Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 02:29 AM EDT

PDB ID	:	5M1C
Title	:	Crystal structure of N-terminally tagged apo-UbiD from E. coli
Authors	:	Marshall, S.A.; Leys, D.
Deposited on	:	2016-10-07
Resolution	:	2.75 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 (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:

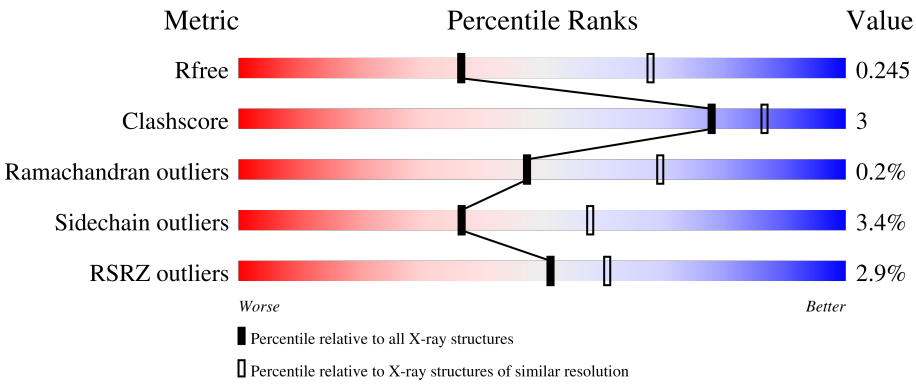
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	517	5% 74% 10% • 15%
1	B	517	% 83% 6% 11%
1	C	517	2% 77% 10% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10633 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 3-octaprenyl-4-hydroxybenzoate carboxy-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	3430	2190	585	638	17	0	0	0
1	B	460	3613	2309	616	671	17	1	0	0
1	C	448	3517	2252	596	652	17	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P0AAB5
A	-18	GLY	-	expression tag	UNP P0AAB5
A	-17	SER	-	expression tag	UNP P0AAB5
A	-16	SER	-	expression tag	UNP P0AAB5
A	-15	HIS	-	expression tag	UNP P0AAB5
A	-14	HIS	-	expression tag	UNP P0AAB5
A	-13	HIS	-	expression tag	UNP P0AAB5
A	-12	HIS	-	expression tag	UNP P0AAB5
A	-11	HIS	-	expression tag	UNP P0AAB5
A	-10	HIS	-	expression tag	UNP P0AAB5
A	-9	SER	-	expression tag	UNP P0AAB5
A	-8	SER	-	expression tag	UNP P0AAB5
A	-7	GLY	-	expression tag	UNP P0AAB5
A	-6	LEU	-	expression tag	UNP P0AAB5
A	-5	VAL	-	expression tag	UNP P0AAB5
A	-4	PRO	-	expression tag	UNP P0AAB5
A	-3	ARG	-	expression tag	UNP P0AAB5
A	-2	GLY	-	expression tag	UNP P0AAB5
A	-1	SER	-	expression tag	UNP P0AAB5
A	0	HIS	-	expression tag	UNP P0AAB5
B	-19	MET	-	initiating methionine	UNP P0AAB5
B	-18	GLY	-	expression tag	UNP P0AAB5
B	-17	SER	-	expression tag	UNP P0AAB5

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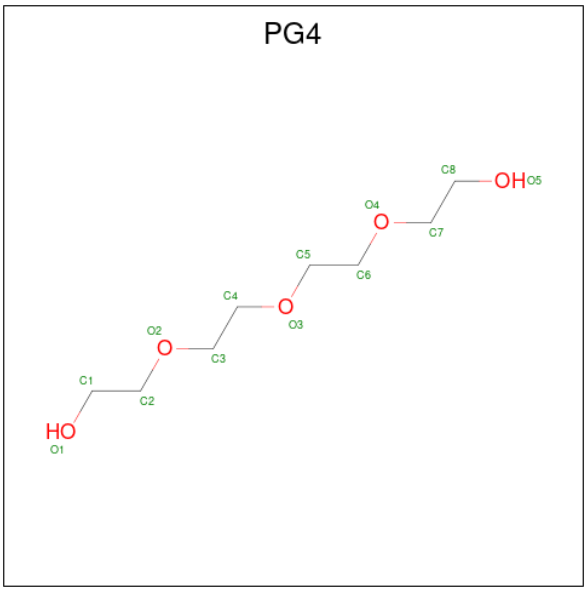
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP P0AAB5
B	-15	HIS	-	expression tag	UNP P0AAB5
B	-14	HIS	-	expression tag	UNP P0AAB5
B	-13	HIS	-	expression tag	UNP P0AAB5
B	-12	HIS	-	expression tag	UNP P0AAB5
B	-11	HIS	-	expression tag	UNP P0AAB5
B	-10	HIS	-	expression tag	UNP P0AAB5
B	-9	SER	-	expression tag	UNP P0AAB5
B	-8	SER	-	expression tag	UNP P0AAB5
B	-7	GLY	-	expression tag	UNP P0AAB5
B	-6	LEU	-	expression tag	UNP P0AAB5
B	-5	VAL	-	expression tag	UNP P0AAB5
B	-4	PRO	-	expression tag	UNP P0AAB5
B	-3	ARG	-	expression tag	UNP P0AAB5
B	-2	GLY	-	expression tag	UNP P0AAB5
B	-1	SER	-	expression tag	UNP P0AAB5
B	0	HIS	-	expression tag	UNP P0AAB5
C	-19	MET	-	initiating methionine	UNP P0AAB5
C	-18	GLY	-	expression tag	UNP P0AAB5
C	-17	SER	-	expression tag	UNP P0AAB5
C	-16	SER	-	expression tag	UNP P0AAB5
C	-15	HIS	-	expression tag	UNP P0AAB5
C	-14	HIS	-	expression tag	UNP P0AAB5
C	-13	HIS	-	expression tag	UNP P0AAB5
C	-12	HIS	-	expression tag	UNP P0AAB5
C	-11	HIS	-	expression tag	UNP P0AAB5
C	-10	HIS	-	expression tag	UNP P0AAB5
C	-9	SER	-	expression tag	UNP P0AAB5
C	-8	SER	-	expression tag	UNP P0AAB5
C	-7	GLY	-	expression tag	UNP P0AAB5
C	-6	LEU	-	expression tag	UNP P0AAB5
C	-5	VAL	-	expression tag	UNP P0AAB5
C	-4	PRO	-	expression tag	UNP P0AAB5
C	-3	ARG	-	expression tag	UNP P0AAB5
C	-2	GLY	-	expression tag	UNP P0AAB5
C	-1	SER	-	expression tag	UNP P0AAB5
C	0	HIS	-	expression tag	UNP P0AAB5

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	13	8	5	0	0

- Molecule 3 is water.

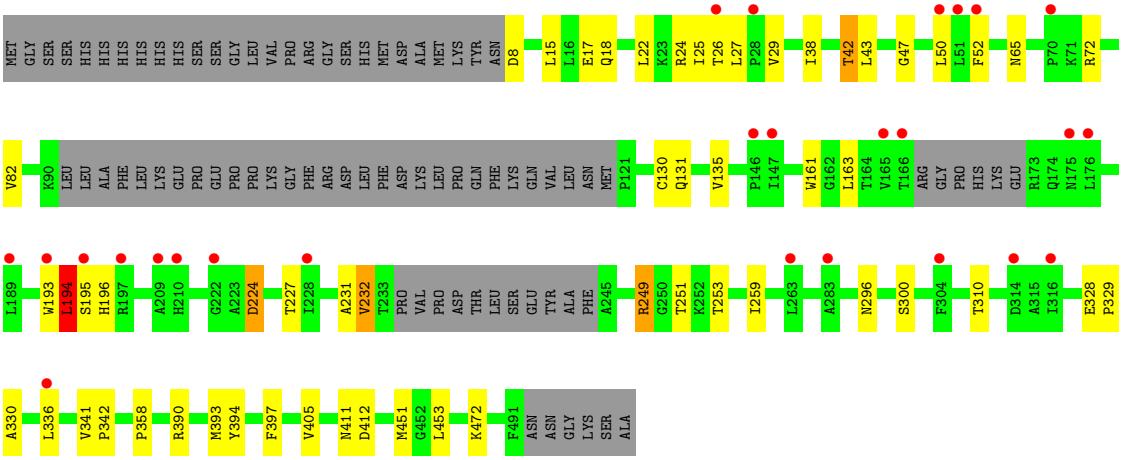
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	11	11	11	0	0
			Total	O		
3	B	27	27	27	0	0
			Total	O		
3	C	22	22	22	0	0

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.

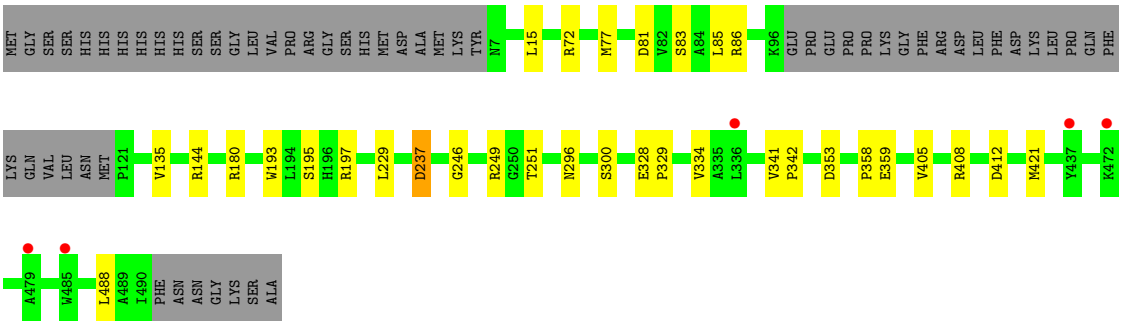
• Molecule 1: 3-octaprenyl-4-hydroxybenzoate carboxy-lyase

Chain A:



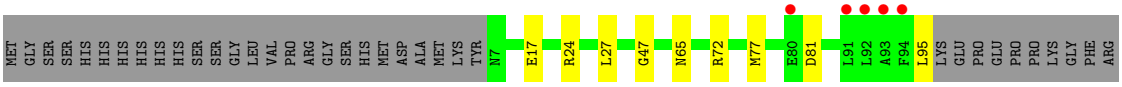
• Molecule 1: 3-octaprenyl-4-hydroxybenzoate carboxy-lyase

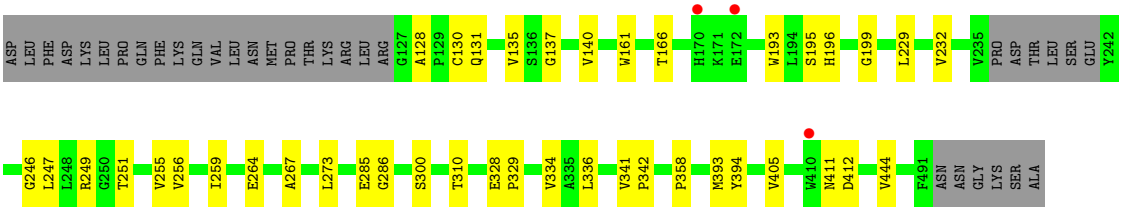
Chain B:



• Molecule 1: 3-octaprenyl-4-hydroxybenzoate carboxy-lyase

Chain C:




ASP
LEU
PHE
ASP
LYS
LEU
PRO
GLN
PHE
LYS
GLN
VAL
LEU
ASN
MET
PRO
THR
LYS
ARG
LEU
ARG
G127
A128
P129
C130
Q131
V135
S136
G137
V140
W161
T166
H170
K171
E172
W193
L194
S195
H196
G199
L229
V232
V235
PRO
ASP
THR
LEU
SER
GLU
Y242
G246
L247
L248
R249
G250
T251
V255
V256
I259
E264
A267
L273
E285
G286
S300
T310
E328
P329
V334
A335
L336
V341
P342
P358
M393
Y394
V405
W410
N411
D412
V444
F491
ASN
ASN
GLY
LYS
SER
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	196.44Å 196.44Å 108.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.41 – 2.75 98.22 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (98.41-2.75) 99.8 (98.22-2.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.213 , 0.246 0.210 , 0.245	Depositor DCC
R_{free} test set	2749 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10633	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4

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	0.64	0/3513	0.82	4/4783 (0.1%)
1	B	0.72	1/3704 (0.0%)	0.82	4/5047 (0.1%)
1	C	0.65	0/3606	0.78	1/4914 (0.0%)
All	All	0.67	1/10823 (0.0%)	0.81	9/14744 (0.1%)

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	2
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	237	ASP	C-O	10.70	1.43	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	197	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	B	237	ASP	O-C-N	-7.44	110.79	122.70
1	A	194	LEU	CA-CB-CG	7.14	131.73	115.30
1	C	286	GLY	N-CA-C	-6.18	97.64	113.10
1	B	72	ARG	CG-CD-NE	5.75	123.86	111.80
1	B	144	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	390	ARG	NE-CZ-NH1	5.71	123.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	A	472	LYS	CD-CE-NZ	5.32	123.93	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	237	ASP	Mainchain
1	B	421	MET	Peptide
1	C	285	GLU	Peptide

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	3430	0	3398	27	0
1	B	3613	0	3585	14	0
1	C	3517	0	3475	22	0
2	B	13	0	18	0	0
3	A	11	0	0	0	0
3	B	27	0	0	0	0
3	C	22	0	0	0	0
All	All	10633	0	10476	61	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 (61) 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:81:ASP:OD1	1:B:83:SER:OG	1.83	0.94
1:C:130:CYS:O	1:C:310:THR:HG22	1.71	0.89
1:A:130:CYS:O	1:A:310:THR:HG22	1.76	0.86
1:C:128:ALA:HB2	1:C:256:VAL:HG21	1.63	0.80
1:C:137:GLY:O	1:C:140:VAL:HG22	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:O	1:A:42:THR:HG23	1.90	0.71
1:A:232:VAL:HG12	1:A:232:VAL:O	1.93	0.69
1:A:131:GLN:HA	1:A:310:THR:CG2	2.24	0.67
1:C:131:GLN:HA	1:C:310:THR:CG2	2.25	0.67
1:A:330:ALA:HB1	1:A:358:PRO:HB3	1.78	0.65
1:C:256:VAL:HG23	1:C:267:ALA:HB2	1.81	0.63
1:A:25:ILE:HD11	1:B:488:LEU:HD23	1.83	0.61
1:B:246:GLY:O	1:B:249:ARG:O	2.19	0.61
1:A:131:GLN:HG2	1:A:310:THR:HG21	1.83	0.60
1:C:131:GLN:HG2	1:C:310:THR:HG21	1.83	0.60
1:A:17:GLU:OE2	1:A:24:ARG:NH1	2.35	0.60
1:A:224:ASP:OD2	1:A:227:THR:HG23	2.02	0.59
1:C:246:GLY:O	1:C:249:ARG:O	2.23	0.57
1:A:397:PHE:HE1	1:A:451:MET:HE1	1.70	0.57
1:C:166:THR:HG21	1:C:199:GLY:HA2	1.86	0.57
1:A:249:ARG:NH2	1:A:253:THR:OG1	2.39	0.56
1:C:232:VAL:HG12	1:C:336:LEU:CD1	2.36	0.55
1:C:128:ALA:CB	1:C:256:VAL:HG21	2.34	0.54
1:A:232:VAL:HG21	1:A:336:LEU:HD13	1.87	0.54
1:B:15:LEU:C	1:B:15:LEU:HD23	2.29	0.53
1:B:405:VAL:HG13	1:B:412:ASP:HB3	1.91	0.52
1:C:405:VAL:HG13	1:C:412:ASP:HB3	1.90	0.52
1:C:341:VAL:HB	1:C:342:PRO:HD3	1.92	0.52
1:A:405:VAL:HG13	1:A:412:ASP:HB3	1.92	0.52
1:A:29:VAL:HG11	1:A:52:PHE:CD1	2.45	0.51
1:B:341:VAL:HB	1:B:342:PRO:HD3	1.92	0.50
1:C:17:GLU:OE1	1:C:24:ARG:NH1	2.44	0.50
1:C:328:GLU:HB3	1:C:329:PRO:HD3	1.94	0.50
1:C:140:VAL:HG23	1:C:140:VAL:O	2.12	0.49
1:A:341:VAL:HB	1:A:342:PRO:HD3	1.95	0.49
1:A:397:PHE:CE1	1:A:451:MET:HE1	2.47	0.49
1:A:15:LEU:C	1:A:15:LEU:HD23	2.33	0.48
1:B:86:ARG:HG2	1:B:342:PRO:HG3	1.95	0.48
1:B:328:GLU:HB3	1:B:329:PRO:HD3	1.97	0.47
1:B:353:ASP:OD1	1:B:408:ARG:NH1	2.47	0.47
1:C:255:VAL:CG2	1:C:264:GLU:HB3	2.45	0.46
1:A:65:ASN:O	1:A:72:ARG:NH1	2.48	0.46
1:A:393:MET:HG3	1:A:394:TYR:CD1	2.50	0.46
1:C:65:ASN:O	1:C:72:ARG:NH1	2.49	0.46
1:A:194:LEU:HD23	1:A:196:HIS:CE1	2.51	0.45
1:A:328:GLU:HB3	1:A:329:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:THR:HG21	1:A:50:LEU:HD11	1.99	0.44
1:A:47:GLY:O	1:A:72:ARG:NH2	2.50	0.44
1:B:180:ARG:HH12	1:B:296:ASN:ND2	2.14	0.44
1:A:411:ASN:OD1	1:B:359:GLU:HG2	2.18	0.43
1:C:77:MET:HG3	1:C:229:LEU:HD13	2.00	0.43
1:C:47:GLY:O	1:C:72:ARG:NH2	2.52	0.43
1:B:86:ARG:CG	1:B:342:PRO:HG3	2.48	0.42
1:C:334:VAL:HG21	1:C:358:PRO:HG3	2.01	0.42
1:A:397:PHE:CD1	1:A:451:MET:HE2	2.55	0.42
1:C:232:VAL:HG12	1:C:336:LEU:HD11	2.00	0.42
1:A:296:ASN:OD1	1:A:296:ASN:O	2.38	0.41
1:A:451:MET:HE3	1:A:453:LEU:HD11	2.02	0.41
1:B:77:MET:HG3	1:B:229:LEU:HD13	2.01	0.41
1:B:334:VAL:HG21	1:B:358:PRO:HG3	2.02	0.40
1:C:393:MET:HG3	1:C:394:TYR:CD1	2.56	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	429/517 (83%)	412 (96%)	15 (4%)	2 (0%)	29 47
1	B	456/517 (88%)	443 (97%)	13 (3%)	0	100 100
1	C	442/517 (86%)	430 (97%)	12 (3%)	0	100 100
All	All	1327/1551 (86%)	1285 (97%)	40 (3%)	2 (0%)	47 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ALA
1	A	232	VAL

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	369/439 (84%)	351 (95%)	18 (5%)	25	43
1	B	389/439 (89%)	383 (98%)	6 (2%)	65	78
1	C	377/439 (86%)	362 (96%)	15 (4%)	31	51
All	All	1135/1317 (86%)	1096 (97%)	39 (3%)	37	58

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	22	LEU
1	A	26	THR
1	A	27	LEU
1	A	42	THR
1	A	43	LEU
1	A	82	VAL
1	A	135	VAL
1	A	161	TRP
1	A	163	LEU
1	A	193	TRP
1	A	194	LEU
1	A	195	SER
1	A	224	ASP
1	A	249	ARG
1	A	251	THR
1	A	259	ILE
1	A	300	SER
1	B	85	LEU
1	B	135	VAL
1	B	193	TRP
1	B	195	SER
1	B	251	THR
1	B	300	SER
1	C	27	LEU
1	C	81	ASP

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Mol	Chain	Res	Type
1	C	95	LEU
1	C	135	VAL
1	C	161	TRP
1	C	193	TRP
1	C	195	SER
1	C	196	HIS
1	C	247	LEU
1	C	251	THR
1	C	259	ILE
1	C	273	LEU
1	C	300	SER
1	C	411	ASN
1	C	444	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	19	GLN
1	A	196	HIS
1	B	296	ASN
1	C	175	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides 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	PG4	B	501	-	12,12,12	0.74	0	11,11,11	0.71	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
2	PG4	B	501	-	-	5/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PG4	O1-C1-C2-O2
2	B	501	PG4	O2-C3-C4-O3
2	B	501	PG4	O3-C5-C6-O4
2	B	501	PG4	O4-C7-C8-O5
2	B	501	PG4	C6-C5-O3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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	437/517 (84%)	0.29	26 (5%)	22	27	39, 89, 129, 156	0
1	B	460/517 (88%)	-0.04	5 (1%)	80	86	39, 58, 104, 136	3 (0%)
1	C	448/517 (86%)	0.02	8 (1%)	68	76	39, 74, 127, 173	0
All	All	1345/1551 (86%)	0.09	39 (2%)	51	61	39, 70, 124, 173	3 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	94	PHE	5.1
1	A	52	PHE	4.1
1	A	50	LEU	4.1
1	A	314	ASP	3.3
1	A	175	ASN	3.3
1	A	316	ILE	3.3
1	A	336	LEU	3.2
1	B	437	TYR	3.2
1	C	91	LEU	3.1
1	A	189	LEU	3.1
1	A	26	THR	3.1
1	C	80	GLU	3.0
1	A	70	PRO	2.9
1	A	195	SER	2.9
1	C	170	HIS	2.8
1	A	166	THR	2.7
1	A	210	HIS	2.7
1	B	336	LEU	2.7
1	A	209	ALA	2.7
1	A	165	VAL	2.7
1	A	193	TRP	2.7
1	B	485	TRP	2.7
1	C	172	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	176	LEU	2.5
1	A	197	ARG	2.5
1	A	147	ILE	2.5
1	A	228	ILE	2.4
1	B	479	ALA	2.4
1	A	263	LEU	2.4
1	A	28	PRO	2.4
1	C	410	TRP	2.3
1	A	222	GLY	2.3
1	A	283	ALA	2.2
1	B	472	LYS	2.2
1	C	92	LEU	2.2
1	A	304	PHE	2.2
1	A	51	LEU	2.1
1	A	146	PRO	2.1
1	C	93	ALA	2.1

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 monosaccharides 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	PG4	B	501	13/13	0.87	0.18	63,73,81,83	0

6.5 Other polymers (i)

There are no such residues in this entry.