Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 05:52 pm BST

PDB ID	:	3BZM
Title	:	Crystal Structure of Open form of Menaquinone-Specific Isochorismate Synthase, MenF
Authors	:	Parsons, J.F.; Shi, K.M.; Ladner, J.E.
Deposited on	:	2008-01-18
Resolution	:	1.95 Å(reported)

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

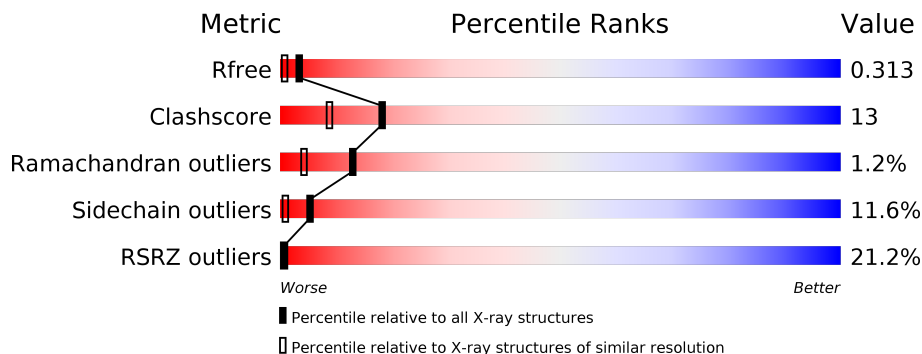|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.95 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	Percentile Ranks	Value
Rfree		0.313
Clashscore		13
Ramachandran outliers		1.2%
Sidechain outliers		11.6%
RSRZ outliers		21.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	A	431	21% · 69% · 23% · 5% ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3546 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 Menaquinone-specific isochorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	3	0
			3432	2163	625	631	13			

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
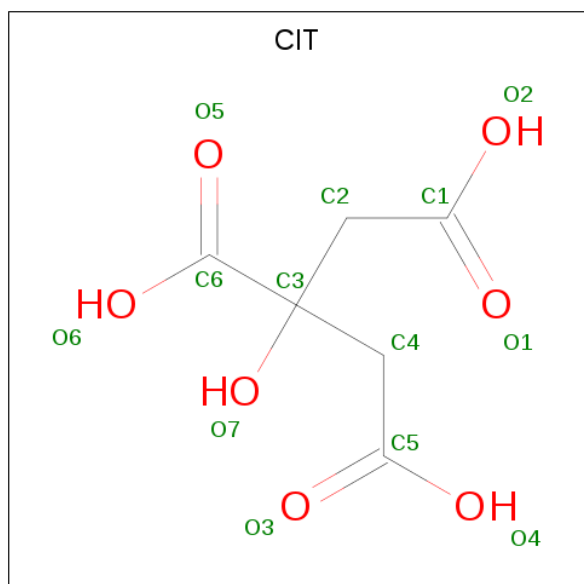
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total	O	0	0
			101	101		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Menaquinone-specific isochorismate synthase

Chain A:
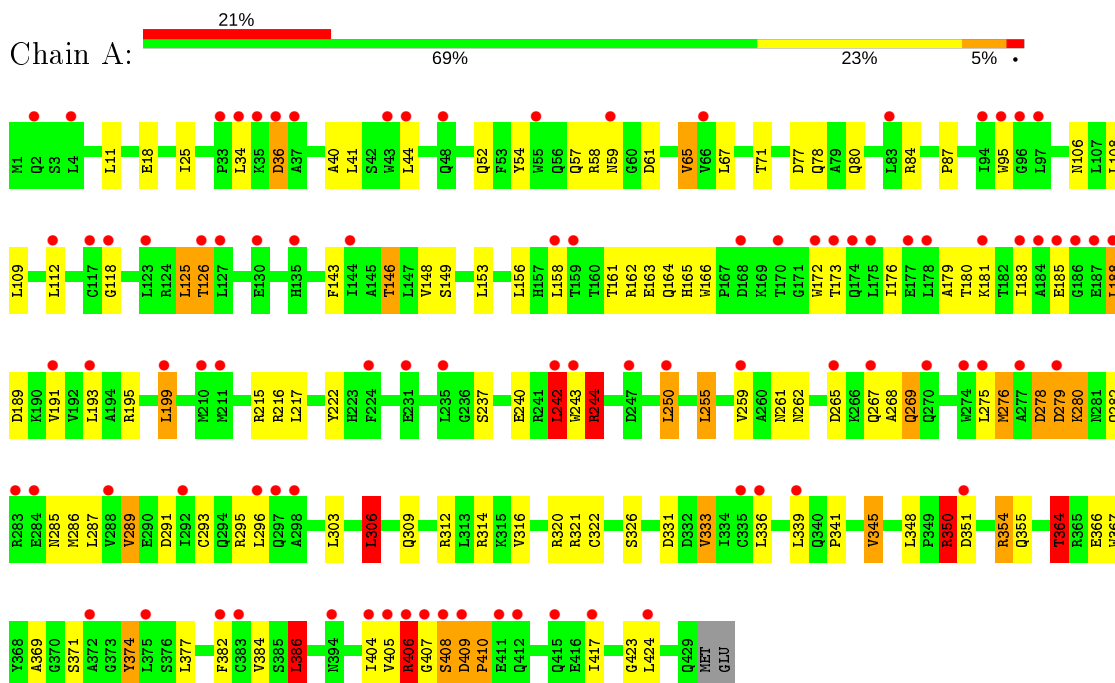
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	72.37Å　　72.37Å　　164.01Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	19.67　–　1.95 19.67　–　1.95	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.67-1.95) 96.4 (19.67-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.58 (at 1.94Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.245　,　0.308 0.254　,　0.313	Depositor DCC
R_{free} test set	1840 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	45.3	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.9	EDS
L-test for twinning[2]	$<\lvert L \rvert> = 0.53, <L^2> = 0.37$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3546	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<\lvert L \rvert>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.95	1/3515 (0.0%)	1.03	20/4773 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	TYR	CD2-CE2	5.50	1.47	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	GLU	N-CA-C	10.06	138.17	111.00
1	A	244	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	189	ASP	N-CA-CB	-9.71	93.12	110.60
1	A	185	GLU	CB-CA-C	-8.05	94.31	110.40
1	A	350	ARG	CB-CA-C	-8.02	94.35	110.40
1	A	188	LEU	CB-CA-C	-6.76	97.36	110.20
1	A	306	LEU	CA-CB-CG	6.31	129.82	115.30
1	A	34	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	244	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	250	LEU	CA-CB-CG	6.07	129.26	115.30
1	A	350	ARG	N-CA-C	5.88	126.87	111.00
1	A	306	LEU	CB-CG-CD2	5.83	120.91	111.00
1	A	364	THR	CB-CA-C	-5.75	96.08	111.60
1	A	331	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	58	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	386	LEU	CB-CG-CD1	5.58	120.48	111.00
1	A	11	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	189	ASP	N-CA-C	-5.29	96.72	111.00
1	A	242	LEU	CA-CB-CG	5.07	126.95	115.30
1	A	354	ARG	NE-CZ-NH1	5.03	122.82	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	A	3432	0	3420	92	0
2	A	13	0	5	1	0
3	A	101	0	0	7	0
All	All	3546	0	3425	92	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 13.

All (92) 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:77[B]:ASP:OD1	3:A:507:HOH:O	1.56	1.18
1:A:405:VAL:O	1:A:406:ARG:HB3	1.54	1.07
1:A:408:SER:O	1:A:409:ASP:HB3	1.60	1.00
1:A:406:ARG:HG3	1:A:407:GLY:N	1.78	0.98
1:A:172:TRP:O	1:A:176:ILE:HG12	1.70	0.92
1:A:255:LEU:HD23	1:A:320:ARG:HB2	1.58	0.85
1:A:179:ALA:O	1:A:183:ILE:HG12	1.78	0.83
1:A:350:ARG:O	1:A:354:ARG:HG3	1.81	0.81
1:A:276:MET:O	1:A:282:GLN:NE2	2.14	0.80
1:A:384:VAL:HG12	1:A:386:LEU:HD13	1.66	0.78
1:A:406:ARG:HG3	1:A:407:GLY:H	1.47	0.78
1:A:408:SER:O	1:A:409:ASP:CB	2.30	0.77
1:A:52:GLN:HG2	1:A:67:LEU:CD1	2.17	0.75
1:A:80:GLN:NE2	1:A:333:VAL:HG13	2.05	0.72
1:A:163:GLU:HG3	1:A:199:LEU:HD12	1.74	0.70
1:A:285:ASN:OD1	1:A:321:ARG:HD2	1.93	0.69
1:A:261:ASN:OD1	1:A:312:ARG:HD2	1.94	0.68
1:A:126:THR:HG23	3:A:439:HOH:O	1.92	0.67
1:A:180:THR:HA	1:A:183:ILE:HG12	1.75	0.67
1:A:164:GLN:HG2	1:A:166:TRP:CZ2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:HG2	1:A:163:GLU:N	2.15	0.61
1:A:279:ASP:O	1:A:280:LYS:HB2	1.99	0.61
1:A:193:LEU:HD12	1:A:404:ILE:HG13	1.82	0.60
1:A:364:THR:HG22	1:A:366:GLU:H	1.67	0.60
1:A:183:ILE:HD13	1:A:188:LEU:HD23	1.82	0.59
1:A:84:ARG:O	1:A:87:PRO:HD3	2.02	0.59
1:A:217:LEU:HD13	1:A:314:ARG:NH2	2.17	0.59
1:A:173:THR:HG23	1:A:410:PRO:HG3	1.86	0.58
1:A:162:ARG:NH2	1:A:164:GLN:OE1	2.34	0.56
1:A:291:ASP:OD2	1:A:295:ARG:NH1	2.36	0.56
1:A:240:GLU:HB2	1:A:255:LEU:HD12	1.88	0.56
1:A:148:VAL:HG22	1:A:149:SER:H	1.70	0.56
1:A:405:VAL:O	1:A:406:ARG:CB	2.39	0.55
1:A:244:ARG:HD2	3:A:468:HOH:O	2.08	0.54
1:A:222:TYR:O	1:A:237:SER:HA	2.08	0.54
1:A:80:GLN:NE2	1:A:333:VAL:CG1	2.72	0.53
1:A:409:ASP:O	1:A:410:PRO:C	2.47	0.52
1:A:279:ASP:O	1:A:280:LYS:CB	2.57	0.52
1:A:65:VAL:O	1:A:65:VAL:HG23	2.10	0.52
1:A:180:THR:HA	1:A:183:ILE:CG1	2.38	0.51
1:A:242:LEU:HD13	1:A:243:TRP:CE3	2.45	0.51
1:A:276:MET:C	1:A:282:GLN:HE21	2.13	0.51
1:A:36:ASP:OD1	1:A:36:ASP:N	2.44	0.51
1:A:162:ARG:HG2	1:A:163:GLU:H	1.76	0.51
1:A:188:LEU:HD21	1:A:191:VAL:HB	1.92	0.51
1:A:44:LEU:HG	1:A:65:VAL:HB	1.93	0.51
1:A:80:GLN:HE22	1:A:333:VAL:HG13	1.77	0.50
1:A:259:VAL:HG22	1:A:275:LEU:HD22	1.94	0.50
1:A:371:SER:HB2	1:A:382:PHE:HB3	1.94	0.50
1:A:293:CYS:HB3	1:A:303:LEU:HD13	1.94	0.49
1:A:262:ASN:O	1:A:268:ALA:HB2	2.12	0.48
1:A:59:ASN:ND2	2:A:432:CIT:H41	2.28	0.48
1:A:163:GLU:HG3	1:A:199:LEU:CD1	2.41	0.48
1:A:54:TYR:HD1	1:A:65:VAL:CG1	2.26	0.48
1:A:384:VAL:CG1	1:A:386:LEU:HD13	2.41	0.48
1:A:52:GLN:HG2	1:A:67:LEU:HD12	1.94	0.47
1:A:261:ASN:OD1	1:A:312:ARG:CD	2.61	0.47
1:A:351:ASP:O	1:A:355:GLN:HG3	2.14	0.47
1:A:406:ARG:CG	1:A:407:GLY:H	2.24	0.47
1:A:143:PHE:O	1:A:146:THR:HB	2.15	0.47
1:A:148:VAL:HG22	1:A:149:SER:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:HB2	1:A:367:TRP:CH2	2.50	0.47
1:A:286:MET:HA	1:A:289:VAL:HG13	1.95	0.46
1:A:306:LEU:HG	1:A:322:CYS:HB2	1.97	0.46
1:A:41:LEU:HD12	1:A:215:ARG:CZ	2.45	0.46
1:A:350:ARG:O	1:A:354:ARG:CG	2.59	0.46
1:A:409:ASP:HA	1:A:410:PRO:HD2	1.65	0.46
1:A:54:TYR:HD1	1:A:65:VAL:HG12	1.82	0.45
1:A:244:ARG:CD	3:A:468:HOH:O	2.65	0.45
1:A:112:LEU:HD13	1:A:125:LEU:HD12	1.98	0.45
1:A:366:GLU:HG2	1:A:367:TRP:CD1	2.51	0.45
1:A:242:LEU:HD13	1:A:243:TRP:CZ3	2.53	0.44
1:A:406:ARG:CG	1:A:407:GLY:N	2.63	0.44
1:A:296:LEU:HD11	1:A:339:LEU:HD21	1.98	0.44
1:A:95:TRP:CE3	1:A:374:TYR:HB3	2.52	0.44
1:A:350:ARG:HG2	3:A:505:HOH:O	2.18	0.43
1:A:57:GLN:OE1	1:A:59:ASN:HB2	2.18	0.43
1:A:265:ASP:O	1:A:269:GLN:HB3	2.19	0.42
1:A:40:ALA:HB1	1:A:65:VAL:HG21	2.01	0.42
1:A:345:VAL:HG21	1:A:369:ALA:HB1	2.01	0.42
1:A:61:ASP:O	1:A:118:GLY:N	2.53	0.42
1:A:40:ALA:HB1	1:A:65:VAL:CG2	2.50	0.42
1:A:278:ASP:OD2	1:A:278:ASP:C	2.58	0.42
1:A:195:ARG:CB	1:A:417:ILE:HD12	2.50	0.42
1:A:216:ARG:NE	3:A:494:HOH:O	2.23	0.42
1:A:366:GLU:HG2	1:A:367:TRP:H	1.84	0.41
1:A:341:PRO:CG	1:A:354:ARG:HD3	2.49	0.41
1:A:165:HIS:ND1	1:A:195:ARG:HD2	2.36	0.41
1:A:423:GLY:HA3	3:A:532:HOH:O	2.20	0.40
1:A:172:TRP:CE2	1:A:176:ILE:HD11	2.55	0.40
1:A:195:ARG:HB3	1:A:417:ILE: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	Percentiles
1	A	430/431 (100%)	403 (94%)	22 (5%)	5 (1%)	13 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	LYS
1	A	406	ARG
1	A	408	SER
1	A	410	PRO
1	A	409	ASP

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	Percentiles
1	A	364/363 (100%)	322 (88%)	42 (12%)	5 1

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	25	ILE
1	A	36	ASP
1	A	65	VAL
1	A	71	THR
1	A	78	GLN
1	A	108	LEU
1	A	109	LEU
1	A	125	LEU
1	A	126	THR
1	A	146	THR
1	A	153	LEU
1	A	156	LEU
1	A	158	LEU

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Mol	Chain	Res	Type
1	A	161	THR
1	A	181	LYS
1	A	199	LEU
1	A	242	LEU
1	A	244	ARG
1	A	250	LEU
1	A	255	LEU
1	A	267	GLN
1	A	269	GLN
1	A	276	MET
1	A	278	ASP
1	A	279	ASP
1	A	287	LEU
1	A	289	VAL
1	A	306	LEU
1	A	309	GLN
1	A	316	VAL
1	A	326	SER
1	A	333	VAL
1	A	336	LEU
1	A	345	VAL
1	A	348	LEU
1	A	350	ARG
1	A	364	THR
1	A	377	LEU
1	A	386	LEU
1	A	406	ARG
1	A	424	LEU

Some 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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	CIT	A	432	-	3,12,12	1.54	0	3,17,17	3.62	1 (33%)

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	CIT	A	432	-	-	4/6/16/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	432	CIT	C3-C2-C1	-6.18	105.09	114.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	432	CIT	C2-C3-C4-C5
2	A	432	CIT	O7-C3-C4-C5
2	A	432	CIT	C6-C3-C4-C5
2	A	432	CIT	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	432	CIT	1	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	429/431 (99%)	1.15	91 (21%)	0	1	32, 46, 73, 81	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	ALA	7.6
1	A	184	ALA	6.4
1	A	405	VAL	5.8
1	A	36	ASP	5.1
1	A	173	THR	4.7
1	A	351	ASP	4.6
1	A	277	ALA	4.6
1	A	118	GLY	4.6
1	A	187	GLU	4.2
1	A	185	GLU	4.2
1	A	170	THR	4.2
1	A	242	LEU	4.2
1	A	406	ARG	4.2
1	A	178	LEU	4.1
1	A	34	LEU	4.0
1	A	339	LEU	3.9
1	A	283	ARG	3.9
1	A	382	PHE	3.9
1	A	279	ASP	3.8
1	A	412	GLN	3.8
1	A	35	LYS	3.8
1	A	411	GLU	3.7
1	A	177	GLU	3.7
1	A	175	LEU	3.7
1	A	188	LEU	3.6
1	A	407	GLY	3.6
1	A	270	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	130	GLU	3.5
1	A	243	TRP	3.5
1	A	274	TRP	3.5
1	A	168	ASP	3.5
1	A	267	GLN	3.4
1	A	112	LEU	3.4
1	A	372	ALA	3.3
1	A	296	LEU	3.3
1	A	375	LEU	3.3
1	A	174	GLN	3.2
1	A	335	CYS	3.2
1	A	409	ASP	3.2
1	A	123	LEU	3.2
1	A	181	LYS	3.2
1	A	292	ILE	3.2
1	A	336	LEU	3.1
1	A	66	VAL	3.0
1	A	117	CYS	3.0
1	A	415	GLN	2.9
1	A	284	GLU	2.9
1	A	183	ILE	2.9
1	A	297	GLN	2.8
1	A	210	MET	2.8
1	A	127	LEU	2.8
1	A	247	ASP	2.7
1	A	235	LEU	2.7
1	A	159	THR	2.7
1	A	94	ILE	2.6
1	A	231	GLU	2.6
1	A	275	LEU	2.5
1	A	44	LEU	2.5
1	A	95	TRP	2.5
1	A	33	PRO	2.4
1	A	408	SER	2.4
1	A	193	LEU	2.4
1	A	259	VAL	2.4
1	A	158	LEU	2.4
1	A	186	GLY	2.4
1	A	250	LEU	2.3
1	A	2	GLN	2.3
1	A	48	GLN	2.3
1	A	144	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	298	ALA	2.3
1	A	126	THR	2.3
1	A	59	ASN	2.3
1	A	265	ASP	2.2
1	A	83	LEU	2.2
1	A	97	LEU	2.2
1	A	55	TRP	2.2
1	A	417	ILE	2.2
1	A	43	TRP	2.1
1	A	394	ASN	2.1
1	A	172	TRP	2.1
1	A	96	GLY	2.1
1	A	383	CYS	2.1
1	A	288	VAL	2.1
1	A	404	ILE	2.1
1	A	211	MET	2.0
1	A	135	HIS	2.0
1	A	224	PHE	2.0
1	A	4	LEU	2.0
1	A	191	VAL	2.0
1	A	199	LEU	2.0
1	A	424	LEU	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 carbohydrates 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
2	CIT	A	432	13/13	0.78	0.19	56,61,67,68	0

6.5 Other polymers (i)

There are no such residues in this entry.