



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 10:50 AM EDT

PDB ID : 3FGP
Title : 2.05 a Crystal Structure of CysM from Mycobacterium Tuberculosis - Open and Closed Conformations
Authors : Agren, D.; Schnell, R.; Schneider, G.
Deposited on : 2008-12-08
Resolution : 2.05 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.23.2
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) : 2.23.2

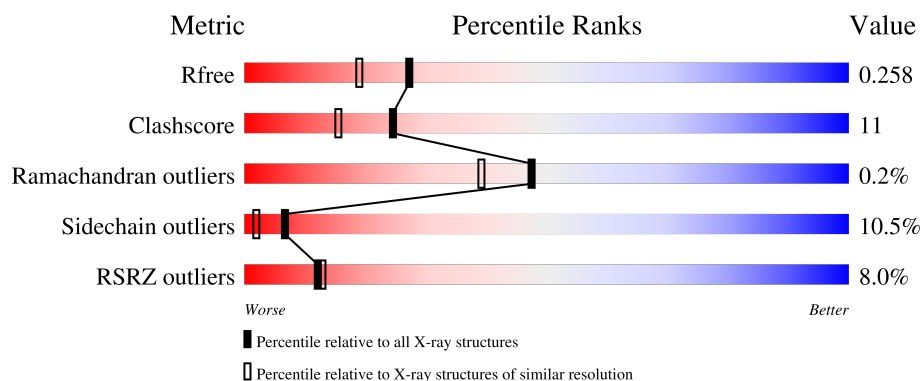
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	326	<div> <div>8%</div> <div>74%</div> <div>18%</div> <div>• •</div> </div>
1	B	326	<div> <div>8%</div> <div>73%</div> <div>21%</div> <div>5% •</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5125 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 Cysteine synthase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	P	S	0	0	0
			2354	1474	417	454	1	8			
1	B	324	Total	C	N	O	P	S	0	0	0
			2447	1533	433	471	1	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P63873
A	-1	SER	-	expression tag	UNP P63873
A	0	HIS	-	expression tag	UNP P63873
A	2	ALA	THR	engineered mutation	UNP P63873
B	-2	GLY	-	expression tag	UNP P63873
B	-1	SER	-	expression tag	UNP P63873
B	0	HIS	-	expression tag	UNP P63873
B	2	ALA	THR	engineered mutation	UNP P63873

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	191	Total	O	0	0
			191	191		
2	B	133	Total	O	0	0
			133	133		

- Molecule 1: Cysteine synthase B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.93Å 89.14Å 99.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.05 49.68 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.05) 97.7 (49.68-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.247 0.218 , 0.258	Depositor DCC
R_{free} test set	2092 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5125	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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: LLP

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	0.62	0/2374	0.75	1/3230 (0.0%)
1	B	0.57	0/2470	0.76	1/3360 (0.0%)
All	All	0.60	0/4844	0.75	2/6590 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	281	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	44	ARG	NE-CZ-NH1	5.11	122.85	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	281	LEU	Peptide

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	2354	0	2318	41	0
1	B	2447	0	2408	64	0
2	A	191	0	0	6	0
2	B	133	0	0	6	0
All	All	5125	0	4726	104	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 11.

All (104) 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:188:THR:O	1:A:192:THR:HG23	1.57	1.02
1:A:22:LEU:HD21	1:A:270:LEU:HD21	1.53	0.90
1:B:102:PRO:O	1:B:105:THR:HG22	1.78	0.84
1:B:25:ARG:NH2	1:B:281:LEU:HD11	1.93	0.83
1:B:125:ALA:CB	1:B:130:ASN:HA	2.12	0.79
1:A:73:THR:HG23	2:A:479:HOH:O	1.83	0.78
1:A:161:HIS:HB3	1:A:192:THR:HG22	1.66	0.78
1:B:309:SER:HB2	2:B:413:HOH:O	1.82	0.78
1:A:33:PRO:HB2	1:A:286:ARG:HB3	1.65	0.77
1:A:25:ARG:NE	2:A:499:HOH:O	2.18	0.76
1:B:303:THR:HG22	1:B:316:ALA:HB1	1.67	0.75
1:A:300:TYR:O	1:A:303:THR:HG22	1.86	0.74
1:B:25:ARG:HH22	1:B:281:LEU:HD11	1.51	0.74
1:A:100:VAL:HG11	1:A:135:THR:HG23	1.70	0.73
1:A:207:ALA:HB3	1:A:239:ARG:HG3	1.69	0.72
1:B:222:MET:HE2	1:B:226:PHE:CD1	2.24	0.72
1:A:73:THR:HG21	2:A:505:HOH:O	1.88	0.72
1:B:158:THR:HG21	2:B:454:HOH:O	1.91	0.71
1:B:133:VAL:HG21	1:B:220:ARG:HD3	1.73	0.70
1:A:123:SER:HB3	1:A:135:THR:HG21	1.76	0.66
1:B:222:MET:CE	1:B:226:PHE:CD1	2.79	0.66
1:B:254:LEU:HD22	1:B:270:LEU:HD21	1.77	0.66
1:B:152:TYR:OH	1:B:219:LEU:HD11	1.96	0.66
1:A:74:ILE:HG21	1:A:149:LEU:HD22	1.77	0.65
1:B:17:VAL:O	1:B:17:VAL:HG23	1.97	0.65
1:A:188:THR:O	1:A:192:THR:CG2	2.39	0.64
1:A:28:ASP:OD2	1:A:34:HIS:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:THR:O	1:B:255:VAL:HG23	1.99	0.62
1:B:76:GLU:HG3	1:B:86:LEU:CD1	2.29	0.62
1:A:197:ARG:HH12	1:A:237:THR:HG23	1.65	0.62
1:B:165:THR:O	1:B:169:LEU:HD13	1.99	0.61
1:B:76:GLU:HG3	1:B:86:LEU:HD13	1.83	0.61
1:A:103:GLU:HB2	1:A:125:ALA:HB2	1.84	0.60
1:B:173:LEU:HD22	1:B:176:ILE:N	2.17	0.59
1:B:129:SER:OG	1:B:218:ALA:O	2.21	0.59
1:B:224:GLU:N	1:B:224:GLU:OE1	2.35	0.59
1:A:197:ARG:NH1	1:A:237:THR:HG23	2.20	0.56
1:B:105:THR:HG23	1:B:122:PHE:CZ	2.39	0.56
1:A:74:ILE:CG2	1:A:149:LEU:HD22	2.36	0.55
1:B:129:SER:CB	1:B:218:ALA:O	2.55	0.54
1:A:242:VAL:HG11	1:A:268:ALA:HA	1.89	0.53
1:B:129:SER:HB3	1:B:218:ALA:O	2.08	0.53
1:B:246:ASP:OD1	1:B:249:ARG:NH1	2.42	0.53
1:A:183:LEU:CD2	1:A:186:THR:HG22	2.39	0.53
1:B:125:ALA:HB1	1:B:130:ASN:HA	1.87	0.53
1:B:222:MET:CE	1:B:226:PHE:CE1	2.92	0.52
1:B:76:GLU:OE1	1:B:150:TYR:N	2.29	0.52
1:A:34:HIS:HE1	1:A:288:ASP:OD2	1.92	0.52
1:A:73:THR:CG2	2:A:479:HOH:O	2.50	0.52
1:B:143:ASN:HD22	1:B:144:PRO:N	2.07	0.52
1:B:173:LEU:HD21	1:B:288:ASP:HB3	1.92	0.51
1:B:75:LEU:O	1:B:148:MET:HA	2.11	0.51
1:B:35:VAL:HG13	1:B:287:ALA:HB3	1.92	0.50
1:A:131:THR:O	1:A:135:THR:HG22	2.11	0.50
1:B:218:ALA:HB3	2:B:431:HOH:O	2.12	0.50
1:B:133:VAL:HG21	1:B:220:ARG:CD	2.40	0.49
1:A:140:ALA:O	2:A:498:HOH:O	2.20	0.48
1:B:158:THR:HG22	1:B:230:LEU:HD13	1.95	0.48
1:A:25:ARG:CZ	2:A:499:HOH:O	2.60	0.48
1:A:129:SER:O	1:A:133:VAL:HG23	2.13	0.48
1:A:51:LLP:H4'1	1:A:51:LLP:OP1	2.13	0.48
1:A:210:PRO:HD3	1:A:219:LEU:HB3	1.96	0.48
1:B:231:TYR:HE1	1:B:236:LEU:HD22	1.79	0.47
1:B:129:SER:O	1:B:130:ASN:HB2	2.15	0.47
1:B:140:ALA:O	2:B:339:HOH:O	2.19	0.47
1:B:65:ASP:HB2	1:B:67:LEU:HD22	1.96	0.46
1:B:143:ASN:HD22	1:B:144:PRO:CD	2.28	0.46
1:B:125:ALA:HB3	1:B:130:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASN:HD22	1:B:143:ASN:C	2.19	0.46
1:A:42:GLU:HG3	1:A:50:ILE:HD12	1.97	0.46
1:A:17:VAL:HG23	1:A:17:VAL:O	2.16	0.46
1:B:105:THR:CG2	1:B:122:PHE:CE2	2.98	0.46
1:A:123:SER:CB	1:A:135:THR:HG21	2.45	0.45
1:B:103:GLU:HG2	1:B:130:ASN:HD21	1.80	0.45
1:B:173:LEU:HD22	1:B:176:ILE:CA	2.47	0.45
1:B:139:LEU:O	1:B:142:THR:HB	2.18	0.44
1:A:51:LLP:H2'1	1:A:81:ASN:ND2	2.32	0.44
1:A:19:LEU:HD22	1:A:258:GLU:HG3	2.00	0.43
1:A:101:MET:O	1:A:122:PHE:HA	2.19	0.43
1:B:51:LLP:H2'1	1:B:81:ASN:ND2	2.33	0.43
1:A:217:TYR:O	1:A:218:ALA:HB3	2.19	0.43
1:B:242:VAL:HG11	1:B:268:ALA:HA	2.01	0.43
1:A:248:VAL:HG21	1:A:313:ALA:HB1	2.01	0.42
1:A:17:VAL:CG2	1:A:39:ALA:HB3	2.49	0.42
1:B:17:VAL:O	1:B:17:VAL:CG2	2.66	0.42
1:B:89:ALA:O	1:B:93:LYS:HB2	2.19	0.42
1:B:281:LEU:HD12	2:B:347:HOH:O	2.19	0.42
1:B:129:SER:O	1:B:130:ASN:CB	2.67	0.42
1:B:212:TYR:CE2	1:B:247:ALA:HB2	2.55	0.42
1:B:216:VAL:HG23	1:B:217:TYR:CD2	2.55	0.42
1:B:61:GLN:HG2	2:B:432:HOH:O	2.19	0.41
1:A:91:ARG:HD3	1:B:256:HIS:O	2.20	0.41
1:B:178:HIS:CD2	1:B:276:VAL:HG11	2.55	0.41
1:A:65:ASP:HB2	1:A:67:LEU:HD22	2.01	0.41
1:B:251:THR:CG2	1:B:306:TYR:HE1	2.34	0.41
1:A:173:LEU:HD12	1:A:290:ALA:HB2	2.02	0.41
1:B:281:LEU:CB	1:B:284:GLY:H	2.34	0.41
1:B:105:THR:HG23	1:B:122:PHE:CE2	2.56	0.40
1:B:75:LEU:HD22	1:B:98:ILE:HB	2.03	0.40
1:B:207:ALA:HB3	1:B:239:ARG:HG2	2.04	0.40
1:A:193:GLY:O	1:A:197:ARG:HG2	2.21	0.40
1:B:75:LEU:HD11	1:B:100:VAL:HG23	2.04	0.40
1:B:114:GLU:HG3	1:B:120:ILE:HG12	2.04	0.40
1:B:125:ALA:HB3	1:B:130:ASN:CG	2.41	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	309/326 (95%)	296 (96%)	13 (4%)	0	100	100
1	B	321/326 (98%)	305 (95%)	15 (5%)	1 (0%)	41	31
All	All	630/652 (97%)	601 (95%)	28 (4%)	1 (0%)	47	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	SER

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	234/243 (96%)	211 (90%)	23 (10%)	8	3
1	B	242/243 (100%)	215 (89%)	27 (11%)	6	1
All	All	476/486 (98%)	426 (90%)	50 (10%)	7	2

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	67	LEU
1	A	69	ARG
1	A	73	THR
1	A	75	LEU

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Mol	Chain	Res	Type
1	A	91	ARG
1	A	105	THR
1	A	106	SER
1	A	109	ARG
1	A	129	SER
1	A	149	LEU
1	A	169	LEU
1	A	173	LEU
1	A	192	THR
1	A	197	ARG
1	A	202	ASN
1	A	219	LEU
1	A	236	LEU
1	A	264	ILE
1	A	281	LEU
1	A	299	LYS
1	A	301	LEU
1	A	314	GLU
1	B	6	SER
1	B	30	ARG
1	B	61	GLN
1	B	67	LEU
1	B	73	THR
1	B	75	LEU
1	B	91	ARG
1	B	93	LYS
1	B	104	ASN
1	B	105	THR
1	B	107	VAL
1	B	109	ARG
1	B	112	LEU
1	B	130	ASN
1	B	142	THR
1	B	143	ASN
1	B	149	LEU
1	B	158	THR
1	B	173	LEU
1	B	175	GLU
1	B	219	LEU
1	B	220	ARG
1	B	236	LEU
1	B	270	LEU

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Mol	Chain	Res	Type
1	B	285	GLU
1	B	299	LYS
1	B	301	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	104	ASN
1	B	104	ASN
1	B	119	GLN
1	B	143	ASN
1	B	221	ASN
1	B	256	HIS
1	B	320	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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$
1	LLP	A	51	1	23,24,25	1.71	4 (17%)	25,32,34	1.69	4 (16%)
1	LLP	B	51	1	23,24,25	1.77	6 (26%)	25,32,34	1.66	5 (20%)

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
1	LLP	A	51	1	-	0/16/17/19	0/1/1/1
1	LLP	B	51	1	-	0/16/17/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	LLP	O3-C3	-5.40	1.24	1.37
1	B	51	LLP	O3-C3	-5.31	1.24	1.37
1	A	51	LLP	C4-C4'	3.22	1.52	1.46
1	A	51	LLP	C2-N1	3.03	1.39	1.33
1	B	51	LLP	C2-N1	2.98	1.39	1.33
1	B	51	LLP	CE-NZ	2.56	1.52	1.46
1	B	51	LLP	C4-C4'	2.52	1.51	1.46
1	B	51	LLP	P-OP2	-2.18	1.46	1.54
1	A	51	LLP	C4'-NZ	2.17	1.34	1.27
1	B	51	LLP	C4'-NZ	2.01	1.34	1.27

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	LLP	OP4-C5'-C5	5.61	120.04	109.35
1	B	51	LLP	OP4-C5'-C5	4.96	118.81	109.35
1	A	51	LLP	OP2-P-OP4	-2.61	99.79	106.73
1	B	51	LLP	C5-C4-C4'	-2.58	117.32	121.56
1	B	51	LLP	C4-C4'-NZ	-2.51	112.77	124.31
1	A	51	LLP	CE-NZ-C4'	-2.30	111.85	118.90
1	B	51	LLP	CE-NZ-C4'	-2.15	112.30	118.90
1	B	51	LLP	C5-C6-N1	-2.14	120.25	123.82
1	A	51	LLP	OP3-P-OP2	2.00	115.30	107.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	51	LLP	2	0
1	B	51	LLP	1	0

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

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, 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	311/326 (95%)	0.51	25 (8%) 12 13	16, 25, 48, 57	0
1	B	323/326 (99%)	0.64	26 (8%) 12 13	20, 31, 41, 52	0
All	All	634/652 (97%)	0.58	51 (8%) 12 13	16, 28, 45, 57	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	GLY	5.6
1	A	125	ALA	5.4
1	A	126	GLU	5.0
1	B	281	LEU	5.0
1	B	31	ASP	4.8
1	A	129	SER	4.5
1	B	30	ARG	4.4
1	B	226	PHE	4.3
1	A	128	GLY	4.3
1	B	127	GLY	4.2
1	B	124	ALA	4.1
1	A	103	GLU	4.0
1	B	129	SER	3.9
1	B	125	ALA	3.8
1	A	71	GLY	3.6
1	B	126	GLU	3.4
1	B	130	ASN	3.3
1	B	225	GLY	3.1
1	B	201	ALA	3.0
1	A	124	ALA	3.0
1	A	105	THR	2.7
1	A	131	THR	2.7
1	B	224	GLU	2.7
1	A	130	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	67	LEU	2.6
1	B	0	HIS	2.5
1	A	108	GLU	2.5
1	A	145	SER	2.5
1	A	109	ARG	2.5
1	A	31	ASP	2.5
1	B	282	ALA	2.5
1	A	127	GLY	2.4
1	B	69	ARG	2.4
1	A	69	ARG	2.4
1	A	111	GLN	2.4
1	B	144	PRO	2.4
1	A	30	ARG	2.3
1	A	122	PHE	2.2
1	A	134	ALA	2.2
1	B	142	THR	2.2
1	A	104	ASN	2.2
1	B	305	ALA	2.2
1	A	144	PRO	2.2
1	B	28	ASP	2.1
1	B	67	LEU	2.1
1	B	141	ALA	2.1
1	A	217	TYR	2.1
1	B	223	ASP	2.1
1	A	141	ALA	2.1
1	B	32	GLY	2.0
1	B	222	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	LLP	B	51	24/25	0.97	0.13	21,22,24,28	0
1	LLP	A	51	24/25	0.98	0.12	16,19,20,21	0

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.