Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 01:56 PM EST

PDB ID	:	4XG1
Title	:	Psychromonas ingrahamii diaminopimelate decarboxylase with LLP
Authors	:	Peverelli, M.G.; Wubben, J.M.; Panjikar, S.; Perugini, M.A.
Deposited on	:	2014-12-30
Resolution	:	2.50 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:

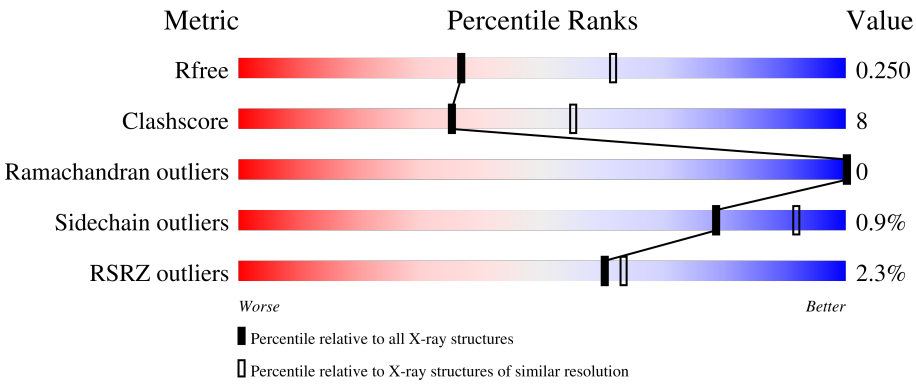
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	427	4% 77% 14% • 8%
1	B	427	% 85% 12% • •
1	C	427	% 82% 13% • •
1	D	427	2% 80% 13% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SCN	C	501	-	-	X	-
2	SCN	C	502	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13006 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 Diaminopimelate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	393	2998	1915	511	559	13	0	0	0
1	B	418	3216	2050	545	607	14	0	0	0
1	C	411	3173	2020	541	598	14	0	0	0
1	D	403	3080	1964	527	575	14	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	HIS	-	expression tag	UNP A1SR00
A	423	HIS	-	expression tag	UNP A1SR00
A	424	HIS	-	expression tag	UNP A1SR00
A	425	HIS	-	expression tag	UNP A1SR00
A	426	HIS	-	expression tag	UNP A1SR00
A	427	HIS	-	expression tag	UNP A1SR00
B	422	HIS	-	expression tag	UNP A1SR00
B	423	HIS	-	expression tag	UNP A1SR00
B	424	HIS	-	expression tag	UNP A1SR00
B	425	HIS	-	expression tag	UNP A1SR00
B	426	HIS	-	expression tag	UNP A1SR00
B	427	HIS	-	expression tag	UNP A1SR00
C	422	HIS	-	expression tag	UNP A1SR00
C	423	HIS	-	expression tag	UNP A1SR00
C	424	HIS	-	expression tag	UNP A1SR00
C	425	HIS	-	expression tag	UNP A1SR00
C	426	HIS	-	expression tag	UNP A1SR00
C	427	HIS	-	expression tag	UNP A1SR00
D	422	HIS	-	expression tag	UNP A1SR00
D	423	HIS	-	expression tag	UNP A1SR00
D	424	HIS	-	expression tag	UNP A1SR00

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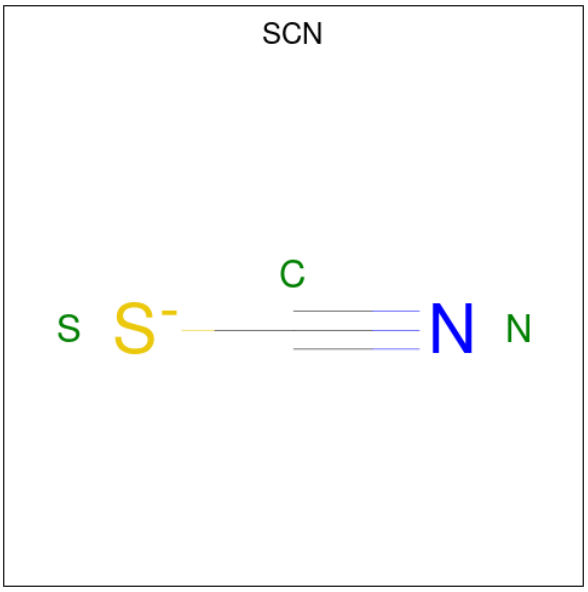
Chain	Residue	Modelled	Actual	Comment	Reference
D	425	HIS	-	expression tag	UNP A1SR00
D	426	HIS	-	expression tag	UNP A1SR00
D	427	HIS	-	expression tag	UNP A1SR00

- Molecule 2 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).

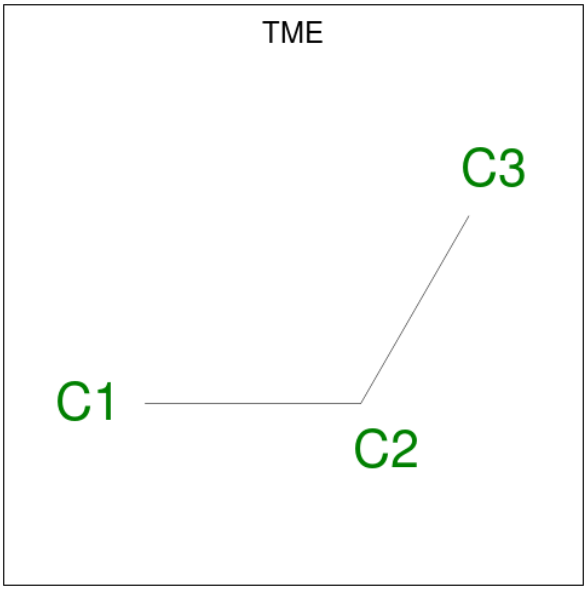


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
2	A	1	3	1	1	1	0	0
			Total	C	N	S		
2	A	1	3	1	1	1	0	0
			Total	C	N	S		
2	A	1	3	1	1	1	0	0
			Total	C	N	S		
2	A	1	3	1	1	1	0	0
			Total	C	N	S		
2	B	1	3	1	1	1	0	0
			Total	C	N	S		
2	B	1	3	1	1	1	0	0
			Total	C	N	S		
2	C	1	3	1	1	1	0	0
			Total	C	N	S		
2	C	1	3	1	1	1	0	0
			Total	C	N	S		
2	D	1	3	1	1	1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

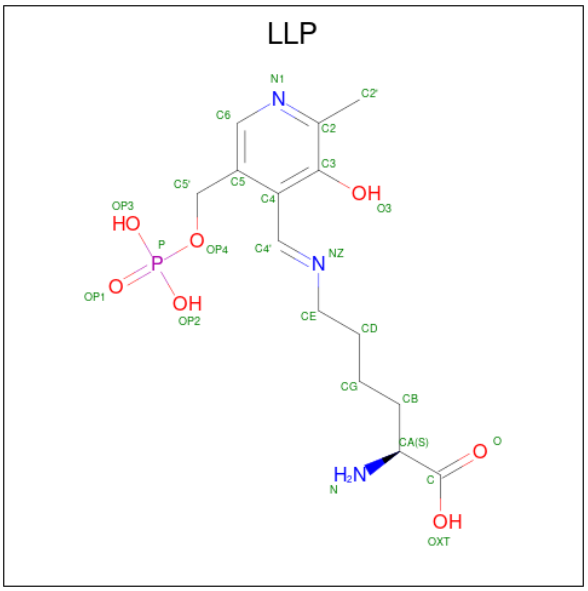
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0

- Molecule 4 is PROPANE (three-letter code: TME) (formula: C_3H_8).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 3 3	0	0
4	B	1	Total C 3 3	0	0
4	B	1	Total C 3 3	0	0
4	B	1	Total C 3 3	0	0
4	D	1	Total C 3 3	0	0

- Molecule 5 is (2S)-2-amino-6-[[3-hydroxy-2-methyl-5-(phosphonooxymethyl)pyridin-4-yl]methylideneamino]hexanoic acid (three-letter code: LLP) (formula: $C_{14}H_{22}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			25	14	3	7	1		
5	B	1	Total	C	N	O	P	0	0
			25	14	3	7	1		
5	C	1	Total	C	N	O	P	0	0
			25	14	3	7	1		
5	D	1	Total	C	N	O	P	0	0
			25	14	3	7	1		

- Molecule 6 is water.

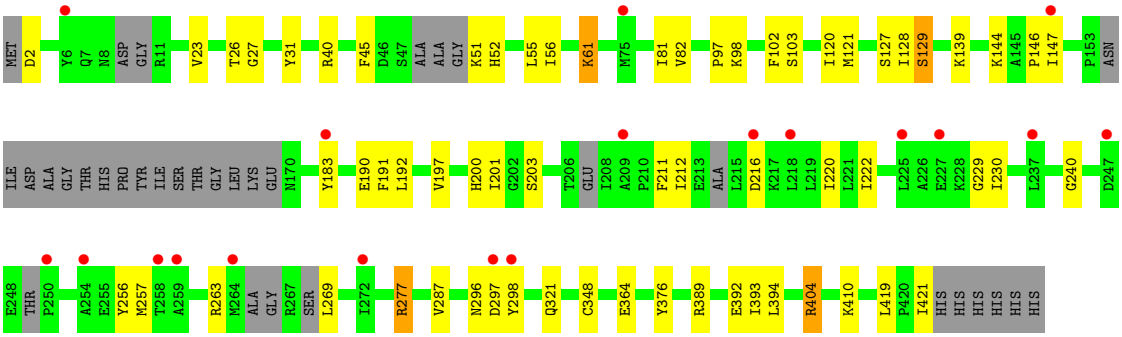
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	103	Total	O	0	0
			103	103		
6	B	106	Total	O	0	0
			106	106		
6	C	117	Total	O	0	0
			117	117		
6	D	65	Total	O	0	0
			65	65		

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.

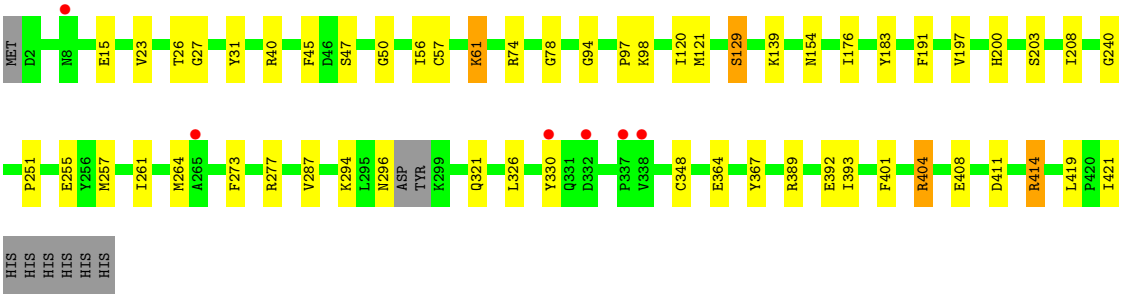
• Molecule 1: Diaminopimelate decarboxylase

Chain A:



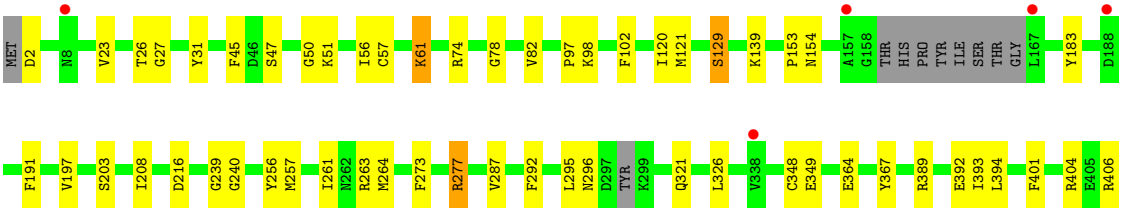
• Molecule 1: Diaminopimelate decarboxylase

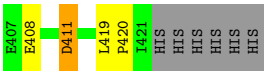
Chain B:



• Molecule 1: Diaminopimelate decarboxylase

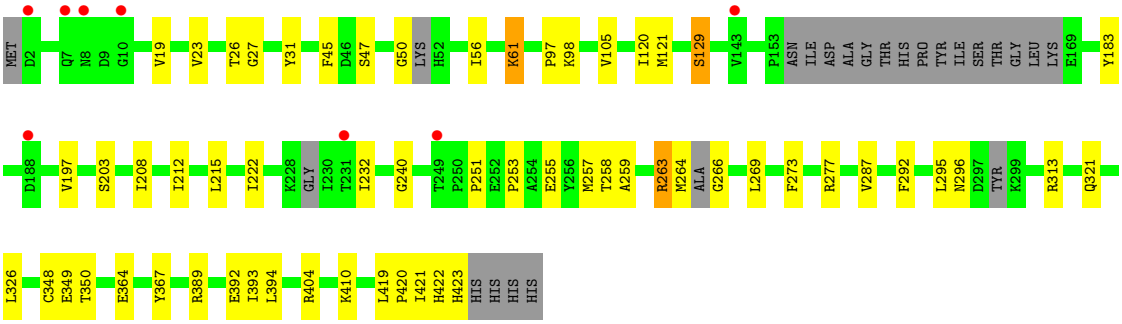
Chain C:





- Molecule 1: Diaminopimelate decarboxylase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.96Å 103.13Å 93.59Å 90.00° 94.77° 90.00°	Depositor
Resolution (Å)	19.85 – 2.50 19.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.85-2.50) 99.7 (19.85-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	7.51 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.211 , 0.246 0.215 , 0.250	Depositor DCC
R_{free} test set	1014 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13006	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: LLP, SCN, TME, K

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	0.65	0/3042	0.77	4/4101 (0.1%)
1	B	0.68	0/3275	0.81	6/4437 (0.1%)
1	C	0.62	0/3228	0.77	5/4367 (0.1%)
1	D	0.58	0/3133	0.75	3/4240 (0.1%)
All	All	0.63	0/12678	0.77	18/17145 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277	ARG	NE-CZ-NH1	-8.50	116.05	120.30
1	C	277	ARG	NE-CZ-NH1	-7.17	116.71	120.30
1	B	414	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	277	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	B	414	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	B	389	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	A	404	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	277	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	C	404	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	D	389	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	B	404	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	B	389	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	D	277	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	D	263	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	389	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	C	277	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	C	411	ASP	CB-CG-OD1	-5.23	113.60	118.30
1	A	389	ARG	NE-CZ-NH2	5.06	122.83	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	2998	0	2970	70	1
1	B	3216	0	3221	48	0
1	C	3173	0	3187	57	0
1	D	3080	0	3061	66	1
2	A	12	0	0	0	0
2	B	6	0	0	1	0
2	C	6	0	0	4	0
2	D	3	0	0	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	3	0	8	3	0
4	B	9	0	24	2	0
4	D	3	0	8	0	0
5	A	25	0	19	1	0
5	B	25	0	18	0	0
5	C	25	0	19	2	0
5	D	25	0	19	6	0
6	A	103	0	0	8	0
6	B	106	0	0	4	0
6	C	117	0	0	3	0
6	D	65	0	0	1	0
All	All	13006	0	12554	206	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 8.

All (206) 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:211:PHE:HE2	1:A:256:TYR:CE1	1.57	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:NZ	1:B:348:CYS:SG	2.12	1.20
1:A:211:PHE:CE2	1:A:256:TYR:CE1	2.31	1.18
1:C:61:LYS:NZ	1:D:348:CYS:SG	2.16	1.18
1:A:348:CYS:SG	1:B:61:LYS:NZ	2.20	1.13
1:A:61:LYS:CE	1:B:348:CYS:SG	2.38	1.11
1:C:348:CYS:SG	1:D:61:LYS:NZ	2.21	1.11
1:A:348:CYS:SG	1:B:61:LYS:CE	2.42	1.07
1:C:61:LYS:CE	1:D:348:CYS:SG	2.43	1.07
1:A:45:PHE:O	1:A:257:MET:CE	2.03	1.06
1:C:348:CYS:SG	1:D:61:LYS:CE	2.44	1.05
1:A:211:PHE:CE2	1:A:256:TYR:HE1	1.72	1.04
1:C:295:LEU:O	1:C:296:ASN:ND2	2.02	0.92
1:A:211:PHE:CE2	1:A:256:TYR:CD1	2.61	0.88
1:A:211:PHE:HE2	1:A:256:TYR:CD1	1.92	0.88
1:A:229:GLY:C	1:A:230:ILE:CA	2.44	0.86
1:A:45:PHE:O	1:A:257:MET:HE2	1.75	0.85
2:C:501:SCN:S	5:D:504:LLP:HE2	2.18	0.84
1:A:222:ILE:HD13	1:A:269:LEU:HD11	1.62	0.80
1:D:264:MET:O	1:D:266:GLY:N	2.16	0.79
1:A:211:PHE:CD2	1:A:256:TYR:HE1	2.02	0.78
1:A:211:PHE:CD2	1:A:256:TYR:CE1	2.73	0.76
1:C:257:MET:O	1:C:261:ILE:HG12	1.85	0.76
1:D:255:GLU:O	1:D:258:THR:HG22	1.86	0.75
1:B:154:ASN:HD22	1:B:176:ILE:HG21	1.51	0.74
1:D:222:ILE:HD13	1:D:269:LEU:CD2	2.19	0.72
1:A:348:CYS:SG	1:B:61:LYS:HE3	2.29	0.72
1:A:61:LYS:HE3	1:B:348:CYS:SG	2.29	0.72
1:A:45:PHE:O	1:A:257:MET:HE1	1.91	0.71
1:D:203:SER:OG	5:D:504:LLP:OP3	2.07	0.71
1:C:239:GLY:HA2	2:C:502:SCN:C	2.21	0.71
1:A:200:HIS:HA	6:A:683:HOH:O	1.91	0.70
1:C:348:CYS:SG	1:D:61:LYS:HE3	2.32	0.70
1:C:74:ARG:HH12	1:D:421:ILE:HB	1.56	0.69
1:C:61:LYS:HE3	1:D:348:CYS:SG	2.33	0.69
1:A:216:ASP:O	1:A:220:ILE:HD13	1.93	0.68
1:D:258:THR:HG23	1:D:259:ALA:N	2.08	0.68
1:D:419:LEU:HB3	1:D:421:ILE:HD11	1.75	0.68
1:A:212:ILE:HG23	1:A:263:ARG:HD2	1.76	0.67
1:A:201:ILE:N	6:A:683:HOH:O	1.92	0.67
1:A:147:ILE:HD11	1:A:192:LEU:HD22	1.77	0.67
1:B:15:GLU:OE1	6:B:619:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LEU:C	1:C:296:ASN:HD22	1.98	0.66
6:A:674:HOH:O	1:C:408:GLU:HG2	1.95	0.65
1:D:419:LEU:HB3	1:D:421:ILE:CD1	2.26	0.65
1:C:411:ASP:OD2	6:C:697:HOH:O	2.15	0.65
1:D:45:PHE:HB3	1:D:56:ILE:HD13	1.79	0.64
1:B:26:THR:HG23	1:B:27:GLY:O	1.98	0.64
1:A:26:THR:HG23	1:A:27:GLY:O	1.98	0.64
1:C:26:THR:HG23	1:C:27:GLY:O	1.98	0.64
1:A:128:ILE:H	4:A:507:TME:H32	1.63	0.64
1:D:26:THR:HG23	1:D:27:GLY:O	1.98	0.63
1:D:222:ILE:HD13	1:D:269:LEU:HD22	1.81	0.62
1:A:61:LYS:HE2	1:B:348:CYS:SG	2.38	0.61
1:A:190:GLU:H	1:A:190:GLU:CD	2.04	0.61
1:A:23:VAL:HA	1:A:26:THR:HG22	1.83	0.61
1:A:51:LYS:O	1:A:52:HIS:C	2.40	0.61
1:B:45:PHE:HB3	1:B:56:ILE:HD13	1.84	0.60
1:A:147:ILE:HD12	1:A:192:LEU:HB3	1.83	0.60
1:C:23:VAL:HA	1:C:26:THR:HG22	1.84	0.60
1:C:45:PHE:HB3	1:C:56:ILE:HD13	1.85	0.59
1:A:45:PHE:HB3	1:A:56:ILE:HD13	1.83	0.59
1:A:212:ILE:HG23	1:A:263:ARG:CD	2.32	0.59
1:B:411:ASP:HA	1:B:414:ARG:HG3	1.83	0.59
1:C:277:ARG:HD2	6:C:658:HOH:O	2.01	0.59
1:B:23:VAL:HA	1:B:26:THR:HG22	1.83	0.59
1:A:82:VAL:C	1:A:102:PHE:HE1	2.07	0.58
1:C:239:GLY:HA2	2:C:502:SCN:S	2.43	0.58
1:D:23:VAL:HA	1:D:26:THR:HG22	1.85	0.57
1:C:61:LYS:HE2	1:D:348:CYS:SG	2.41	0.55
1:B:255:GLU:OE1	6:B:691:HOH:O	2.18	0.55
1:C:74:ARG:NH1	1:D:421:ILE:HB	2.20	0.55
1:C:348:CYS:SG	1:D:61:LYS:HE2	2.42	0.55
1:D:45:PHE:HB3	1:D:56:ILE:CD1	2.36	0.55
1:A:127:SER:HB2	4:A:507:TME:H33	1.88	0.54
1:C:394:LEU:HD23	1:D:419:LEU:HD13	1.89	0.54
1:D:258:THR:CG2	1:D:259:ALA:N	2.69	0.54
1:C:277:ARG:NH1	5:C:504:LLP:OXT	2.30	0.54
1:A:348:CYS:SG	1:B:61:LYS:HE2	2.41	0.54
1:B:94:GLY:HA3	1:D:420:PRO:HB2	1.89	0.54
1:A:55:LEU:HA	6:A:688:HOH:O	2.08	0.54
1:A:296:ASN:OD1	1:A:298:TYR:N	2.29	0.54
1:A:147:ILE:CD1	1:A:192:LEU:HD22	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:PRO:O	1:B:120:ILE:HA	2.09	0.53
1:B:408:GLU:OE2	1:D:410:LYS:NZ	2.38	0.53
1:D:232:ILE:O	1:D:269:LEU:CD1	2.57	0.53
1:C:82:VAL:C	1:C:102:PHE:HE1	2.11	0.53
1:D:45:PHE:CE1	1:D:253:PRO:HB3	2.44	0.52
1:C:129:SER:OG	1:D:364:GLU:OE2	2.15	0.52
1:B:330:TYR:OH	2:B:502:SCN:S	2.63	0.51
1:D:97:PRO:O	1:D:120:ILE:HA	2.10	0.51
1:B:208:ILE:H	4:B:505:TME:C3	2.23	0.51
1:D:105:VAL:HG22	6:D:634:HOH:O	2.10	0.51
1:C:2:ASP:OD1	6:C:609:HOH:O	2.19	0.51
1:A:2:ASP:N	1:A:40:ARG:HH22	2.08	0.51
1:C:97:PRO:O	1:C:120:ILE:HA	2.10	0.51
1:D:212:ILE:CG2	1:D:263:ARG:CZ	2.89	0.51
5:C:504:LLP:N	1:D:349:GLU:OE2	2.44	0.51
1:A:376:TYR:CE1	5:A:508:LLP:HG3	2.45	0.50
1:C:349:GLU:HG2	5:D:504:LLP:HD3	1.93	0.50
1:A:55:LEU:HD12	6:A:688:HOH:O	2.09	0.50
1:D:208:ILE:HG13	1:D:251:PRO:CG	2.41	0.50
1:A:211:PHE:CD2	1:A:256:TYR:CD1	2.99	0.50
1:C:216:ASP:OD1	1:C:263:ARG:HD2	2.12	0.50
1:A:129:SER:OG	1:B:364:GLU:OE2	2.18	0.50
1:D:47:SER:O	1:D:50:GLY:N	2.45	0.50
1:C:26:THR:HG21	1:C:393:ILE:HD11	1.94	0.49
1:A:410:LYS:NZ	1:C:406:ARG:O	2.45	0.49
1:D:26:THR:HG21	1:D:393:ILE:HD11	1.93	0.49
1:D:183:TYR:OH	1:D:197:VAL:HG22	2.12	0.49
1:A:103:SER:HB3	6:A:614:HOH:O	2.12	0.49
1:C:47:SER:O	1:C:50:GLY:N	2.46	0.49
1:A:97:PRO:O	1:A:120:ILE:HA	2.12	0.49
1:D:212:ILE:CG2	1:D:263:ARG:NH1	2.76	0.49
1:A:421:ILE:HD13	1:B:74:ARG:CZ	2.43	0.49
1:B:183:TYR:OH	1:B:197:VAL:HG22	2.13	0.48
1:A:56:ILE:N	6:A:688:HOH:O	2.06	0.48
1:B:47:SER:O	1:B:50:GLY:N	2.45	0.48
1:A:183:TYR:OH	1:A:197:VAL:HG22	2.12	0.48
1:C:45:PHE:HB3	1:C:56:ILE:CD1	2.43	0.48
1:C:216:ASP:OD2	1:C:263:ARG:NH1	2.48	0.47
1:D:350:THR:HG23	2:D:501:SCN:N	2.28	0.47
1:A:45:PHE:HB3	1:A:56:ILE:CD1	2.43	0.47
1:B:45:PHE:HB3	1:B:56:ILE:CD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:TYR:OH	1:C:197:VAL:HG22	2.15	0.47
1:D:232:ILE:O	1:D:269:LEU:HD11	2.14	0.47
1:D:326:LEU:HD22	1:D:367:TYR:HB2	1.97	0.47
1:A:203:SER:OG	1:A:277:ARG:NH2	2.48	0.46
1:A:2:ASP:N	1:A:40:ARG:NH2	2.63	0.46
1:C:129:SER:HB3	1:D:292:PHE:CD1	2.49	0.46
1:A:190:GLU:HG2	1:A:191:PHE:CD2	2.50	0.46
1:B:26:THR:HG21	1:B:393:ILE:HD11	1.97	0.46
1:B:139:LYS:HG3	1:B:191:PHE:CE2	2.51	0.46
1:A:26:THR:HG21	1:A:393:ILE:HD11	1.96	0.46
1:C:203:SER:OG	1:C:277:ARG:NH2	2.48	0.46
1:D:215:LEU:HD23	1:D:263:ARG:HG3	1.98	0.46
1:C:349:GLU:CG	5:D:504:LLP:HD3	2.45	0.46
1:D:258:THR:CG2	1:D:259:ALA:H	2.29	0.46
1:D:212:ILE:HG21	1:D:263:ARG:CZ	2.47	0.45
1:A:394:LEU:HD23	1:B:419:LEU:HD13	1.98	0.45
1:C:326:LEU:HD22	1:C:367:TYR:HB2	1.97	0.45
1:D:23:VAL:HG11	1:D:287:VAL:HG11	1.98	0.45
1:B:208:ILE:HG13	1:B:251:PRO:CG	2.47	0.45
1:A:296:ASN:OD1	1:A:297:ASP:N	2.50	0.44
1:C:31:TYR:HB2	1:C:392:GLU:HG2	1.98	0.44
1:A:31:TYR:HB2	1:A:392:GLU:HG2	1.99	0.44
1:D:232:ILE:HG22	1:D:269:LEU:HD11	1.99	0.44
1:D:257:MET:SD	1:D:273:PHE:CZ	3.10	0.44
1:A:222:ILE:CD1	1:A:269:LEU:HD11	2.40	0.44
1:D:203:SER:HA	1:D:240:GLY:HA2	1.98	0.44
1:D:313:ARG:HH21	5:D:504:LLP:HN2	1.64	0.44
1:A:419:LEU:HD11	1:B:401:PHE:HB3	2.00	0.44
1:A:23:VAL:HG11	1:A:287:VAL:HG11	1.99	0.44
1:A:146:PRO:C	1:A:147:ILE:HG13	2.38	0.44
1:C:364:GLU:OE2	1:D:129:SER:OG	2.27	0.44
1:C:419:LEU:HG	1:C:420:PRO:HD2	1.99	0.44
1:C:261:ILE:O	1:C:264:MET:HB2	2.18	0.43
1:B:255:GLU:CD	6:B:691:HOH:O	2.55	0.43
1:C:23:VAL:HG11	1:C:287:VAL:HG11	2.00	0.43
1:A:81:ILE:HG13	1:A:102:PHE:CD1	2.53	0.43
1:D:222:ILE:HD13	1:D:269:LEU:HD21	1.98	0.43
2:C:501:SCN:S	5:D:504:LLP:CE	3.01	0.43
1:A:364:GLU:OE2	1:B:129:SER:OG	2.24	0.43
1:B:23:VAL:HG11	1:B:287:VAL:HG11	2.00	0.43
1:A:61:LYS:NZ	1:B:348:CYS:CB	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:GLU:HB2	1:B:404:ARG:HB3	2.01	0.43
1:D:422:HIS:O	1:D:423:HIS:HB2	2.19	0.43
1:A:203:SER:HA	1:A:240:GLY:HA2	2.00	0.42
1:C:153:PRO:O	1:C:154:ASN:HB2	2.19	0.42
1:B:57:CYS:HA	1:B:78:GLY:C	2.39	0.42
1:C:74:ARG:NH1	1:D:421:ILE:HD13	2.34	0.42
1:A:98:LYS:O	1:A:121:MET:HB2	2.20	0.42
1:B:200:HIS:HA	6:B:627:HOH:O	2.18	0.42
1:C:292:PHE:CD1	1:D:129:SER:HB3	2.55	0.42
1:C:57:CYS:HA	1:C:78:GLY:C	2.40	0.42
1:C:208:ILE:HD13	1:C:256:TYR:HA	2.01	0.42
1:D:31:TYR:HB2	1:D:392:GLU:HG2	2.01	0.42
4:A:507:TME:H33	1:B:294:LYS:HG2	2.02	0.42
1:B:31:TYR:HB2	1:B:392:GLU:HG2	2.01	0.42
1:B:261:ILE:O	1:B:264:MET:HB2	2.19	0.42
1:B:98:LYS:O	1:B:121:MET:HB2	2.19	0.42
1:B:296:ASN:OD1	1:B:296:ASN:C	2.57	0.42
1:A:103:SER:CB	6:A:614:HOH:O	2.68	0.42
1:B:326:LEU:HD22	1:B:367:TYR:HB2	2.01	0.42
1:C:419:LEU:HD13	1:D:394:LEU:HD23	2.01	0.41
1:D:98:LYS:O	1:D:121:MET:HB2	2.19	0.41
1:B:203:SER:HA	1:B:240:GLY:HA2	2.02	0.41
1:C:98:LYS:O	1:C:121:MET:HB2	2.21	0.41
1:D:45:PHE:CD1	1:D:253:PRO:HB3	2.56	0.41
1:B:421:ILE:O	1:B:421:ILE:HG13	2.20	0.41
1:C:139:LYS:HG3	1:C:191:PHE:CE2	2.55	0.41
1:B:40:ARG:HB2	4:B:507:TME:H31	2.02	0.41
1:B:408:GLU:OE2	1:D:410:LYS:CE	2.69	0.41
1:A:392:GLU:HB2	1:A:404:ARG:HB3	2.03	0.41
1:C:401:PHE:CD2	1:D:419:LEU:HD11	2.56	0.41
1:C:74:ARG:CZ	1:D:421:ILE:HD13	2.51	0.41
1:D:392:GLU:HB2	1:D:404:ARG:HB3	2.04	0.40
1:A:139:LYS:HG3	1:A:191:PHE:CE2	2.56	0.40
1:B:257:MET:SD	1:B:273:PHE:CZ	3.14	0.40
1:D:19:VAL:HB	1:D:326:LEU:HD11	2.03	0.40
1:D:222:ILE:CD1	1:D:269:LEU:CD2	2.95	0.40
1:D:295:LEU:O	1:D:296:ASN:ND2	2.53	0.40
1:A:144:LYS:HE2	1:A:190:GLU:O	2.22	0.40
1:C:51:LYS:HA	1:C:51:LYS:HD3	1.97	0.40
1:C:203:SER:HA	1:C:240:GLY:HA2	2.03	0.40
1:C:257:MET:SD	1:C:273:PHE:CZ	3.15	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)
1:A:139:LYS:O	1:D:263:ARG:NH2[2_655]	1.85	0.35

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	374/427 (88%)	362 (97%)	12 (3%)	0	100	100
1	B	414/427 (97%)	399 (96%)	15 (4%)	0	100	100
1	C	405/427 (95%)	390 (96%)	15 (4%)	0	100	100
1	D	391/427 (92%)	376 (96%)	15 (4%)	0	100	100
All	All	1584/1708 (93%)	1527 (96%)	57 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	311/355 (88%)	308 (99%)	3 (1%)	76	90
1	B	340/355 (96%)	337 (99%)	3 (1%)	78	92
1	C	337/355 (95%)	334 (99%)	3 (1%)	78	92
1	D	321/355 (90%)	318 (99%)	3 (1%)	78	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1309/1420 (92%)	1297 (99%)	12 (1%)	78 92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	129	SER
1	A	321	GLN
1	B	61	LYS
1	B	129	SER
1	B	321	GLN
1	C	61	LYS
1	C	129	SER
1	C	321	GLN
1	D	61	LYS
1	D	129	SER
1	D	321	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	B	21	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 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	TME	B	506	-	2,2,2	0.32	0	0,1,1	-	-
5	LLP	B	508	-	24,25,25	2.40	5 (20%)	31,34,34	1.53	5 (16%)
2	SCN	A	504	-	1,2,2	0.58	0	0,1,1	-	-
5	LLP	A	508	-	24,25,25	2.07	4 (16%)	31,34,34	2.41	12 (38%)
2	SCN	A	501	-	1,2,2	0.25	0	0,1,1	-	-
2	SCN	C	502	-	1,2,2	0.98	0	0,1,1	-	-
2	SCN	C	501	-	1,2,2	0.09	0	0,1,1	-	-
2	SCN	D	501	-	1,2,2	0.49	0	0,1,1	-	-
5	LLP	D	504	-	24,25,25	2.79	5 (20%)	31,34,34	2.32	12 (38%)
2	SCN	A	502	-	1,2,2	1.09	0	0,1,1	-	-
5	LLP	C	504	-	24,25,25	2.19	5 (20%)	31,34,34	1.65	8 (25%)
2	SCN	A	503	-	1,2,2	0.92	0	0,1,1	-	-
2	SCN	B	502	-	1,2,2	0.53	0	0,1,1	-	-
4	TME	A	507	-	2,2,2	0.30	0	0,1,1	-	-
4	TME	D	503	-	2,2,2	0.28	0	0,1,1	-	-
2	SCN	B	501	-	1,2,2	0.27	0	0,1,1	-	-
4	TME	B	507	-	2,2,2	0.62	0	0,1,1	-	-
4	TME	B	505	-	2,2,2	0.59	0	0,1,1	-	-

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
5	LLP	B	508	-	-	4/19/19/19	0/1/1/1
5	LLP	C	504	-	-	1/19/19/19	0/1/1/1
5	LLP	A	508	-	-	4/19/19/19	0/1/1/1
5	LLP	D	504	-	-	7/19/19/19	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	504	LLP	C3-C2	9.20	1.50	1.40
5	B	508	LLP	C3-C2	7.08	1.48	1.40
5	A	508	LLP	C3-C2	6.88	1.47	1.40
5	C	504	LLP	C3-C2	6.80	1.47	1.40
5	D	504	LLP	C4-C3	5.60	1.49	1.40
5	B	508	LLP	C4'-NZ	5.41	1.45	1.27
5	D	504	LLP	C4'-NZ	5.36	1.45	1.27
5	C	504	LLP	C4-C5	5.12	1.48	1.42
5	B	508	LLP	C4-C5	4.92	1.48	1.42
5	D	504	LLP	C4-C5	4.84	1.48	1.42
5	C	504	LLP	C4'-NZ	4.78	1.43	1.27
5	A	508	LLP	C4'-NZ	4.51	1.42	1.27
5	B	508	LLP	C4-C3	4.20	1.47	1.40
5	A	508	LLP	C4-C5	3.80	1.46	1.42
5	D	504	LLP	C4-C4'	2.89	1.52	1.46
5	B	508	LLP	OXT-C	-2.48	1.22	1.30
5	C	504	LLP	C4-C3	2.48	1.44	1.40
5	C	504	LLP	C4-C4'	2.24	1.50	1.46
5	A	508	LLP	OXT-C	-2.12	1.23	1.30

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	508	LLP	C5-C4-C4'	6.29	131.91	121.56
5	D	504	LLP	C4-C3-C2	-5.85	116.56	120.19
5	A	508	LLP	C3-C4-C4'	-4.98	111.13	120.41
5	D	504	LLP	CB-CA-N	4.47	121.88	110.17
5	D	504	LLP	C3-C4-C4'	3.92	127.72	120.41
5	D	504	LLP	OP4-C5'-C5	3.63	116.27	109.35
5	A	508	LLP	O3-C3-C2	3.61	125.36	117.49
5	D	504	LLP	C5-C4-C4'	-3.59	115.65	121.56
5	B	508	LLP	OXT-C-O	-3.56	116.01	124.09
5	A	508	LLP	OP2-P-OP4	-3.39	97.70	106.73
5	A	508	LLP	C2'-C2-C3	-3.37	116.73	120.89
5	D	504	LLP	O-C-CA	-3.34	110.33	122.14
5	D	504	LLP	OXT-C-O	3.33	131.64	124.09
5	C	504	LLP	C4-C3-C2	-3.32	118.13	120.19
5	C	504	LLP	OP2-P-OP4	-3.30	97.95	106.73
5	A	508	LLP	OP3-P-OP1	3.25	123.39	110.68
5	A	508	LLP	C4-C3-C2	-3.20	118.21	120.19
5	A	508	LLP	CB-CA-C	-2.98	103.21	110.30
5	D	504	LLP	CD-CE-NZ	2.98	118.22	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	508	LLP	CD-CE-NZ	2.97	118.22	110.93
5	C	504	LLP	OXT-C-O	-2.91	117.48	124.09
5	C	504	LLP	C3-C4-C5	-2.86	116.07	118.26
5	A	508	LLP	OXT-C-CA	2.76	122.77	113.38
5	B	508	LLP	C6-N1-C2	2.71	124.18	119.17
5	B	508	LLP	OXT-C-CA	2.65	122.39	113.38
5	C	504	LLP	O3-C3-C2	2.56	123.08	117.49
5	A	508	LLP	OXT-C-O	-2.55	118.30	124.09
5	C	504	LLP	C4-C4'-NZ	-2.37	113.42	124.31
5	C	504	LLP	OP2-P-OP1	2.31	119.71	110.68
5	C	504	LLP	OXT-C-CA	2.24	121.03	113.38
5	D	504	LLP	CG-CB-CA	-2.20	106.27	113.35
5	A	508	LLP	C5'-C5-C6	2.17	122.95	119.37
5	D	504	LLP	OP3-P-OP2	2.14	115.83	107.64
5	A	508	LLP	CB-CA-N	2.14	115.78	110.17
5	D	504	LLP	C3-C4-C5	-2.12	116.63	118.26
5	B	508	LLP	C3-C2-N1	-2.12	118.03	120.77
5	D	504	LLP	OP3-P-OP4	-2.00	101.40	106.73

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	508	LLP	N-CA-CB-CG
5	A	508	LLP	C-CA-CB-CG
5	C	504	LLP	CD-CE-NZ-C4'
5	D	504	LLP	C4-C4'-NZ-CE
5	B	508	LLP	CD-CE-NZ-C4'
5	D	504	LLP	CG-CD-CE-NZ
5	A	508	LLP	CE-CD-CG-CB
5	D	504	LLP	CE-CD-CG-CB
5	B	508	LLP	CA-CB-CG-CD
5	D	504	LLP	OXT-C-CA-CB
5	A	508	LLP	C4-C4'-NZ-CE
5	B	508	LLP	C4-C4'-NZ-CE
5	B	508	LLP	C-CA-CB-CG
5	D	504	LLP	C-CA-CB-CG
5	D	504	LLP	N-CA-CB-CG
5	D	504	LLP	O-C-CA-CB

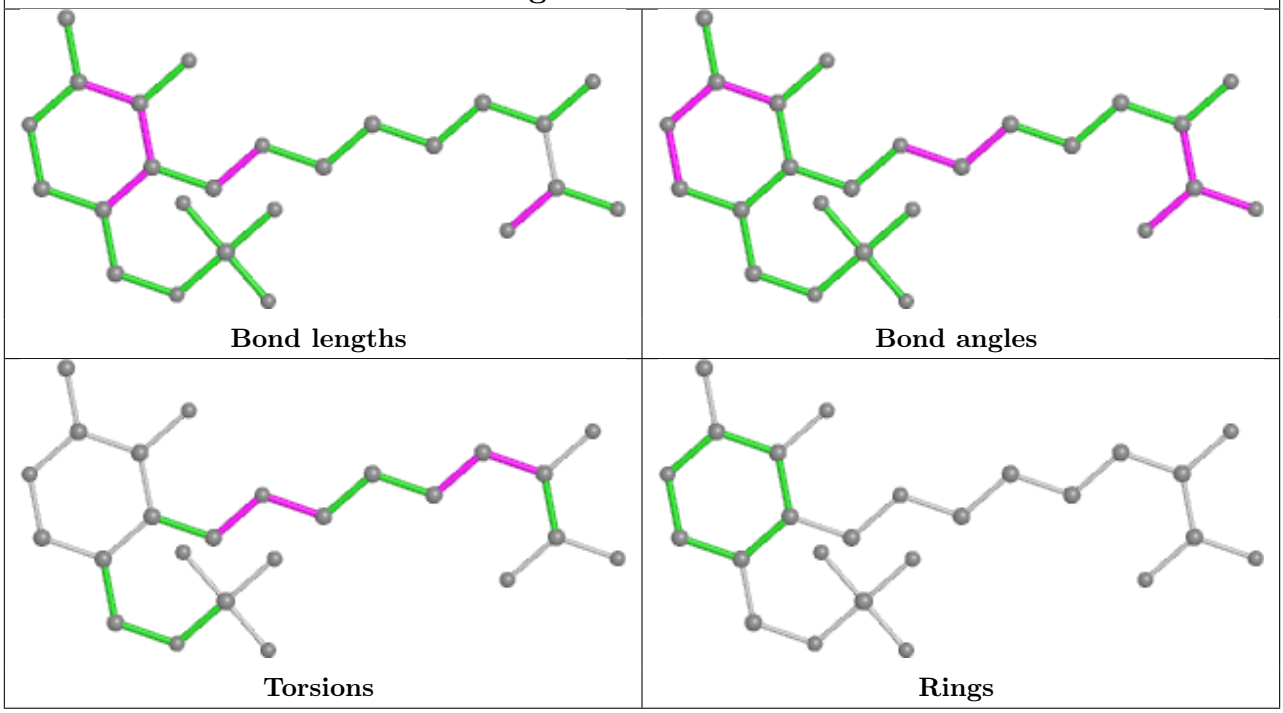
There are no ring outliers.

10 monomers are involved in 18 short contacts:

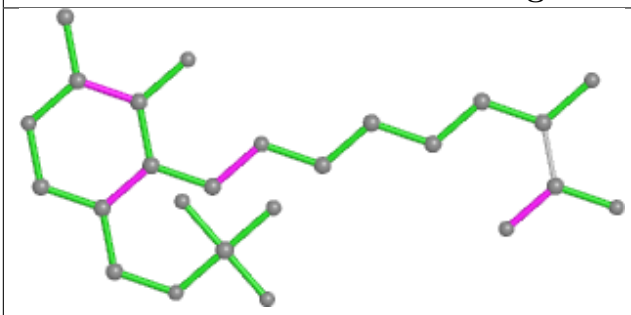
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	508	LLP	1	0
2	C	502	SCN	2	0
2	C	501	SCN	2	0
2	D	501	SCN	1	0
5	D	504	LLP	6	0
5	C	504	LLP	2	0
2	B	502	SCN	1	0
4	A	507	TME	3	0
4	B	507	TME	1	0
4	B	505	TME	1	0

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 LLP B 508



Ligand LLP A 508



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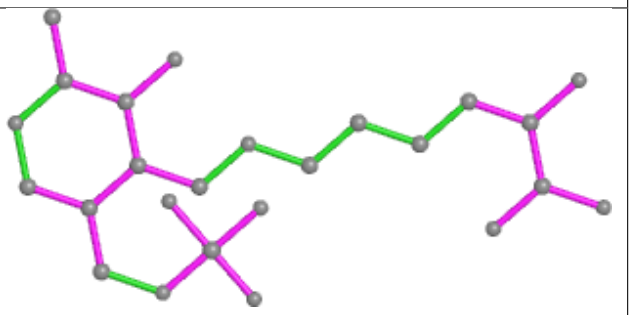
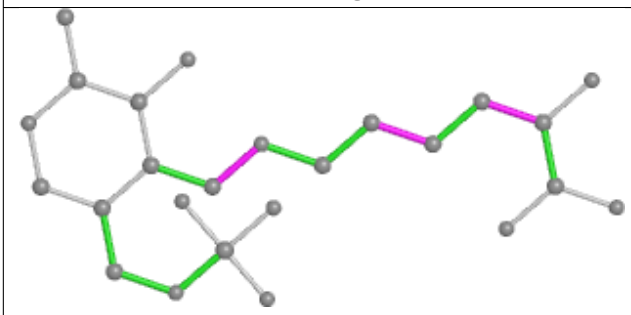
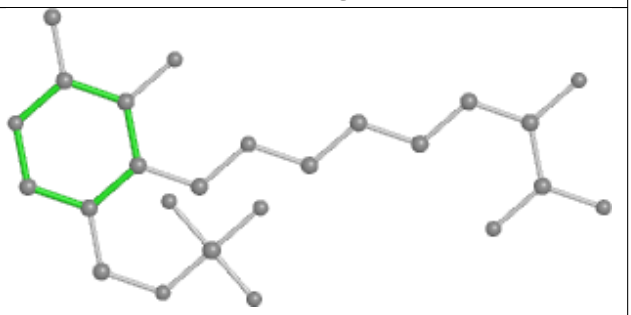


Bond angles

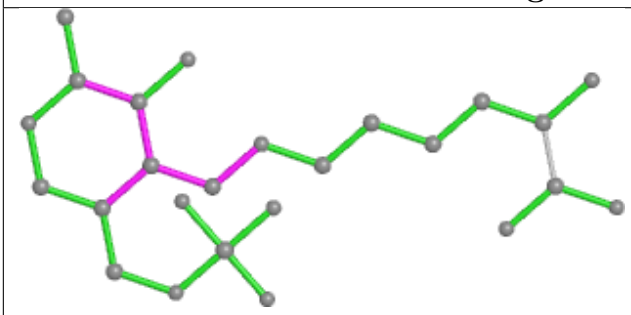


Torsions

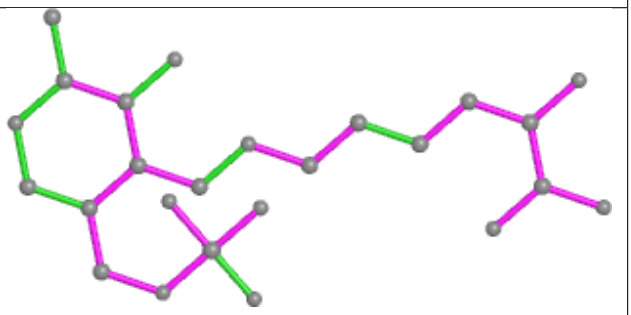


Rings

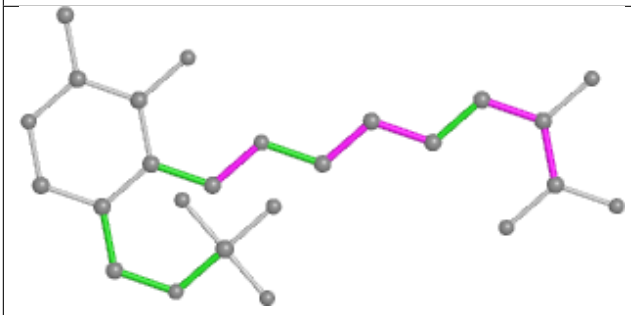
Ligand LLP D 504



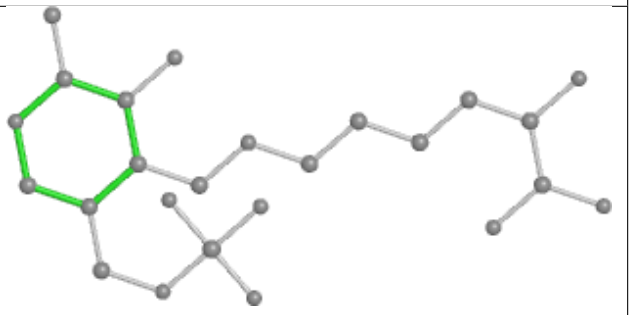
Bond lengths



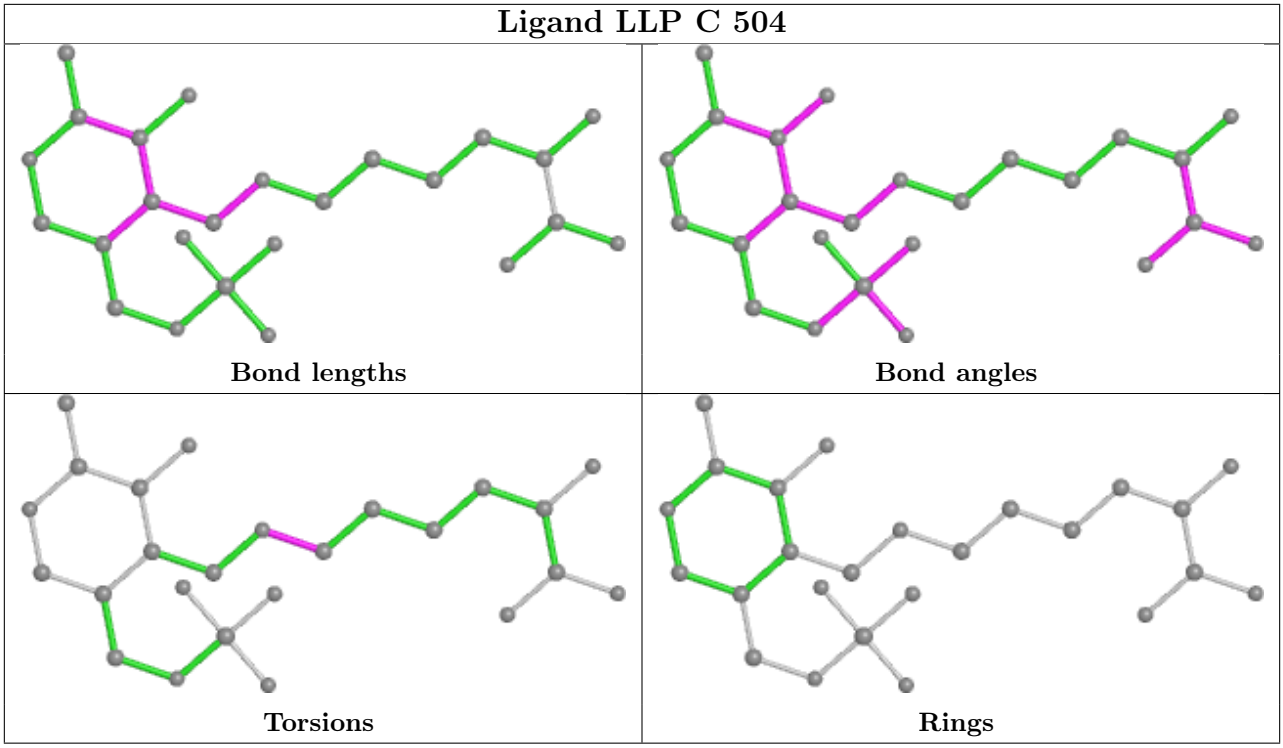
Bond angles



Torsions



Rings



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	393/427 (92%)	0.16	19 (4%)	30	32	5, 30, 60, 79	0
1	B	418/427 (97%)	-0.15	6 (1%)	75	77	6, 24, 54, 72	0
1	C	411/427 (96%)	-0.20	5 (1%)	79	80	11, 26, 56, 76	0
1	D	403/427 (94%)	0.21	8 (1%)	65	68	12, 38, 68, 79	0
All	All	1625/1708 (95%)	0.00	38 (2%)	60	63	5, 29, 61, 79	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	GLU	3.4
1	C	8	ASN	3.4
1	B	338	VAL	3.3
1	A	259	ALA	3.2
1	D	10	GLY	3.2
1	C	157	ALA	3.1
1	A	209	ALA	2.8
1	D	231	THR	2.8
1	B	337	PRO	2.6
1	A	225	LEU	2.6
1	A	218	LEU	2.6
1	C	167	LEU	2.6
1	C	188	ASP	2.5
1	A	298	TYR	2.4
1	D	188	ASP	2.4
1	B	265	ALA	2.4
1	C	338	VAL	2.4
1	D	8	ASN	2.4
1	D	2	ASP	2.3
1	A	247	ASP	2.3
1	A	75	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	272	ILE	2.3
1	A	216	ASP	2.3
1	B	332	ASP	2.3
1	B	330	TYR	2.3
1	A	250	PRO	2.3
1	A	254	ALA	2.2
1	A	258	THR	2.2
1	A	183	TYR	2.2
1	D	7	GLN	2.2
1	A	297	ASP	2.2
1	B	8	ASN	2.2
1	A	237	LEU	2.2
1	A	6	TYR	2.1
1	D	249	THR	2.1
1	A	147	ILE	2.0
1	A	264	MET	2.0
1	D	143	VAL	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
4	TME	D	503	3/3	0.70	0.17	38,38,40,40	0
4	TME	B	507	3/3	0.73	0.28	24,24,25,25	0
4	TME	B	505	3/3	0.79	0.23	20,20,20,20	0
4	TME	B	506	3/3	0.81	0.32	34,34,35,36	0
2	SCN	B	502	3/3	0.82	0.24	59,59,66,68	0
2	SCN	A	504	3/3	0.84	0.20	45,45,51,58	0

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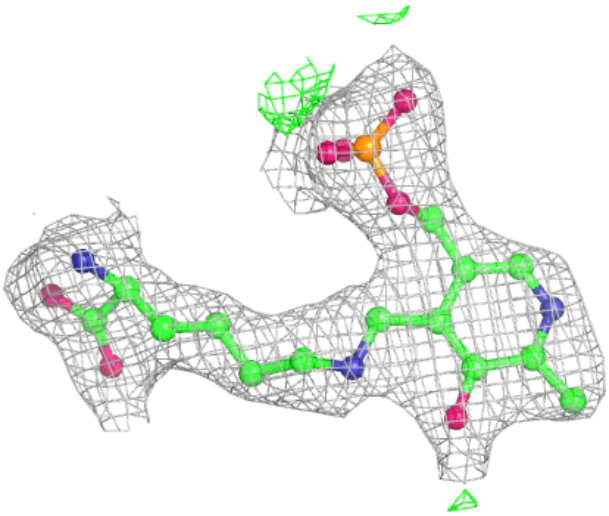
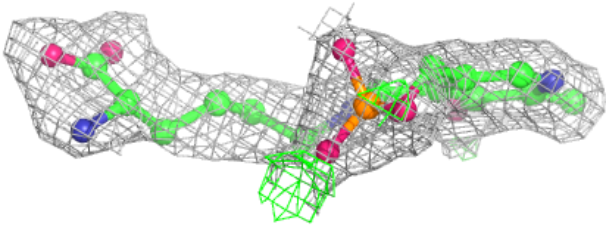
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SCN	B	501	3/3	0.90	0.19	21,21,29,41	0
2	SCN	A	503	3/3	0.90	0.24	41,41,48,51	0
3	K	A	505	1/1	0.91	0.07	45,45,45,45	0
4	TME	A	507	3/3	0.91	0.19	14,14,14,15	0
2	SCN	D	501	3/3	0.91	0.17	29,29,34,44	0
2	SCN	C	501	3/3	0.92	0.22	55,55,56,56	0
3	K	D	502	1/1	0.93	0.12	40,40,40,40	0
2	SCN	C	502	3/3	0.93	0.17	29,29,39,42	0
3	K	C	503	1/1	0.93	0.12	50,50,50,50	0
3	K	B	504	1/1	0.94	0.15	56,56,56,56	0
2	SCN	A	501	3/3	0.94	0.14	42,42,53,65	0
5	LLP	D	504	25/25	0.95	0.12	18,20,24,25	0
5	LLP	A	508	25/25	0.96	0.13	19,22,25,30	0
2	SCN	A	502	3/3	0.96	0.20	25,25,32,35	0
3	K	B	503	1/1	0.97	0.04	33,33,33,33	0
5	LLP	B	508	25/25	0.98	0.10	6,9,9,9	0
5	LLP	C	504	25/25	0.98	0.09	11,13,16,17	0
3	K	A	506	1/1	0.98	0.04	23,23,23,23	0

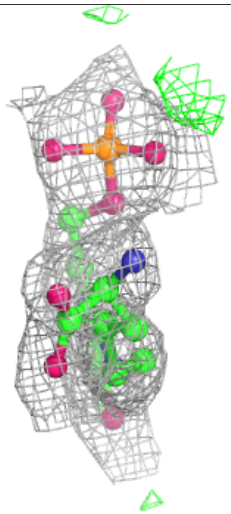
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LLP D 504:

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

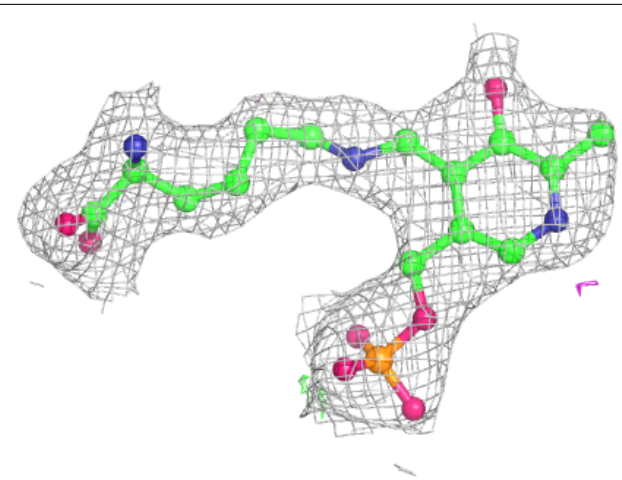


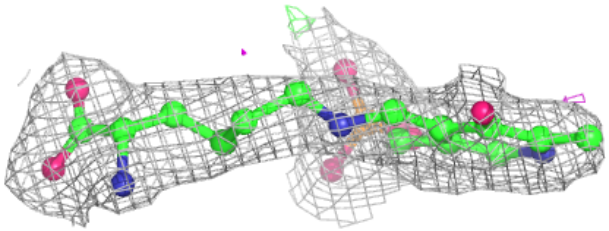


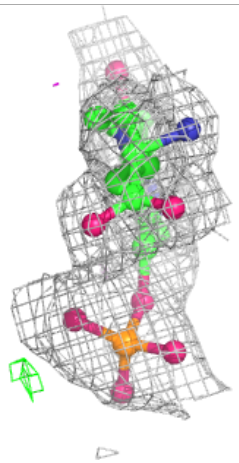


Electron density around LLP A 508:

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

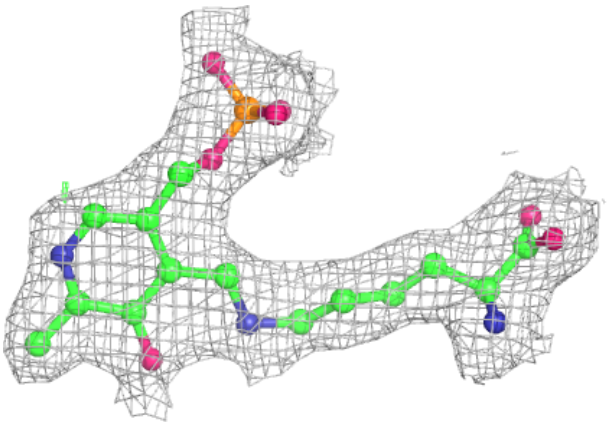


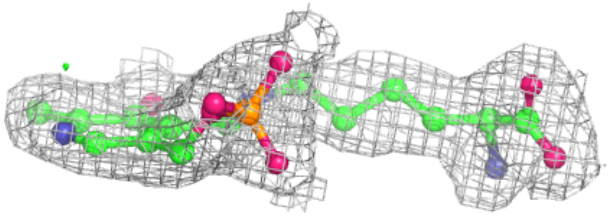


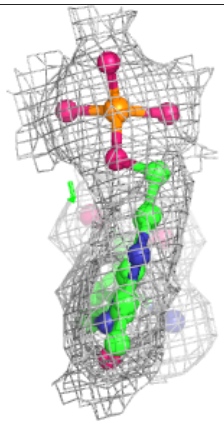


Electron density around LLP B 508:

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







Electron density around LLP C 504:

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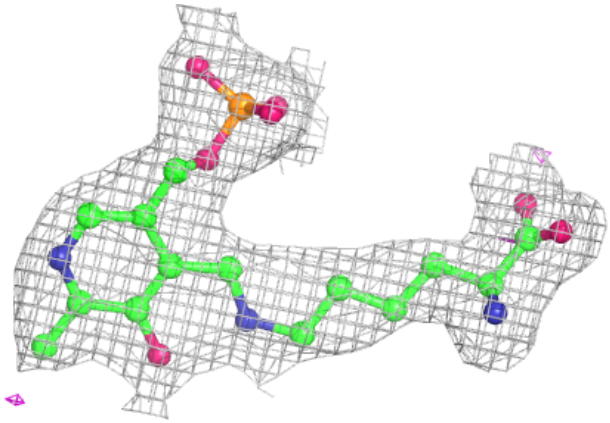
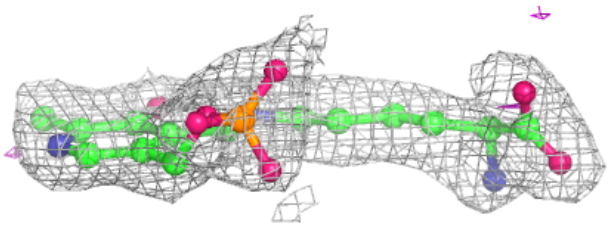
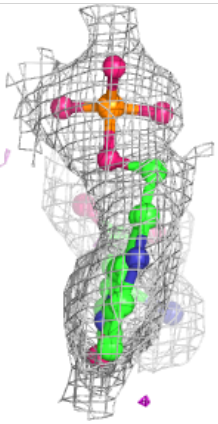
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.