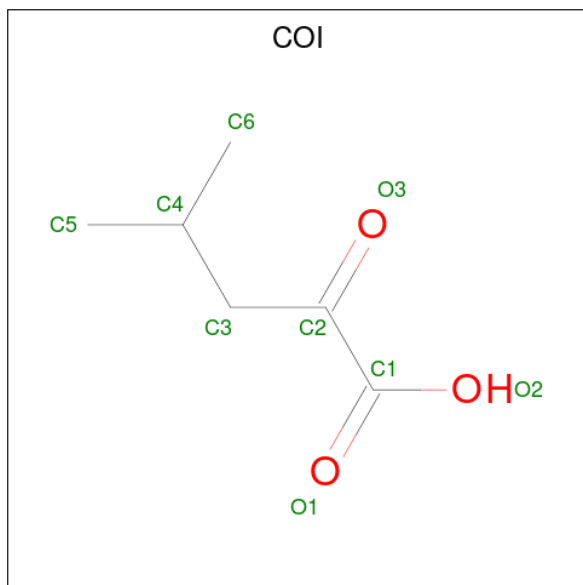


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	6	1	2		
2	B	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 2-OXO-4-METHYLPENTANOIC ACID (CCD ID: COI) (formula: $C_6H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	6	3		
4	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	552	Total	O	0	0
			552	552		
6	B	499	Total	O	0	0
			499	499		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.41Å 154.85Å 68.88Å 90.00° 97.65° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.00-1.80) 90.6 (50.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.158 , 0.205 0.158 , 0.205	Depositor DCC
R_{free} test set	4754 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9868	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GOL, COI

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	0.92	4/4476 (0.1%)	0.95	7/6114 (0.1%)
1	B	0.88	2/4510 (0.0%)	0.92	3/6154 (0.0%)
All	All	0.90	6/8986 (0.1%)	0.93	10/12268 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	25	PRO	CA-C	8.98	1.56	1.51
1	A	240	ALA	CA-CB	6.67	1.57	1.52
1	A	408	VAL	CA-CB	6.14	1.58	1.54
1	A	28	VAL	CA-CB	5.98	1.61	1.54
1	A	19	ILE	CA-CB	5.32	1.60	1.53
1	B	77	VAL	CA-CB	5.11	1.60	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	MET	CG-SD-CE	-9.96	78.99	100.90
1	A	492	VAL	CB-CA-C	7.32	117.95	110.70
1	B	492	VAL	CB-CA-C	7.31	117.93	110.70
1	A	254	THR	N-CA-C	-5.61	105.17	111.28
1	A	407	GLN	CA-C-N	-5.29	118.25	122.85
1	A	407	GLN	C-N-CA	-5.29	118.25	122.85
1	A	193	THR	N-CA-CB	-5.21	102.45	110.16
1	A	624	ALA	N-CA-C	5.17	112.87	108.22
1	A	193	THR	OG1-CB-CG2	5.07	119.44	109.30
1	B	492	VAL	N-CA-C	-5.06	108.35	113.20

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	4369	0	4175	33	0
1	B	4398	0	4223	23	0
2	A	9	0	10	0	0
2	B	9	0	10	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	9	0	9	0	0
4	B	9	0	9	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	552	0	0	12	0
6	B	499	0	0	5	0
All	All	9868	0	8452	54	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.

All (54) 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:27:ARG:HH11	1:A:27:ARG:HG3	1.15	1.09
1:A:193:THR:HG23	1:A:197:ARG:NH1	1.79	0.98
1:A:193:THR:HG23	1:A:197:ARG:HH12	1.25	0.98
1:B:114:PHE:HE2	6:B:964:HOH:O	1.66	0.79
1:A:26:PRO:HG3	6:A:987:HOH:O	1.85	0.74
1:B:426:ILE:HG21	1:B:461:ILE:HG21	1.69	0.71
1:A:488:TYR:CE1	1:A:641:ARG:HD3	2.26	0.70
1:A:27:ARG:HG3	1:A:27:ARG:NH1	1.93	0.70
1:A:373:THR:HB	6:A:798:HOH:O	1.91	0.69
1:A:520:ILE:HD12	1:A:547:PHE:HE1	1.56	0.68
1:B:500:GLN:HB2	1:B:514:ILE:HD11	1.75	0.68
1:A:193:THR:HG21	6:A:902:HOH:O	1.94	0.67
1:A:97:ARG:HD3	6:A:974:HOH:O	1.94	0.67
1:A:193:THR:CG2	1:A:197:ARG:HH12	2.06	0.63
1:A:104:ARG:HG3	6:A:1208:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LYS:HE2	6:A:678:HOH:O	2.00	0.61
1:B:463:LYS:NZ	6:B:947:HOH:O	2.35	0.59
1:A:56:ILE:HD13	1:A:265:ASP:OD2	2.02	0.59
1:B:475:VAL:HG22	1:B:479:GLU:HB2	1.85	0.59
1:B:37:ARG:NE	6:B:1086:HOH:O	2.33	0.56
1:A:190:ALA:HA	1:A:193:THR:HG22	1.89	0.55
1:B:114:PHE:CE2	6:B:964:HOH:O	2.47	0.55
6:A:723:HOH:O	1:B:19:ILE:HG12	2.08	0.52
1:B:373:THR:HG23	1:B:425:VAL:HG23	1.93	0.51
1:A:535:LEU:O	1:A:539:VAL:HG13	2.12	0.50
1:A:576:THR:HG23	1:A:614:THR:HA	1.94	0.49
1:B:514:ILE:HD13	1:B:515:THR:N	2.28	0.48
1:B:63:TRP:HB3	1:B:303:ALA:HA	1.94	0.48
1:A:21:LYS:CE	6:A:678:HOH:O	2.60	0.48
1:A:488:TYR:CD1	1:A:641:ARG:HD3	2.48	0.48
1:B:453:LEU:HD23	1:B:453:LEU:O	2.14	0.48
1:A:405:LEU:HD11	1:B:47:ARG:HG3	1.95	0.47
1:B:441:MET:HE1	1:B:481:TRP:HZ3	1.78	0.47
1:A:84:GLN:HG3	1:A:84:GLN:O	2.14	0.47
1:B:565:ALA:O	2:B:703:LEU:HD13	2.16	0.46
1:A:163:ARG:NH1	6:A:737:HOH:O	2.49	0.45
1:A:114:PHE:HE2	6:A:1012:HOH:O	1.99	0.44
1:B:499:ARG:HD2	6:B:661:HOH:O	2.18	0.43
1:A:72:PRO:HG3	1:A:308:ILE:HD12	2.00	0.43
1:A:18:THR:HA	1:B:344:ASN:HD22	1.84	0.42
1:B:514:ILE:HD13	1:B:515:THR:C	2.44	0.42
1:B:426:ILE:HG21	1:B:461:ILE:CG2	2.44	0.42
1:A:450:PRO:O	1:A:454:GLN:HG3	2.19	0.41
1:B:173:SER:O	1:B:177:ARG:HG3	2.20	0.41
1:A:27:ARG:CG	6:A:1000:HOH:O	2.68	0.41
1:A:199:CYS:HB3	1:A:213:PHE:CE2	2.55	0.41
1:A:173:SER:O	1:A:177:ARG:HG3	2.21	0.41
1:B:22:PRO:HB3	1:B:39:SER:HA	2.01	0.41
1:A:27:ARG:HA	1:A:27:ARG:HD2	1.74	0.40
1:A:426:ILE:HD12	6:A:856:HOH:O	2.20	0.40
1:B:567:ALA:HB2	2:B:703:LEU:HD12	2.03	0.40
1:B:441:MET:HE1	1:B:481:TRP:CZ3	2.55	0.40
1:A:80:ARG:HD2	1:A:80:ARG:C	2.45	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	571/644 (89%)	555 (97%)	16 (3%)	0	100	100
1	B	573/644 (89%)	562 (98%)	11 (2%)	0	100	100
All	All	1144/1288 (89%)	1117 (98%)	27 (2%)	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	452/520 (87%)	436 (96%)	16 (4%)	32	19
1	B	456/520 (88%)	448 (98%)	8 (2%)	51	43
All	All	908/1040 (87%)	884 (97%)	24 (3%)	37	28

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

Mol	Chain	Res	Type
1	A	27	ARG
1	A	87	ILE
1	A	193	THR
1	A	365	PRO
1	A	392	LEU
1	A	401	VAL
1	A	404	MET
1	A	411	LEU

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Mol	Chain	Res	Type
1	A	426	ILE
1	A	475	VAL
1	A	492	VAL
1	A	515	THR
1	A	525	THR
1	A	539	VAL
1	A	552	LEU
1	A	641	ARG
1	B	274	LEU
1	B	282	LEU
1	B	358	LEU
1	B	376	SER
1	B	387	LEU
1	B	492	VAL
1	B	495	LEU
1	B	514	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	210	GLN
1	A	273	ASN
1	A	521	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
4	COI	B	702	3	8,8,8	1.73	1 (12%)	10,10,10	1.21	1 (10%)
5	GOL	A	704	-	5,5,5	0.40	0	5,5,5	0.66	0
2	LEU	A	703	-	6,8,8	1.09	1 (16%)	5,10,10	1.76	2 (40%)
2	LEU	B	703	-	6,8,8	1.11	1 (16%)	5,10,10	1.34	0
4	COI	A	702	3	8,8,8	1.61	1 (12%)	10,10,10	1.41	1 (10%)
5	GOL	B	704	-	5,5,5	0.47	0	5,5,5	0.59	0

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
4	COI	B	702	3	-	2/8/8/8	-
5	GOL	A	704	-	-	0/4/4/4	-
2	LEU	A	703	-	-	5/8/8/8	-
2	LEU	B	703	-	-	5/8/8/8	-
4	COI	A	702	3	-	3/8/8/8	-
5	GOL	B	704	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	COI	C2-C1	-4.41	1.46	1.53
4	A	702	COI	C2-C1	-3.93	1.47	1.53
2	B	703	LEU	OXT-C	-2.48	1.22	1.30
2	A	703	LEU	OXT-C	-2.42	1.22	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	COI	C3-C2-C1	3.49	122.11	115.89
2	A	703	LEU	OXT-C-O	-2.84	117.64	124.08
4	B	702	COI	C3-C2-C1	2.50	120.34	115.89
2	A	703	LEU	CD1-CG-CB	2.47	119.96	111.08

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	703	LEU	N-CA-CB-CG
2	B	703	LEU	N-CA-CB-CG
4	B	702	COI	C2-C3-C4-C5
2	A	703	LEU	CA-CB-CG-CD1
2	B	703	LEU	CA-CB-CG-CD1
4	A	702	COI	C2-C3-C4-C5
4	A	702	COI	C1-C2-C3-C4
2	A	703	LEU	C-CA-CB-CG
2	A	703	LEU	CA-CB-CG-CD2
2	B	703	LEU	C-CA-CB-CG
4	A	702	COI	O3-C2-C3-C4
2	B	703	LEU	CA-CB-CG-CD2
4	B	702	COI	C1-C2-C3-C4
2	A	703	LEU	OXT-C-CA-N
2	B	703	LEU	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	703	LEU	2	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 [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, 95th 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	575/644 (89%)	-0.43	10 (1%) 69 69	7, 16, 31, 47	4 (0%)
1	B	577/644 (89%)	-0.47	4 (0%) 84 85	7, 16, 31, 47	6 (1%)
All	All	1152/1288 (89%)	-0.45	14 (1%) 76 77	7, 16, 31, 47	10 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	579	SER	4.1
1	A	464	ILE	3.7
1	A	460	VAL	3.5
1	A	426	ILE	3.1
1	A	28	VAL	2.5
1	A	434	LYS	2.4
1	A	458	SER	2.3
1	B	463	LYS	2.2
1	A	18	THR	2.2
1	B	614	THR	2.2
1	B	18	THR	2.1
1	A	614	THR	2.0
1	A	396	ALA	2.0
1	A	435	GLY	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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
4	COI	B	702	9/9	0.93	0.10	17,24,26,27	0
4	COI	A	702	9/9	0.95	0.07	20,21,23,24	0
2	LEU	A	703	9/9	0.96	0.06	12,12,14,15	0
5	GOL	A	704	6/6	0.96	0.05	14,15,16,17	0
2	LEU	B	703	9/9	0.97	0.05	11,12,13,15	0
5	GOL	B	704	6/6	0.97	0.06	11,14,16,16	0
3	ZN	A	701	1/1	1.00	0.03	18,18,18,18	0
3	ZN	B	701	1/1	1.00	0.03	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.