Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 02:10 am GMT

PDB ID	:	5M1D
Title	:	Crystal structure of N-terminally tagged UbiD from E. coli reconstituted with prFMN cofactor
Authors	:	Marshall, S.A.; Leys, D.
Deposited on	:	2016-10-07
Resolution	:	2.70 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:

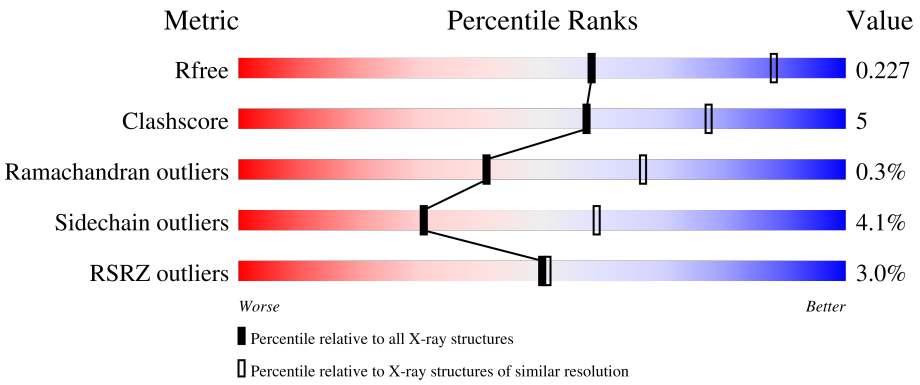
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	517	4% 81% 9% 9%
1	B	517	% 80% 8% • 10%
1	C	517	3% 76% 10% • 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11153 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	469	3660	2338	624	680	18	0	0	1
1	B	465	3651	2333	622	678	18	0	0	0
1	C	459	3588	2293	609	669	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

Continued on next page...

Continued from previous page...

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 MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

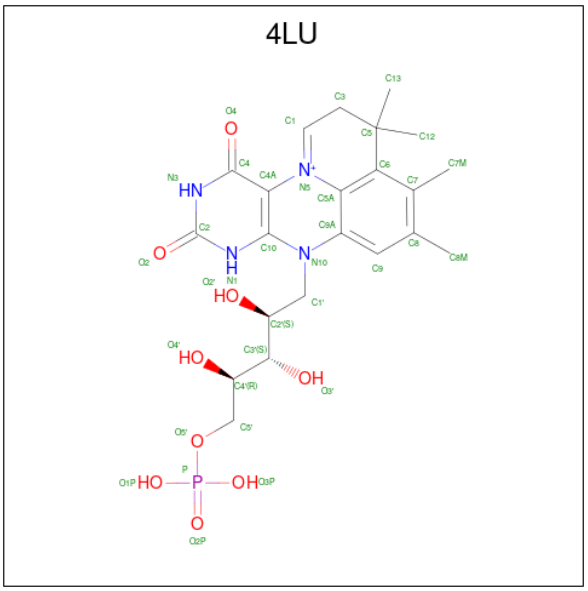
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0

- Molecule 3 is 1-deoxy-5-O-phosphono-1-(3,3,4,5-tetramethyl-9,11-dioxo-2,3,8,9,10,11-hexah ydro-7H-quinolino[1,8-fg]pteridin-12-ium-7-y l)-D-ribitol (three-letter code: 4LU) (formula: $C_{22}H_{30}N_4O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 36 22 4 9 1	0	0
3	B	1	Total C N O P 36 22 4 9 1	0	0
3	C	1	Total C N O P 36 22 4 9 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

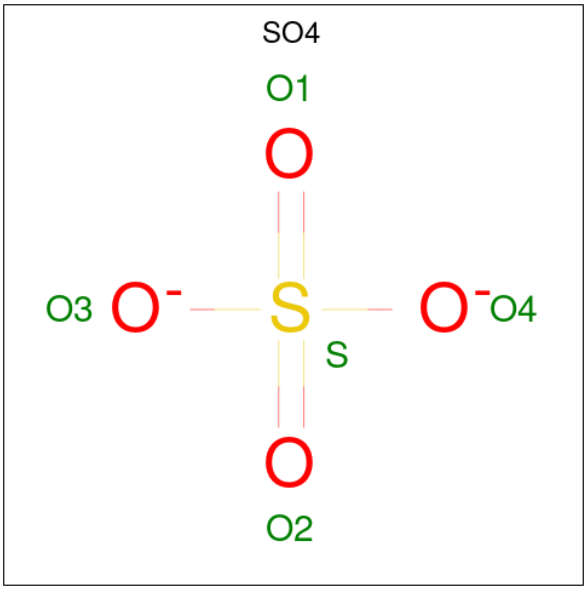
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

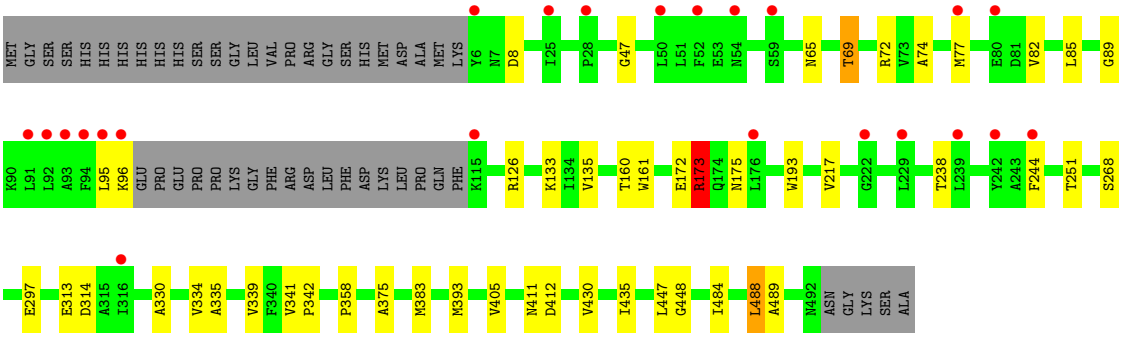
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	38	Total O 38 38	0	0
6	B	65	Total O 65 65	0	0
6	C	32	Total O 32 32	0	0

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.

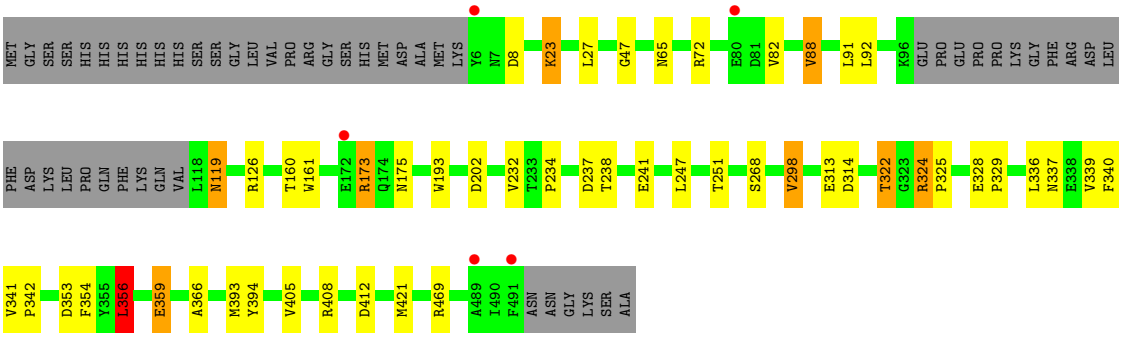
• Molecule 1: 3-octaprenyl-4-hydroxybenzoate carboxy-lyase

Chain A:



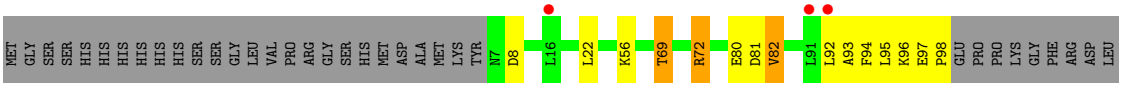
• Molecule 1: 3-octaprenyl-4-hydroxybenzoate carboxy-lyase

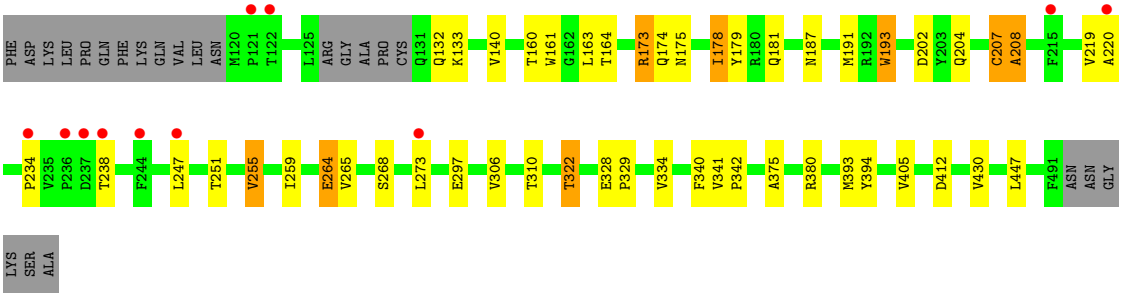
Chain B:



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

Chain C:




PHE ASP LYS LEU PRO GLN PHE LYS GLN VAL LEU ASN M120 P121 T122 L125 ARG GLY ALA PRO CYS Q131 Q132 K133 V140 T160 W161 G162 L163 T164 R173 Q174 N175 I178 Y179 R180 Q181 N187 M191 R192 W193 D202 Y203 Q204 C207 A208 F215 V219 A220
P234 V235 P236 D237 T238 F244 L247 T251 V255 I259 E264 V265 S268 L273 E297 V306 T310 T322 E328 P329 V334 F340 V341 P342 A375 R380 M393 Y394 V405 D412 V430 L447 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	194.20Å 194.20Å 107.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	137.32 – 2.70 137.32 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (137.32-2.70) 99.9 (137.32-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.195 , 0.226 0.194 , 0.227	Depositor DCC
R_{free} test set	2805 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11153	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: 4LU, NA, SO4, MN

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	0.60	0/3752	0.75	1/5115 (0.0%)
1	B	0.65	0/3743	0.80	4/5101 (0.1%)
1	C	0.63	1/3677 (0.0%)	0.78	5/5013 (0.1%)
All	All	0.63	1/11172 (0.0%)	0.78	10/15229 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	297	GLU	CD-OE1	5.42	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	178	ILE	CG1-CB-CG2	-7.86	94.10	111.40
1	B	241	GLU	OE1-CD-OE2	-7.79	113.96	123.30
1	A	173	ARG	CG-CD-NE	6.49	125.42	111.80
1	B	356	LEU	CB-CG-CD1	6.04	121.27	111.00
1	B	298	VAL	CB-CA-C	-6.03	99.95	111.40
1	B	359	GLU	CB-CA-C	-5.69	99.01	110.40
1	C	22	LEU	CA-CB-CG	5.46	127.86	115.30
1	C	207	CYS	N-CA-C	-5.19	96.98	111.00
1	C	72	ARG	CG-CD-NE	5.14	122.60	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	98	PRO	N-CA-CB	5.06	109.37	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	421	MET	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	3660	0	3603	30	0
1	B	3651	0	3612	32	0
1	C	3588	0	3527	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	36	0	28	4	0
3	B	36	0	28	5	0
3	C	36	0	28	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	5	0	0	0	0
6	A	38	0	0	1	0
6	B	65	0	0	0	1
6	C	32	0	0	0	0
All	All	11153	0	10826	106	1

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 5.

All (106) 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)
3:B:502:4LU:H14	3:B:502:4LU:H13	1.25	1.13
3:C:502:4LU:H13	3:C:502:4LU:H14	1.24	1.11
3:A:502:4LU:H14	3:A:502:4LU:H13	1.32	1.05
1:C:164:THR:HG21	1:C:191:MET:HE2	1.48	0.95
3:C:502:4LU:H14	3:C:502:4LU:C12	2.06	0.86
3:B:502:4LU:H14	3:B:502:4LU:C12	2.03	0.84
3:A:502:4LU:H14	3:A:502:4LU:C12	2.11	0.80
1:C:164:THR:HG21	1:C:191:MET:CE	2.18	0.74
1:A:488:LEU:HD13	1:B:27:LEU:HD12	1.71	0.71
1:C:140:VAL:HG11	1:C:306:VAL:HG13	1.73	0.70
1:C:174:GLN:HE22	1:C:264:GLU:H	1.41	0.67
1:C:179:TYR:HD2	1:C:191:MET:HE1	1.59	0.67
1:C:173:ARG:NH2	1:C:202:ASP:OD2	2.28	0.66
1:A:330:ALA:HB1	1:A:358:PRO:HB3	1.77	0.66
1:C:393:MET:HG3	1:C:394:TYR:CD1	2.32	0.65
1:B:393:MET:HG3	1:B:394:TYR:CD1	2.31	0.65
1:B:91:LEU:HD21	1:B:247:LEU:HD13	1.79	0.65
1:C:219:VAL:HG22	1:C:273:LEU:HB2	1.78	0.64
1:A:173:ARG:HD2	1:A:173:ARG:C	2.17	0.64
1:C:174:GLN:NE2	1:C:264:GLU:H	1.96	0.63
1:A:95:LEU:O	1:A:96:LYS:HG3	1.99	0.63
1:A:8:ASP:HB2	1:A:268:SER:HB2	1.81	0.62
1:B:322:THR:HG23	1:B:329:PRO:HG2	1.81	0.62
1:B:173:ARG:NH2	1:B:202:ASP:OD2	2.29	0.62
1:C:207:CYS:O	1:C:208:ALA:HB3	2.00	0.61
3:C:502:4LU:H13	3:C:502:4LU:C7M	2.15	0.61
1:B:313:GLU:O	1:B:314:ASP:HB2	2.02	0.59
1:C:191:MET:HE3	1:C:193:TRP:CE3	2.38	0.59
1:B:8:ASP:HB2	1:B:268:SER:HB2	1.85	0.59
1:C:322:THR:HG23	1:C:329:PRO:HG2	1.83	0.59
1:C:8:ASP:HB2	1:C:268:SER:HB2	1.84	0.59
1:C:207:CYS:O	1:C:208:ALA:CB	2.50	0.59
1:A:484:ILE:HG13	1:A:488:LEU:HD22	1.86	0.58
1:B:119:ASN:C	1:B:119:ASN:HD22	2.07	0.58
1:C:81:ASP:OD1	1:C:82:VAL:N	2.38	0.57
1:A:133:LYS:HE3	1:A:313:GLU:OE1	2.05	0.57
1:C:219:VAL:CG2	1:C:273:LEU:HD12	2.35	0.56
1:C:219:VAL:HG21	1:C:273:LEU:HD12	1.87	0.56
1:A:47:GLY:O	1:A:72:ARG:NH2	2.39	0.56
1:B:232:VAL:HG12	1:B:336:LEU:HD11	1.87	0.56
1:C:179:TYR:HD2	1:C:191:MET:CE	2.19	0.56
1:B:405:VAL:HG13	1:B:412:ASP:HB3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ASN:C	1:B:119:ASN:ND2	2.60	0.54
1:B:160:THR:O	3:B:502:4LU:H4	2.08	0.54
3:B:502:4LU:C12	3:B:502:4LU:C7M	2.81	0.53
1:A:69:THR:HG22	1:A:72:ARG:H	1.73	0.52
1:A:313:GLU:O	1:A:314:ASP:HB2	2.09	0.52
1:B:47:GLY:O	1:B:72:ARG:NH2	2.42	0.52
1:A:65:ASN:O	1:A:72:ARG:NH1	2.43	0.52
1:C:163:LEU:HD12	1:C:220:ALA:O	2.10	0.52
1:C:160:THR:O	3:C:502:4LU:H4	2.09	0.52
1:A:411:ASN:OD1	1:B:359:GLU:HG3	2.10	0.51
1:A:405:VAL:HG13	1:A:412:ASP:HB3	1.92	0.51
1:B:356:LEU:HD13	1:B:366:ALA:HB2	1.92	0.51
1:A:173:ARG:HD2	1:A:173:ARG:O	2.12	0.50
1:A:489:ALA:O	1:B:23:LYS:HE3	2.12	0.50
1:C:219:VAL:CG2	1:C:273:LEU:HB2	2.40	0.50
1:B:341:VAL:HB	1:B:342:PRO:HD3	1.93	0.50
1:C:179:TYR:CD2	1:C:191:MET:CE	2.95	0.49
1:C:405:VAL:HG13	1:C:412:ASP:HB3	1.93	0.49
1:A:435:ILE:HG23	6:A:635:HOH:O	2.12	0.49
1:C:234:PRO:CG	1:C:340:PHE:HZ	2.25	0.49
1:B:353:ASP:OD2	1:B:408:ARG:NH1	2.45	0.49
1:B:234:PRO:CG	1:B:340:PHE:HZ	2.26	0.48
1:A:95:LEU:O	1:A:96:LYS:CG	2.61	0.48
1:A:393:MET:HG2	1:C:380:ARG:HD2	1.96	0.48
1:B:65:ASN:O	1:B:72:ARG:NH1	2.46	0.48
1:C:69:THR:HG22	1:C:72:ARG:H	1.78	0.48
1:C:204:GLN:O	1:C:207:CYS:O	2.31	0.48
1:C:178:ILE:HB	3:C:502:4LU:O2'	2.13	0.47
1:B:88:VAL:HG22	1:B:339:VAL:HG22	1.96	0.47
1:A:447:LEU:HD13	1:C:375:ALA:HB1	1.96	0.47
1:B:354:PHE:CE2	1:B:356:LEU:HD21	2.50	0.47
1:C:174:GLN:HE22	1:C:264:GLU:HG3	1.79	0.47
1:C:255:VAL:HG22	1:C:265:VAL:O	2.14	0.46
1:A:89:GLY:HA2	1:A:339:VAL:HG13	1.98	0.46
1:A:411:ASN:HA	1:B:359:GLU:HG2	1.97	0.45
1:B:173:ARG:CZ	1:B:175:ASN:HB2	2.46	0.45
1:A:173:ARG:CZ	1:A:175:ASN:HB2	2.46	0.45
1:A:85:LEU:HD13	1:A:335:ALA:O	2.16	0.45
1:C:341:VAL:HB	1:C:342:PRO:HD3	1.99	0.45
1:C:132:GLN:HB2	1:C:310:THR:CG2	2.46	0.45
1:C:173:ARG:CZ	1:C:175:ASN:HB2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:THR:O	3:A:502:4LU:H4	2.18	0.44
3:B:502:4LU:H13	3:B:502:4LU:C7M	2.17	0.44
1:C:306:VAL:HG13	1:C:306:VAL:O	2.18	0.44
1:A:341:VAL:HB	1:A:342:PRO:HD3	2.00	0.44
1:A:74:ALA:HA	1:A:77:MET:HE2	2.00	0.44
1:C:187:ASN:CA	1:C:306:VAL:HG12	2.48	0.44
1:B:356:LEU:CD2	1:B:356:LEU:N	2.81	0.43
1:B:324:ARG:HG2	1:B:325:PRO:HD2	2.00	0.43
1:A:375:ALA:HB1	1:C:447:LEU:HD13	1.99	0.43
3:A:502:4LU:C12	3:A:502:4LU:C7M	2.87	0.43
1:C:328:GLU:HB3	1:C:329:PRO:HD3	2.00	0.43
1:B:234:PRO:HG3	1:B:340:PHE:HZ	1.84	0.42
1:B:173:ARG:HD3	1:B:237:ASP:O	2.19	0.42
3:C:502:4LU:C12	3:C:502:4LU:C7M	2.82	0.42
1:C:234:PRO:HG3	1:C:340:PHE:HZ	1.84	0.42
1:C:181:GLN:HE22	1:C:219:VAL:HG11	1.84	0.42
1:A:435:ILE:HG13	1:A:448:GLY:HA3	2.02	0.41
1:B:313:GLU:O	1:B:314:ASP:CB	2.67	0.41
1:B:328:GLU:HB3	1:B:329:PRO:HD3	2.03	0.41
1:A:383:MET:HE1	1:C:430:VAL:HG21	2.02	0.41
1:C:93:ALA:O	1:C:95:LEU:N	2.54	0.40
1:A:297:GLU:OE2	1:B:469:ARG:NH1	2.54	0.40
1:B:119:ASN:ND2	1:B:119:ASN:O	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:605:HOH:O	6:B:605:HOH:O[8_554]	1.29	0.91

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	465/517 (90%)	452 (97%)	13 (3%)	0	100	100
1	B	461/517 (89%)	449 (97%)	12 (3%)	0	100	100
1	C	453/517 (88%)	437 (96%)	12 (3%)	4 (1%)	17	40
All	All	1379/1551 (89%)	1338 (97%)	37 (3%)	4 (0%)	41	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	97	GLU
1	C	208	ALA
1	C	94	PHE
1	C	96	LYS

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	390/439 (89%)	375 (96%)	15 (4%)	33	62
1	B	392/439 (89%)	376 (96%)	16 (4%)	30	59
1	C	383/439 (87%)	366 (96%)	17 (4%)	28	56
All	All	1165/1317 (88%)	1117 (96%)	48 (4%)	30	59

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	THR
1	A	82	VAL
1	A	126	ARG
1	A	135	VAL
1	A	161	TRP
1	A	172	GLU
1	A	173	ARG
1	A	193	TRP
1	A	217	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	238	THR
1	A	244	PHE
1	A	251	THR
1	A	334	VAL
1	A	430	VAL
1	A	488	LEU
1	B	23	LYS
1	B	82	VAL
1	B	88	VAL
1	B	92	LEU
1	B	119	ASN
1	B	126	ARG
1	B	161	TRP
1	B	173	ARG
1	B	193	TRP
1	B	238	THR
1	B	251	THR
1	B	298	VAL
1	B	322	THR
1	B	324	ARG
1	B	337	ASN
1	B	356	LEU
1	C	56	LYS
1	C	69	THR
1	C	80	GLU
1	C	82	VAL
1	C	92	LEU
1	C	133	LYS
1	C	161	TRP
1	C	173	ARG
1	C	193	TRP
1	C	238	THR
1	C	247	LEU
1	C	251	THR
1	C	255	VAL
1	C	259	ILE
1	C	264	GLU
1	C	322	THR
1	C	334	VAL

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	54	ASN
1	B	119	ASN
1	B	131	GLN
1	C	174	GLN

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)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	4LU	B	502	2,4	35,39,39	1.41	1 (2%)	46,62,62	1.70	8 (17%)
5	SO4	B	504	-	4,4,4	0.47	0	6,6,6	0.38	0
3	4LU	C	502	4	35,39,39	1.67	6 (17%)	46,62,62	2.06	11 (23%)
3	4LU	A	502	2,4	35,39,39	1.54	2 (5%)	46,62,62	1.71	8 (17%)

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	4LU	B	502	2,4	-	1/18/30/30	0/4/4/4
3	4LU	C	502	4	-	3/18/30/30	0/4/4/4
3	4LU	A	502	2,4	-	1/18/30/30	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	4LU	O2-C2	7.06	1.38	1.23
3	C	502	4LU	O2-C2	6.91	1.37	1.23
3	B	502	4LU	O2-C2	6.43	1.36	1.23
3	C	502	4LU	C5A-C6	3.39	1.42	1.39
3	A	502	4LU	C10-N10	3.18	1.44	1.38
3	C	502	4LU	C10-N10	3.00	1.43	1.38
3	C	502	4LU	C9A-N10	2.39	1.45	1.41
3	C	502	4LU	C4-N3	-2.36	1.34	1.38
3	C	502	4LU	C9-C9A	2.11	1.43	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	4LU	C5-C6-C5A	-7.05	113.78	121.48
3	A	502	4LU	C5-C6-C5A	-6.22	114.68	121.48
3	C	502	4LU	C12-C5-C3	-5.37	100.30	109.60
3	B	502	4LU	C4-C4A-C10	-5.32	116.81	121.08
3	C	502	4LU	C4A-C4-N3	3.99	120.11	111.79
3	C	502	4LU	C4-N3-C2	-3.88	120.74	126.34
3	B	502	4LU	C4A-C4-N3	3.87	119.87	111.79
3	A	502	4LU	C4A-C4-N3	3.83	119.78	111.79
3	B	502	4LU	C5-C6-C5A	-3.67	117.47	121.48
3	A	502	4LU	C4-N3-C2	-3.60	121.15	126.34
3	C	502	4LU	O3P-P-O5'	-3.58	97.20	106.73
3	A	502	4LU	O4-C4-C4A	-3.44	120.30	128.06
3	B	502	4LU	C4-N3-C2	-3.33	121.54	126.34
3	B	502	4LU	N1-C2-N3	3.26	121.05	115.80
3	C	502	4LU	N1-C2-N3	3.20	120.95	115.80
3	B	502	4LU	C12-C5-C3	-3.17	104.10	109.60
3	C	502	4LU	O1P-P-O3P	3.01	119.12	107.64
3	A	502	4LU	C12-C5-C3	-2.78	104.79	109.60
3	C	502	4LU	C4-C4A-C10	-2.72	118.89	121.08
3	B	502	4LU	O4-C4-C4A	-2.66	122.07	128.06
3	C	502	4LU	O2-C2-N3	-2.43	117.24	121.82
3	C	502	4LU	O4-C4-C4A	-2.41	122.62	128.06
3	A	502	4LU	N1-C2-N3	2.34	119.56	115.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	4LU	C3-C5-C6	2.29	112.62	107.38
3	A	502	4LU	C4-C4A-C10	-2.20	119.32	121.08
3	B	502	4LU	O2-C2-N3	-2.14	117.79	121.82
3	C	502	4LU	P-O5'-C5'	2.09	124.05	118.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	4LU	C2'-C1'-N10-C10
3	C	502	4LU	C2'-C1'-N10-C10
3	C	502	4LU	N10-C1'-C2'-O2'
3	B	502	4LU	C2'-C1'-N10-C10
3	C	502	4LU	C2'-C3'-C4'-C5'

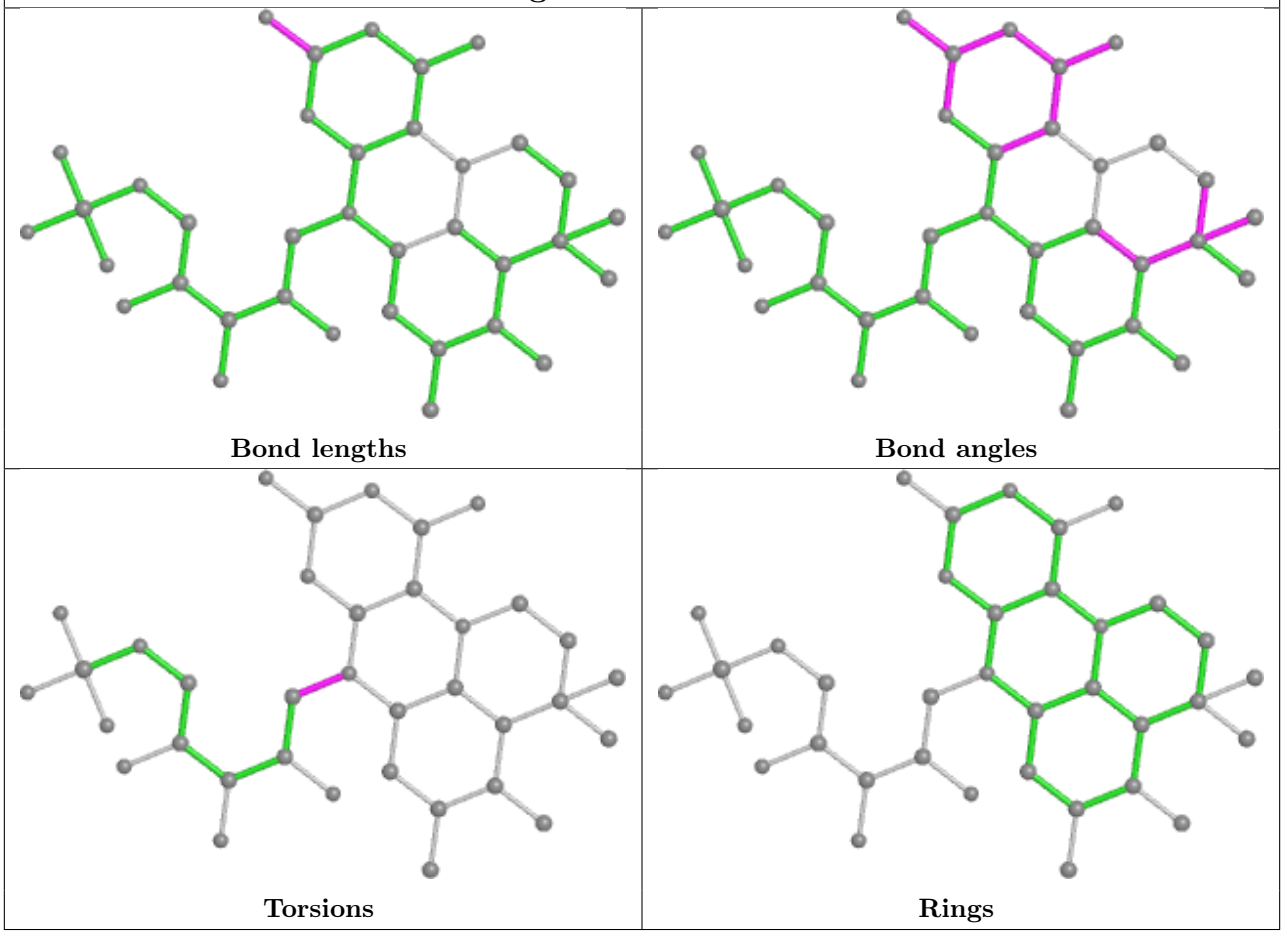
There are no ring outliers.

3 monomers are involved in 15 short contacts:

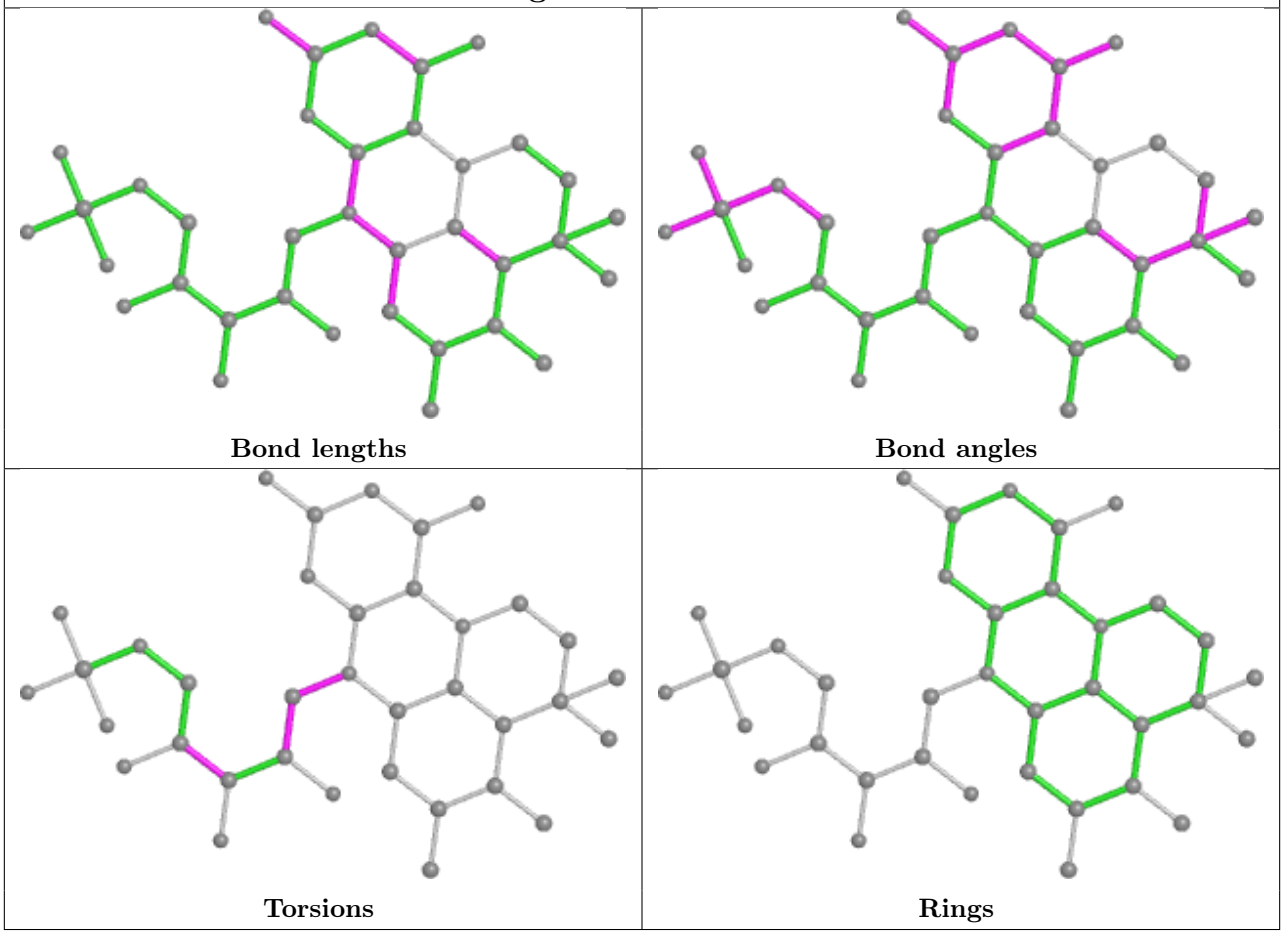
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	4LU	5	0
3	C	502	4LU	6	0
3	A	502	4LU	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

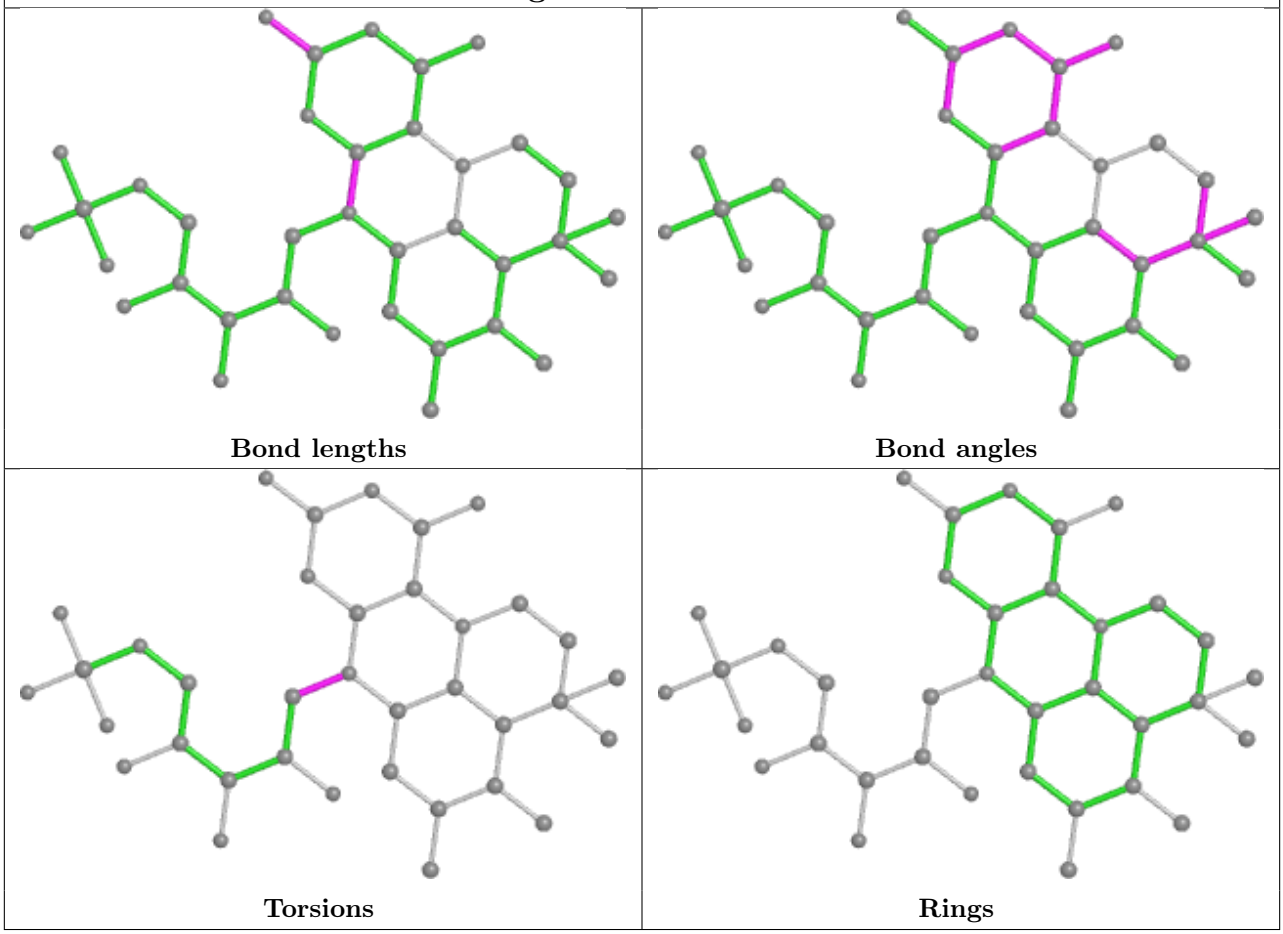
Ligand 4LU B 502



Ligand 4LU C 502



Ligand 4LU A 502



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	469/517 (90%)	0.20	23 (4%)	29	28	35, 74, 126, 159	0
1	B	465/517 (89%)	-0.07	5 (1%)	80	82	34, 51, 90, 130	0
1	C	459/517 (88%)	0.16	14 (3%)	49	49	34, 69, 137, 170	0
All	All	1393/1551 (89%)	0.10	42 (3%)	50	51	34, 62, 126, 170	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	234	PRO	4.7
1	A	91	LEU	4.6
1	A	176	LEU	4.6
1	A	6	TYR	4.3
1	C	238	THR	3.8
1	A	52	PHE	3.7
1	A	316	ILE	3.7
1	C	92	LEU	3.6
1	A	244	PHE	3.5
1	A	94	PHE	3.5
1	A	50	LEU	3.2
1	A	59	SER	3.2
1	A	96	LYS	3.1
1	A	28	PRO	3.1
1	A	115	LYS	3.1
1	B	6	TYR	3.0
1	A	25	ILE	3.0
1	A	239	LEU	3.0
1	A	95	LEU	2.9
1	A	92	LEU	2.9
1	A	77	MET	2.8
1	C	215	PHE	2.8
1	C	91	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	122	THR	2.7
1	B	80	GLU	2.7
1	A	80	GLU	2.6
1	C	244	PHE	2.5
1	C	247	LEU	2.5
1	C	220	ALA	2.5
1	B	489	ALA	2.4
1	A	222	GLY	2.3
1	A	93	ALA	2.3
1	A	242	TYR	2.3
1	B	491	PHE	2.3
1	B	172	GLU	2.2
1	C	236	PRO	2.2
1	A	54	ASN	2.2
1	C	273	LEU	2.1
1	C	237	ASP	2.1
1	A	229	LEU	2.1
1	C	121	PRO	2.1
1	C	16	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 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	MN	A	501	1/1	0.37	0.17	110,110,110,110	1
4	NA	A	503	1/1	0.65	0.30	60,60,60,60	1
4	NA	C	503	1/1	0.82	0.12	56,56,56,56	1
2	MN	B	501	1/1	0.86	0.10	95,95,95,95	0

Continued on next page...

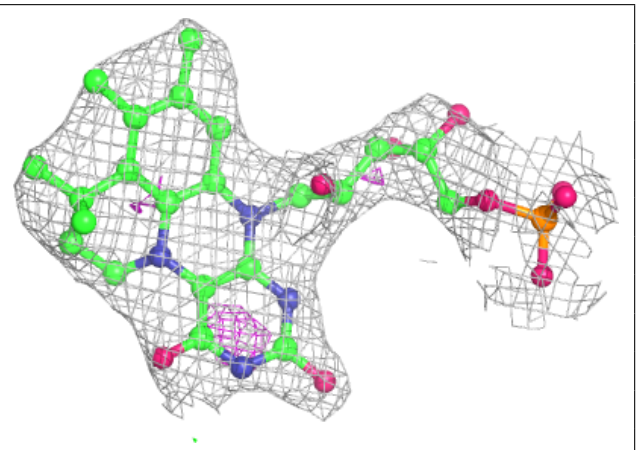
Continued from previous page...

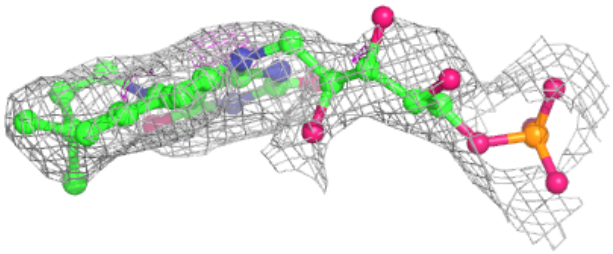
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	C	501	1/1	0.88	0.06	107,107,107,107	1
3	4LU	C	502	36/36	0.90	0.26	55,76,105,110	0
5	SO4	B	504	5/5	0.90	0.17	43,45,56,56	5
3	4LU	A	502	36/36	0.93	0.29	83,97,117,119	0
4	NA	B	503	1/1	0.97	0.14	66,66,66,66	0
3	4LU	B	502	36/36	0.98	0.14	35,42,53,59	0

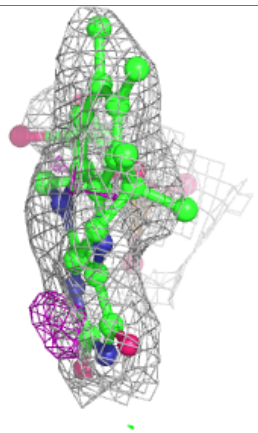
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 4LU C 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

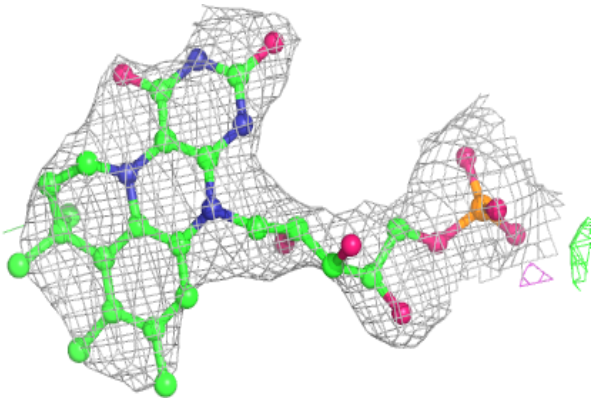


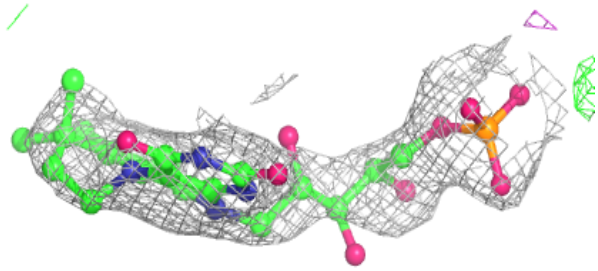


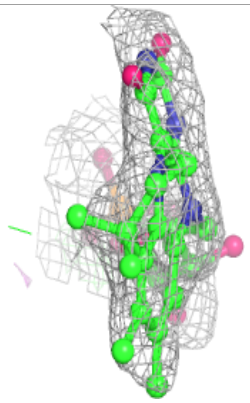


Electron density around 4LU A 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

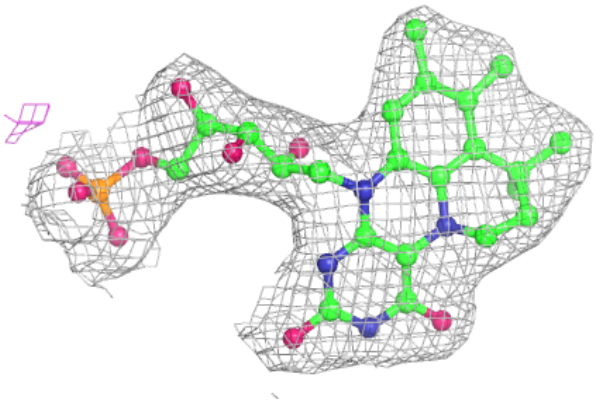


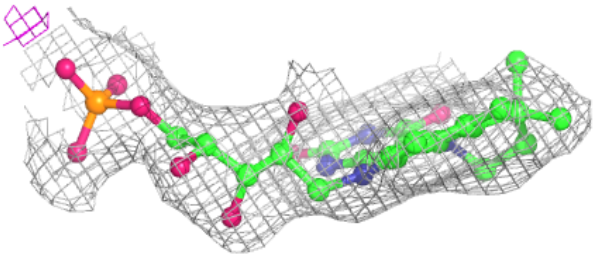


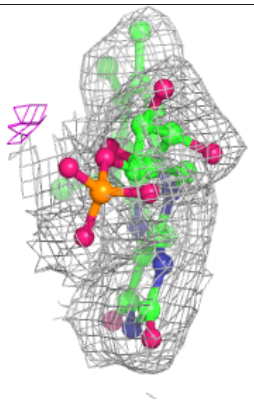


Electron density around 4LU B 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.