Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2022 – 11:48 am GMT

PDB ID	:	7A0Y
Title	:	Structure of dimeric sodium proton antiporter NhaA K300R variant, at pH 8.2, crystallized with chimeric Fab antibodies
Authors	:	Fippel, A.; Mir, S.H.; Lentes, C.J.; Wirth, C.; Hunte, C.
Deposited on	:	2020-08-11
Resolution	:	2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

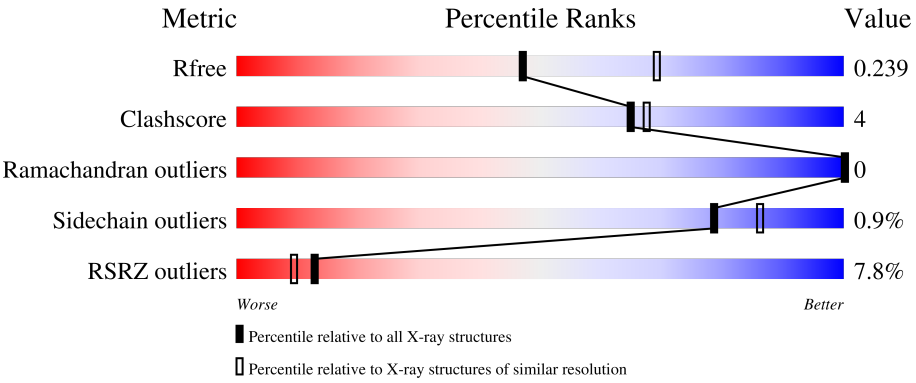
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	411	7% 77% 13% 9%
1	B	411	9% 77% 13% 9%
2	C	252	8% 81% 15%
2	E	252	4% 78% 11% 12%
3	D	210	13% 90% 9%

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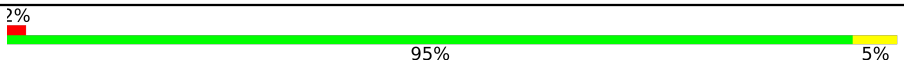
Mol	Chain	Length	Quality of chain
3	F	210	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 12300 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 Na(+)/H(+) antiporter NhaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	62	3	0
			2814	1877	460	463	14			
1	B	373	Total	C	N	O	S	68	2	0
			2806	1870	457	465	14			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP Q8ZRZ3
A	-3	ASN	-	expression tag	UNP Q8ZRZ3
A	-2	LEU	-	expression tag	UNP Q8ZRZ3
A	-1	GLY	-	expression tag	UNP Q8ZRZ3
A	0	ILE	-	expression tag	UNP Q8ZRZ3
A	1	LEU	-	expression tag	UNP Q8ZRZ3
A	300	ARG	LYS	engineered mutation	UNP Q8ZRZ3
A	389	SER	-	expression tag	UNP Q8ZRZ3
A	390	GLU	-	expression tag	UNP Q8ZRZ3
A	391	ASN	-	expression tag	UNP Q8ZRZ3
A	392	LEU	-	expression tag	UNP Q8ZRZ3
A	393	TYR	-	expression tag	UNP Q8ZRZ3
A	394	PHE	-	expression tag	UNP Q8ZRZ3
A	395	GLN	-	expression tag	UNP Q8ZRZ3
A	396	GLY	-	expression tag	UNP Q8ZRZ3
A	397	GLY	-	expression tag	UNP Q8ZRZ3
A	398	ARG	-	expression tag	UNP Q8ZRZ3
A	399	GLY	-	expression tag	UNP Q8ZRZ3
A	400	SER	-	expression tag	UNP Q8ZRZ3
A	401	HIS	-	expression tag	UNP Q8ZRZ3
A	402	HIS	-	expression tag	UNP Q8ZRZ3
A	403	HIS	-	expression tag	UNP Q8ZRZ3
A	404	HIS	-	expression tag	UNP Q8ZRZ3
A	405	HIS	-	expression tag	UNP Q8ZRZ3
A	406	HIS	-	expression tag	UNP Q8ZRZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP Q8ZRZ3
B	-3	ASN	-	expression tag	UNP Q8ZRZ3
B	-2	LEU	-	expression tag	UNP Q8ZRZ3
B	-1	GLY	-	expression tag	UNP Q8ZRZ3
B	0	ILE	-	expression tag	UNP Q8ZRZ3
B	1	LEU	-	expression tag	UNP Q8ZRZ3
B	300	ARG	LYS	engineered mutation	UNP Q8ZRZ3
B	389	SER	-	expression tag	UNP Q8ZRZ3
B	390	GLU	-	expression tag	UNP Q8ZRZ3
B	391	ASN	-	expression tag	UNP Q8ZRZ3
B	392	LEU	-	expression tag	UNP Q8ZRZ3
B	393	TYR	-	expression tag	UNP Q8ZRZ3
B	394	PHE	-	expression tag	UNP Q8ZRZ3
B	395	GLN	-	expression tag	UNP Q8ZRZ3
B	396	GLY	-	expression tag	UNP Q8ZRZ3
B	397	GLY	-	expression tag	UNP Q8ZRZ3
B	398	ARG	-	expression tag	UNP Q8ZRZ3
B	399	GLY	-	expression tag	UNP Q8ZRZ3
B	400	SER	-	expression tag	UNP Q8ZRZ3
B	401	HIS	-	expression tag	UNP Q8ZRZ3
B	402	HIS	-	expression tag	UNP Q8ZRZ3
B	403	HIS	-	expression tag	UNP Q8ZRZ3
B	404	HIS	-	expression tag	UNP Q8ZRZ3
B	405	HIS	-	expression tag	UNP Q8ZRZ3
B	406	HIS	-	expression tag	UNP Q8ZRZ3

- Molecule 2 is a protein called chimeric antibody Fab-F6, heavy chain,chimeric antibody Fab-F6, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	213	Total	C	N	O	S	28	1	0
			1573	987	271	310	5			
2	E	223	Total	C	N	O	S	5	1	0
			1633	1020	282	326	5			

- Molecule 3 is a protein called chimeric antibody Fab-F6, light chain,chimeric antibody Fab-F6, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	207	Total	C	N	O	S	27	1	0
			1561	976	263	318	4			

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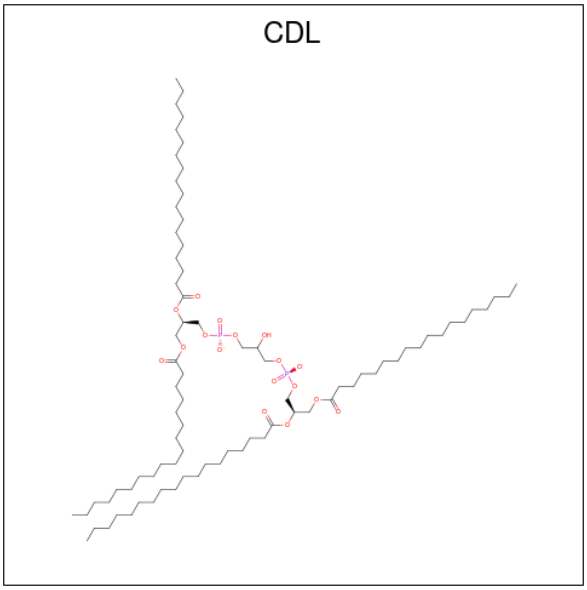
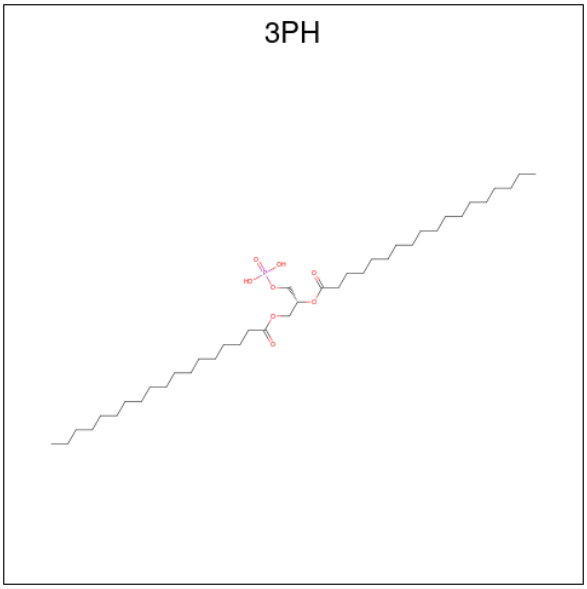
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	209	Total	C	N	O	S	4	0	0
			1568	979	265	320	4			

- Molecule 4 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



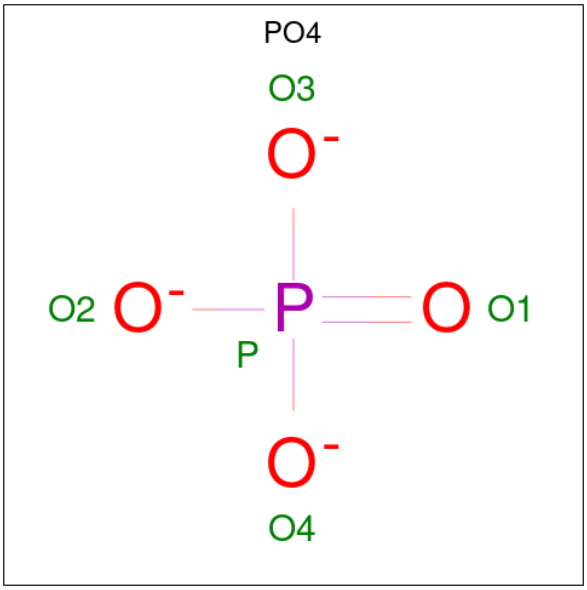
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			53	34	17	2		

- Molecule 5 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



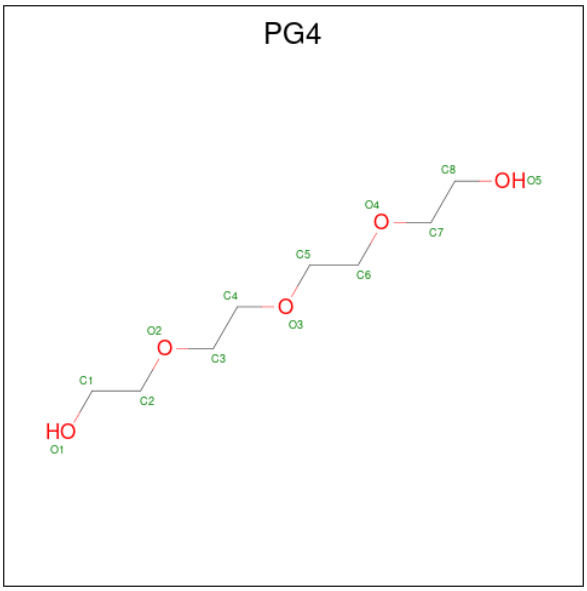
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O P 27 18 8 1	0	0
5	B	1	Total C O P 23 14 8 1	0	0
5	B	1	Total C O P 27 18 8 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



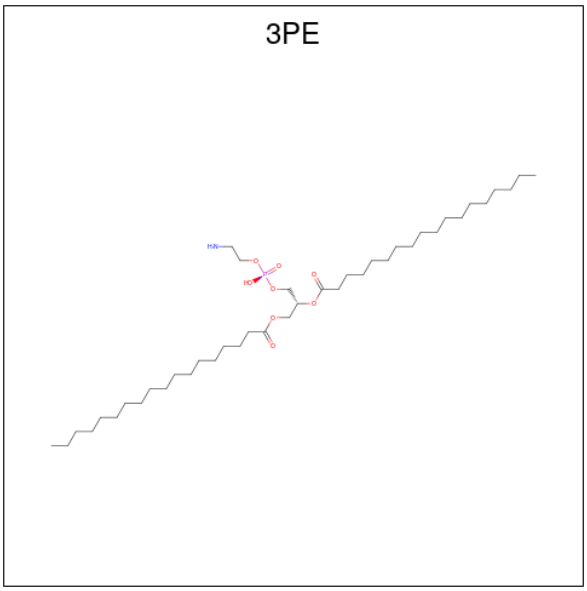
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 18 1 8 1	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	3	Total Cl 3 3	0	0
9	E	1	Total Cl 1 1	0	0

- Molecule 10 is water.

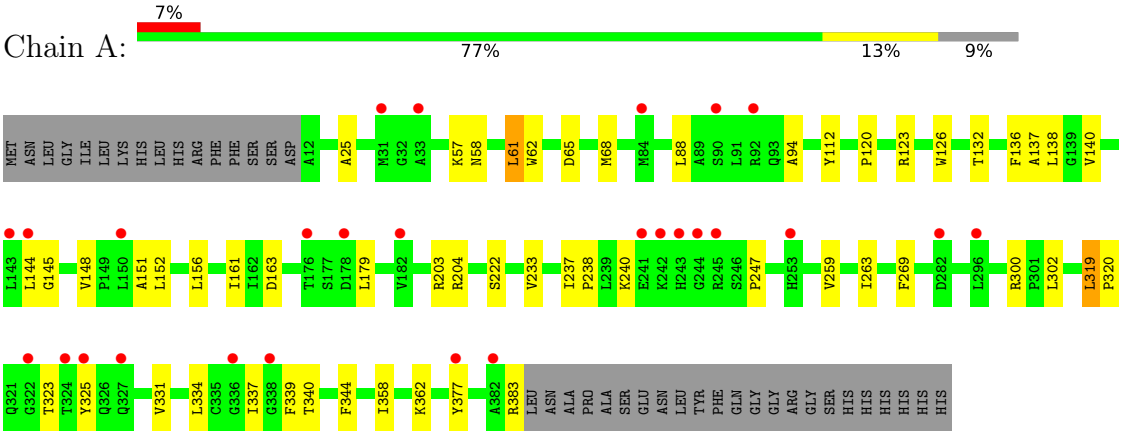
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	10	Total O 10 10	0	0
10	C	31	Total O 31 31	0	0
10	D	28	Total O 28 28	0	0
10	E	48	Total O 48 48	0	0
10	F	30	Total O 30 30	0	0

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.

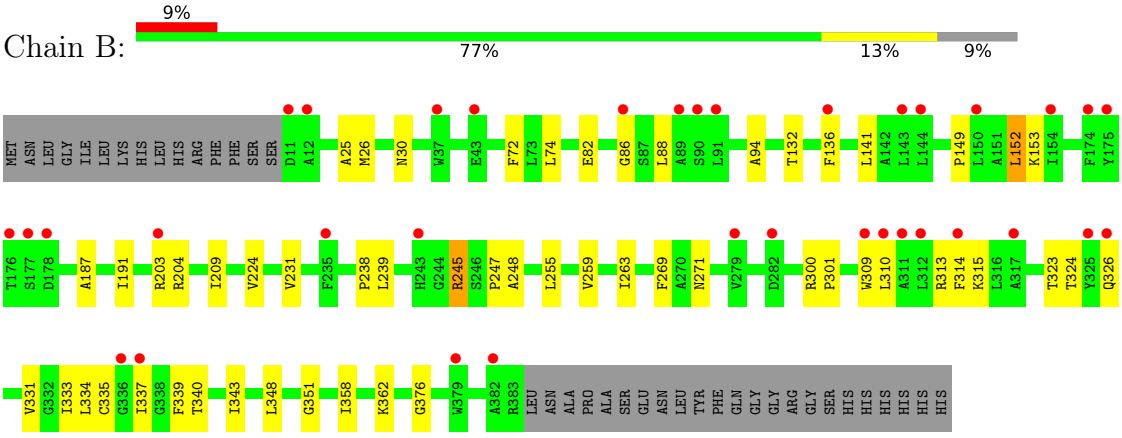
• Molecule 1: Na(+)/H(+) antiporter NhaA

Chain A:



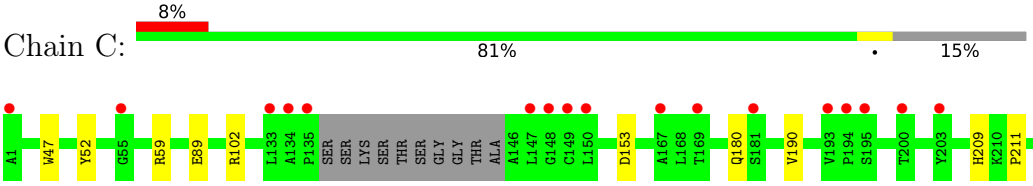
• Molecule 1: Na(+)/H(+) antiporter NhaA

Chain B:



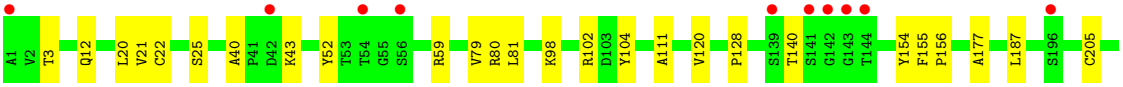
• Molecule 2: chimeric antibody Fab-F6, heavy chain,chimeric antibody Fab-F6, heavy chain

Chain C:



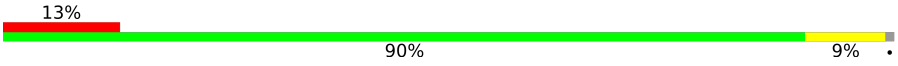
• Molecule 2: chimeric antibody Fab-F6, heavy chain,chimeric antibody Fab-F6, heavy chain

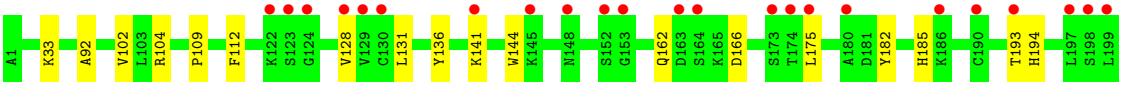
Chain E:

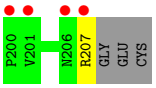


• Molecule 3: chimeric antibody Fab-F6, light chain,chimeric antibody Fab-F6, light chain

Chain D:

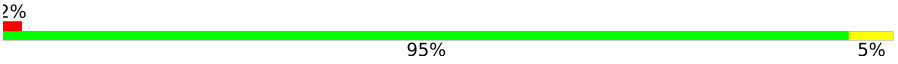


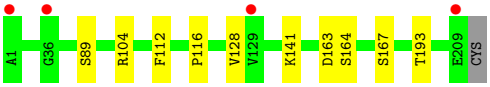




• Molecule 3: chimeric antibody Fab-F6, light chain,chimeric antibody Fab-F6, light chain

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	112.04Å 91.68Å 138.29Å 90.00° 110.08° 90.00°	Depositor
Resolution (Å)	24.74 – 2.45 24.74 – 2.45	Depositor EDS
% Data completeness (in resolution range)	59.4 (24.74-2.45) 59.4 (24.74-2.45)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.44Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.203 , 0.241 0.203 , 0.239	Depositor DCC
R_{free} test set	1746 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å^2)	58.6	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	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	0.93	EDS
Total number of atoms	12300	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PG4, PO4, 3PE, 3PH, CDL

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	0.24	0/2884	0.38	0/3933
1	B	0.24	0/2873	0.39	0/3917
2	C	0.25	0/1611	0.44	0/2191
2	E	0.25	0/1672	0.45	0/2274
3	D	0.25	0/1599	0.44	0/2177
3	F	0.24	0/1603	0.44	0/2182
All	All	0.24	0/12242	0.42	0/16674

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2814	0	2995	30	0
1	B	2806	0	2994	32	0
2	C	1573	0	1541	7	0
2	E	1633	0	1600	15	0
3	D	1561	0	1517	12	0
3	F	1568	0	1520	6	0
4	A	53	0	50	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	27	0	27	0	0
5	B	50	0	46	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	13	0	18	0	0
7	B	13	0	18	0	0
8	B	28	0	30	2	0
9	C	3	0	0	1	0
9	E	1	0	0	0	0
10	A	10	0	0	0	0
10	C	31	0	0	0	0
10	D	28	0	0	0	0
10	E	48	0	0	0	0
10	F	30	0	0	0	0
All	All	12300	0	12356	98	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 4.

All (98) 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)
2:E:98:LYS:HB3	2:E:111:ALA:HB3	1.75	0.67
1:A:204:ARG:NH1	4:A:501:CDL:OB4	2.28	0.65
3:D:112:PHE:HB2	3:D:131:LEU:HB3	1.79	0.65
4:A:501:CDL:H142	1:B:209:ILE:HD12	1.78	0.64
3:D:182:TYR:O	3:D:207:ARG:NH2	2.30	0.64
2:E:52:TYR:OH	2:E:102:ARG:NH1	2.30	0.64
2:C:52:TYR:OH	2:C:102:ARG:NH1	2.31	0.63
1:B:149:PRO:HG2	1:B:152:LEU:HB2	1.81	0.63
2:E:40:ALA:HB3	2:E:43:LYS:HB2	1.80	0.62
1:A:238:PRO:HG2	1:A:247:PRO:HG2	1.81	0.60
1:A:339:PHE:HD2	1:A:340:THR:HG23	1.66	0.60
3:D:128:VAL:HG13	3:D:175:LEU:HB3	1.83	0.60
1:B:82:GLU:HA	1:B:86:GLY:HA3	1.81	0.60
3:D:104:ARG:NH1	3:D:166:ASP:O	2.35	0.59
1:A:179:LEU:HD21	1:A:222:SER:HB2	1.84	0.59
1:A:323:THR:HG22	1:A:325:TYR:H	1.68	0.59
1:B:301:PRO:HG3	1:B:333:ILE:HA	1.84	0.58
3:F:141:LYS:HB3	3:F:193:THR:HB	1.85	0.58
1:A:58:ASN:HD21	1:A:61:LEU:HD23	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:HG13	1:A:362:LYS:HE3	1.85	0.57
1:B:238:PRO:HG2	1:B:247:PRO:HG2	1.86	0.57
1:B:203:ARG:HD3	1:B:245:ARG:HE	1.68	0.57
3:D:33:LYS:HE3	3:D:162:GLN:HB3	1.85	0.56
3:F:116:PRO:HD3	3:F:128:VAL:HG22	1.87	0.56
1:B:224:VAL:HG22	1:B:348:LEU:HD13	1.87	0.54
1:B:358:ILE:HG13	1:B:362:LYS:HE3	1.89	0.54
3:D:141:LYS:HB3	3:D:193:THR:HB	1.89	0.54
1:B:88:LEU:HA	1:B:94:ALA:HB3	1.89	0.54
3:D:185:HIS:O	3:D:207:ARG:NH2	2.41	0.53
1:B:25:ALA:HB2	1:B:269:PHE:HA	1.89	0.53
1:A:88:LEU:HA	1:A:94:ALA:HB2	1.90	0.53
3:D:102:VAL:O	3:D:136:TYR:OH	2.25	0.53
2:E:22:CYS:HB3	2:E:79:VAL:HG13	1.91	0.53
1:B:132:THR:OG1	1:B:300:ARG:NH1	2.44	0.51
1:B:334:LEU:HD13	1:B:376:GLY:HA3	1.93	0.51
1:A:151:ALA:HB1	1:A:320:PRO:HB2	1.93	0.51
1:A:203:ARG:NH2	1:A:240:LYS:O	2.43	0.50
1:A:152:LEU:HD22	1:A:331:VAL:HG21	1.92	0.50
2:C:89:GLU:OE1	2:C:89:GLU:N	2.42	0.50
1:B:245:ARG:HD2	1:B:247:PRO:HD3	1.94	0.50
3:F:104:ARG:NH1	3:F:167:SER:OG	2.45	0.49
1:B:351:GLY:O	2:E:102:ARG:NH2	2.45	0.49
1:A:144:LEU:HD11	1:A:377:TYR:CZ	2.48	0.49
4:A:501:CDL:H141	8:B:501:3PE:H31	1.95	0.49
1:A:132:THR:OG1	1:A:300:ARG:NH1	2.46	0.48
1:A:140:VAL:HG11	1:A:334:LEU:HD11	1.95	0.48
2:E:59:ARG:HG3	2:E:104:TYR:OH	2.13	0.48
1:B:141:LEU:HD23	1:B:153:LYS:HG2	1.97	0.47
1:A:163:ASP:OD2	1:A:300:ARG:NH2	2.47	0.47
1:B:74:LEU:HD13	1:B:255:LEU:HB3	1.96	0.47
2:E:20:LEU:HD12	2:E:81:LEU:HD23	1.96	0.47
2:C:47:TRP:CD2	3:D:92:ALA:HB3	2.50	0.46
1:A:145:GLY:HA2	1:A:148:VAL:HG13	1.97	0.46
2:C:190:VAL:HG21	3:D:131:LEU:HD13	1.97	0.46
3:D:144:TRP:CE2	3:D:175:LEU:HB2	2.51	0.46
1:B:136:PHE:HB3	1:B:337:ILE:HG21	1.98	0.46
3:F:163:ASP:OD1	3:F:164:SER:N	2.49	0.46
1:A:259:VAL:HA	1:A:263:ILE:HB	1.98	0.46
1:A:25:ALA:HB2	1:A:269:PHE:HA	1.98	0.46
2:E:140:THR:HB	3:F:112:PHE:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:VAL:O	1:B:335:CYS:N	2.49	0.45
2:C:153:ASP:OD1	2:C:180:GLN:NE2	2.36	0.45
1:B:187:ALA:O	1:B:191:ILE:HG12	2.16	0.45
1:B:314:PHE:O	1:B:315:LYS:HG2	2.17	0.45
2:E:3:THR:OG1	2:E:25:SER:OG	2.34	0.45
2:E:21:VAL:HG13	2:E:80[B]:ARG:HG2	1.99	0.45
2:E:128:PRO:HB3	2:E:154:TYR:HB3	1.99	0.44
2:E:59:ARG:NH1	3:F:89:SER:O	2.50	0.44
1:B:26:MET:O	1:B:30:ASN:ND2	2.38	0.44
1:A:137:ALA:HB1	1:A:156:LEU:HD21	2.00	0.44
1:B:309:TRP:CE3	1:B:310:LEU:HD23	2.53	0.44
1:A:136:PHE:CD1	1:A:337:ILE:HG21	2.53	0.43
1:B:259:VAL:HA	1:B:263:ILE:HB	2.00	0.43
2:E:12:GLN:O	2:E:120:VAL:HA	2.18	0.43
1:B:339:PHE:HD2	1:B:340:THR:HG23	1.84	0.43
1:B:72:PHE:HB3	1:B:231:VAL:HG13	2.01	0.43
1:A:57:LYS:HB2	1:A:62:TRP:NE1	2.34	0.43
2:C:209:HIS:CD2	2:C:211:PRO:HD2	2.53	0.43
3:D:109:PRO:HD3	3:D:194:HIS:ND1	2.33	0.43
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.68	0.43
1:B:204:ARG:NH1	8:B:501:3PE:O14	2.52	0.43
1:B:309:TRP:CH2	1:B:313:ARG:HD3	2.53	0.42
2:C:59:ARG:HD3	9:C:302:CL:CL	2.56	0.42
1:A:323:THR:C	1:A:325:TYR:H	2.22	0.42
2:E:177:ALA:HA	2:E:187:LEU:HB3	2.01	0.42
1:B:152:LEU:HD23	1:B:152:LEU:HA	1.81	0.42
1:A:233:VAL:O	1:A:237:ILE:HG12	2.21	0.41
1:A:203:ARG:HH12	1:A:240:LYS:HB2	1.84	0.41
2:E:155:PHE:HA	2:E:156:PRO:HA	1.87	0.41
1:A:138:LEU:HD23	1:A:156:LEU:HD23	2.02	0.41
1:A:57:LYS:NZ	1:A:65:ASP:OD2	2.47	0.41
1:A:120:PRO:HA	1:A:123:ARG:HG2	2.03	0.41
1:B:271:ASN:HB3	1:B:343:ILE:HG21	2.02	0.41
1:A:112:TYR:CD1	1:A:126:TRP:HA	2.56	0.40
1:B:239:LEU:HD13	1:B:248:ALA:HB3	2.03	0.40
1:A:68:MET:HG3	1:A:344:PHE:CE1	2.56	0.40
1:B:309:TRP:HE3	1:B:310:LEU:HD23	1.86	0.40
1:B:334:LEU:HD12	1:B:334:LEU:HA	1.96	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	373/411 (91%)	352 (94%)	21 (6%)	0	100	100
1	B	373/411 (91%)	357 (96%)	16 (4%)	0	100	100
2	C	210/252 (83%)	201 (96%)	9 (4%)	0	100	100
2	E	222/252 (88%)	214 (96%)	8 (4%)	0	100	100
3	D	206/210 (98%)	197 (96%)	9 (4%)	0	100	100
3	F	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
All	All	1591/1746 (91%)	1517 (95%)	74 (5%)	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	288/318 (91%)	283 (98%)	5 (2%)	60	73
1	B	288/318 (91%)	283 (98%)	5 (2%)	60	73
2	C	170/199 (85%)	170 (100%)	0	100	100
2	E	177/199 (89%)	175 (99%)	2 (1%)	73	82
3	D	177/178 (99%)	177 (100%)	0	100	100
3	F	177/178 (99%)	177 (100%)	0	100	100
All	All	1277/1390 (92%)	1265 (99%)	12 (1%)	78	86

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

Mol	Chain	Res	Type
1	A	61	LEU
1	A	161	ILE
1	A	302	LEU
1	A	319	LEU
1	A	383	ARG
1	B	152	LEU
1	B	245	ARG
1	B	323	THR
1	B	324	THR
1	B	326	GLN
2	E	205	CYS
2	E	208	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\#\|Z\|>2$
5	3PH	B	502	-	22,22,47	0.29	0	26,27,52	0.48	0
5	3PH	A	502	-	26,26,47	0.26	0	30,31,52	0.43	0
5	3PH	B	503	-	26,26,47	0.26	0	30,31,52	0.42	0
6	PO4	A	503	-	4,4,4	0.91	0	6,6,6	0.43	0
7	PG4	A	504	-	12,12,12	0.46	0	11,11,11	0.28	0
8	3PE	B	501	-	27,27,50	0.40	0	30,32,55	0.35	0
6	PO4	B	504	-	4,4,4	0.91	0	6,6,6	0.42	0
4	CDL	A	501	-	52,52,99	1.26	4 (7%)	58,64,111	1.26	5 (8%)
7	PG4	B	505	-	12,12,12	0.45	0	11,11,11	0.29	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
5	3PH	B	502	-	-	4/24/24/49	-
5	3PH	A	502	-	-	3/28/28/49	-
5	3PH	B	503	-	-	1/28/28/49	-
7	PG4	A	504	-	-	1/10/10/10	-
8	3PE	B	501	-	-	7/31/31/54	-
4	CDL	A	501	-	-	18/63/63/110	-
7	PG4	B	505	-	-	1/10/10/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	CDL	OA8-CA7	4.27	1.45	1.33
4	A	501	CDL	OB8-CB7	4.27	1.45	1.33
4	A	501	CDL	OB6-CB5	4.14	1.46	1.34
4	A	501	CDL	OA6-CA5	4.03	1.45	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	CDL	OA6-CA5-C11	4.14	120.42	111.50
4	A	501	CDL	OB6-CB5-C51	3.72	119.52	111.50
4	A	501	CDL	CA4-OA6-CA5	-2.93	110.58	117.79
4	A	501	CDL	OA8-CA7-C31	2.82	120.75	111.91
4	A	501	CDL	OB8-CB7-C71	2.56	119.95	111.91

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	CDL	CA2-OA2-PA1-OA3
4	A	501	CDL	CA2-OA2-PA1-OA5
4	A	501	CDL	CA3-OA5-PA1-OA3
4	A	501	CDL	CA3-OA5-PA1-OA4
5	A	502	3PH	C1-O11-P-O13
5	A	502	3PH	C1-O11-P-O14
8	B	501	3PE	C1-O11-P-O14
8	B	501	3PE	C11-O13-P-O12
8	B	501	3PE	C11-O13-P-O14
4	A	501	CDL	CA3-OA5-PA1-OA2
4	A	501	CDL	CB3-OB5-PB2-OB2
8	B	501	3PE	C11-O13-P-O11
4	A	501	CDL	CA5-C11-C12-C13
4	A	501	CDL	C11-CA5-OA6-CA4
4	A	501	CDL	OA7-CA5-OA6-CA4
5	A	502	3PH	C1-O11-P-O12
5	B	502	3PH	O11-C1-C2-O21
4	A	501	CDL	OB5-CB3-CB4-CB6
4	A	501	CDL	OA6-CA4-CA6-OA8
4	A	501	CDL	C31-C32-C33-C34
5	B	502	3PH	O11-C1-C2-C3
4	A	501	CDL	OB5-CB3-CB4-OB6
4	A	501	CDL	CB3-OB5-PB2-OB3
5	B	502	3PH	C1-O11-P-O12
4	A	501	CDL	CB2-OB2-PB2-OB5
7	A	504	PG4	O2-C3-C4-O3
5	B	502	3PH	O31-C31-C32-C33
8	B	501	3PE	O21-C2-C3-O31
4	A	501	CDL	CA3-CA4-CA6-OA8
7	B	505	PG4	O2-C3-C4-O3
5	B	503	3PH	O11-C1-C2-C3
8	B	501	3PE	C1-O11-P-O13
4	A	501	CDL	CB2-OB2-PB2-OB3
8	B	501	3PE	C12-C11-O13-P
4	A	501	CDL	OB7-CB5-OB6-CB4

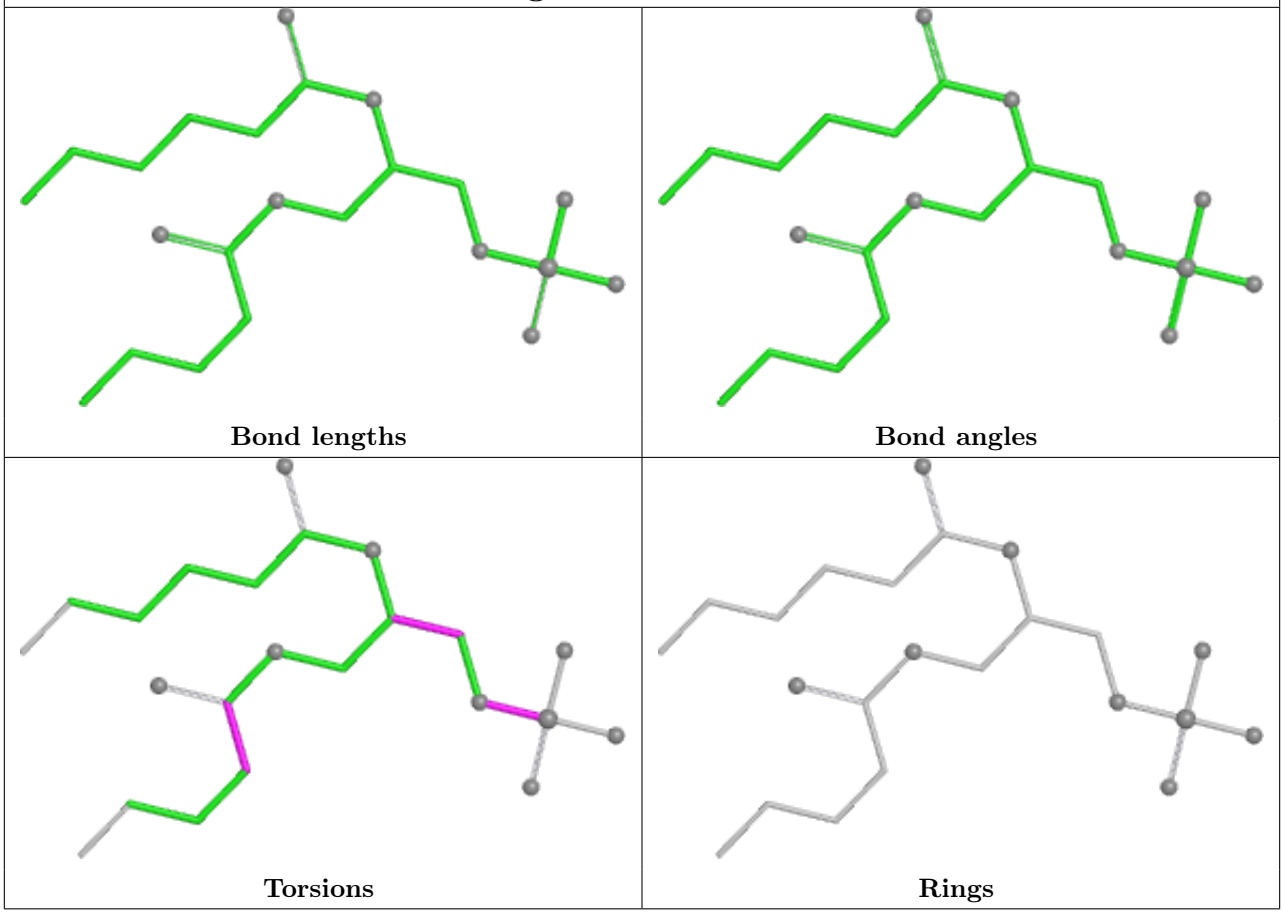
There are no ring outliers.

2 monomers are involved in 4 short contacts:

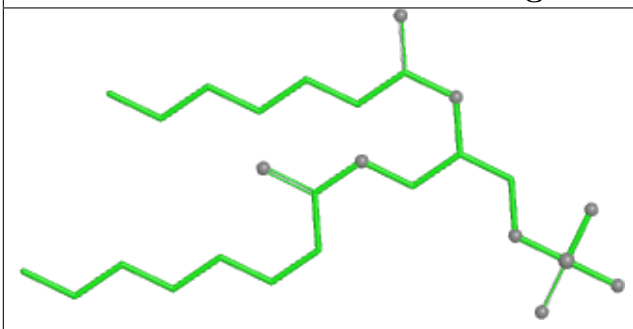
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	3PE	2	0
4	A	501	CDL	3	0

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.

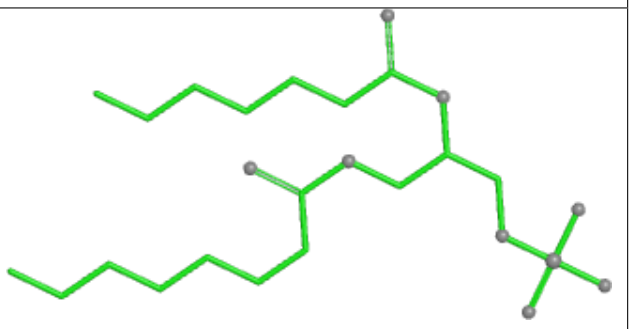
Ligand 3PH B 502



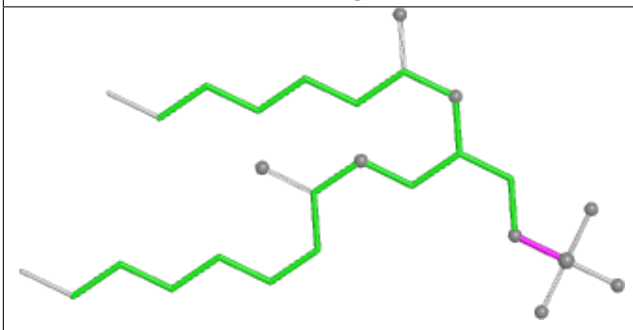
Ligand 3PH A 502



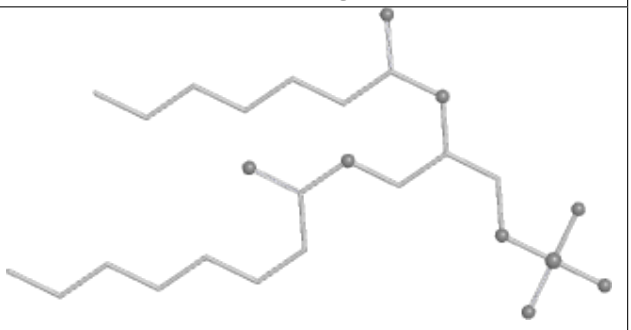
Bond lengths



Bond angles

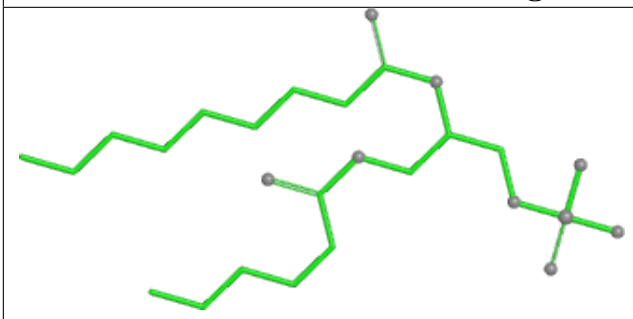


Torsions

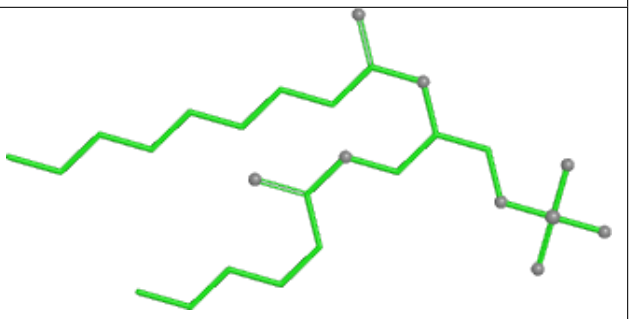


Rings

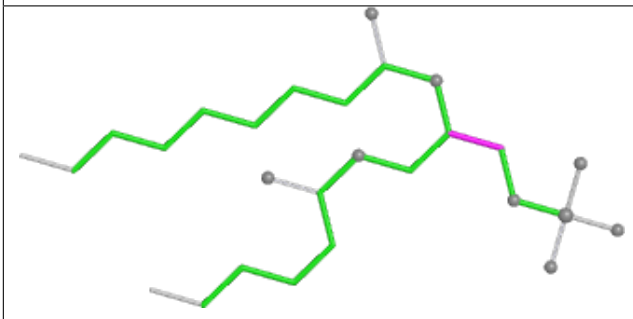
Ligand 3PH B 503



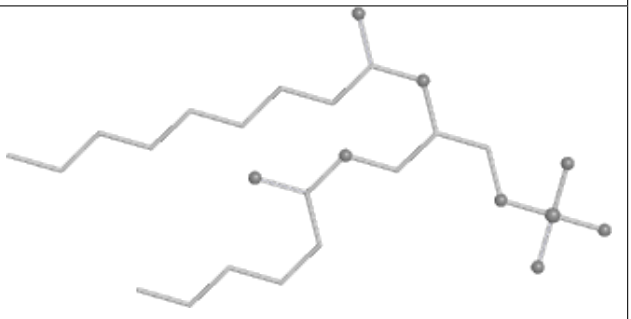
Bond lengths



Bond angles

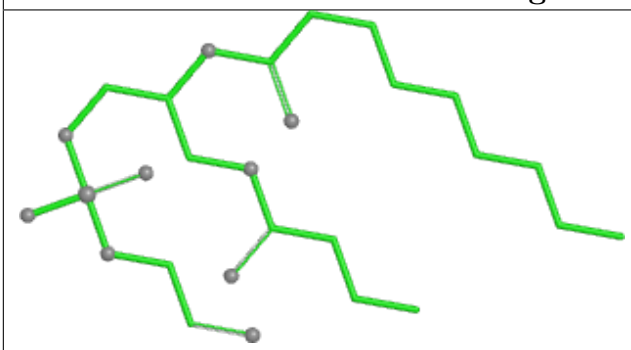


Torsions

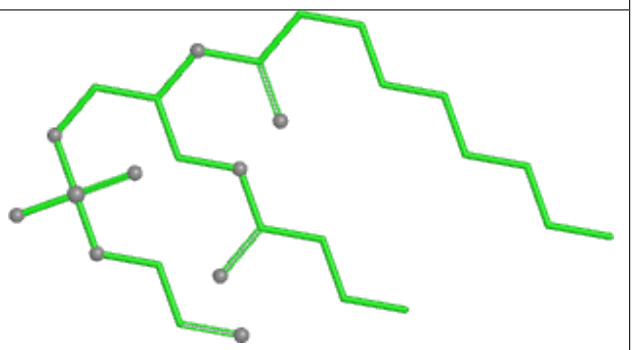


Rings

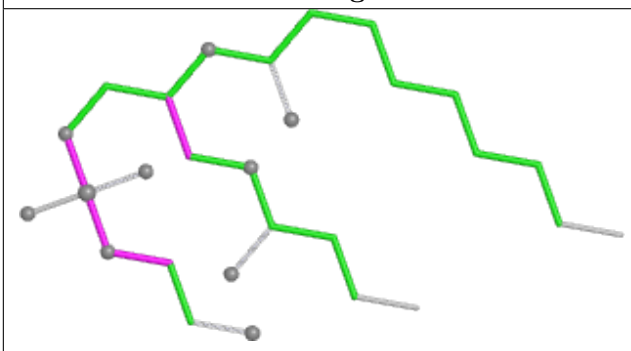
Ligand 3PE B 501



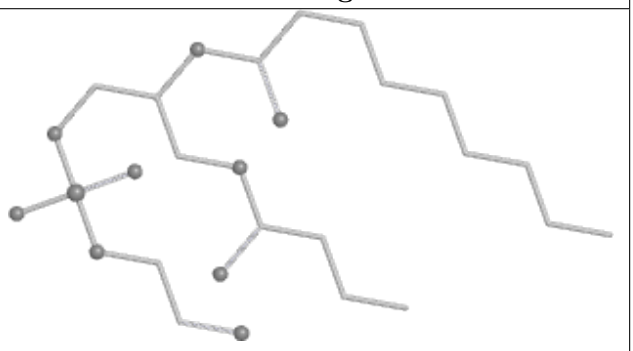
Bond lengths



Bond angles

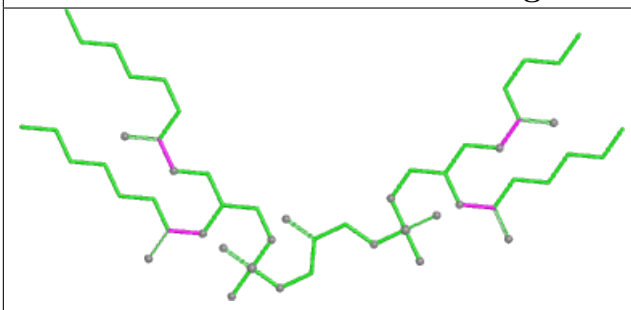


Torsions

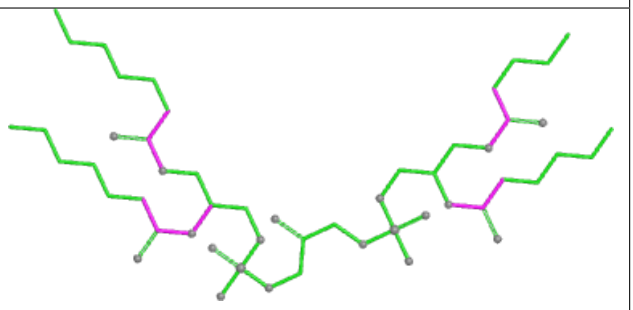


Rings

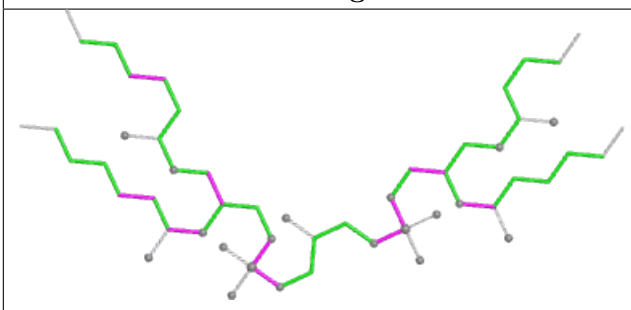
Ligand CDL A 501



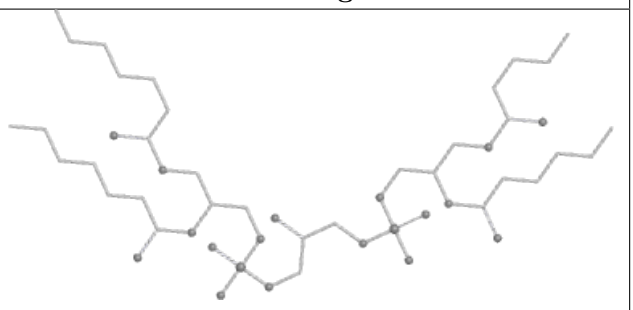
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	372/411 (90%)	0.08	27 (7%) 15 11	33, 74, 133, 170	13 (3%)
1	B	370/411 (90%)	0.19	35 (9%) 8 5	50, 85, 136, 174	13 (3%)
2	C	210/252 (83%)	0.25	21 (10%) 7 4	24, 54, 138, 172	2 (0%)
2	E	223/252 (88%)	-0.12	10 (4%) 33 30	26, 46, 87, 141	2 (0%)
3	D	206/210 (98%)	0.37	27 (13%) 3 2	28, 70, 145, 175	6 (2%)
3	F	209/210 (99%)	-0.30	4 (1%) 66 64	29, 51, 79, 106	1 (0%)
All	All	1590/1746 (91%)	0.09	124 (7%) 13 9	24, 68, 134, 175	37 (2%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	221	GLU	6.7
1	A	324	THR	5.7
1	B	91	LEU	5.6
1	B	175	TYR	5.4
3	D	164	SER	5.3
2	C	149	CYS	5.3
1	A	178	ASP	5.1
1	B	144	LEU	5.0
2	C	222	PRO	5.0
3	D	128	VAL	5.0
3	D	193	THR	4.9
3	F	1	ALA	4.9
1	B	325	TYR	4.9
1	A	244	GLY	4.9
1	B	150	LEU	4.8
3	D	123	SER	4.7
3	D	141	LYS	4.6
1	A	382	ALA	4.4
2	C	147	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	243	HIS	4.1
2	E	139	SER	3.9
3	D	201	VAL	3.9
1	B	310	LEU	3.9
2	E	143	GLY	3.8
3	D	148	ASN	3.8
3	D	130	CYS	3.7
3	D	124	GLY	3.7
2	C	135	PRO	3.7
1	B	203	ARG	3.7
1	A	150	LEU	3.6
3	D	197	LEU	3.6
3	D	129	VAL	3.6
3	D	199	LEU	3.6
1	B	311	ALA	3.6
2	C	150	LEU	3.5
3	D	186	LYS	3.5
1	B	176	THR	3.4
2	C	193	VAL	3.4
1	A	322	GLY	3.4
1	B	143	LEU	3.4
1	B	235	PHE	3.4
2	C	203	TYR	3.4
1	B	174	PHE	3.3
2	E	196	SER	3.3
1	A	92	ARG	3.3
2	C	181	SER	3.2
2	E	141	SER	3.2
3	F	209	GLU	3.2
1	A	253	HIS	3.2
3	D	180	ALA	3.2
3	D	200	PRO	3.1
1	A	241	GLU	3.1
1	A	176	THR	3.0
1	B	312	LEU	3.0
2	E	42	ASP	3.0
1	B	243	HIS	3.0
2	C	223	LYS	3.0
2	C	134	ALA	3.0
1	A	327	GLN	3.0
1	B	37	TRP	2.9
2	E	56	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	142	GLY	2.9
1	B	317	ALA	2.9
3	D	145	LYS	2.9
1	B	382	ALA	2.9
3	D	198	SER	2.8
3	D	163	ASP	2.8
1	A	242	LYS	2.8
3	D	122	LYS	2.8
2	C	169	THR	2.7
3	D	190	CYS	2.7
2	C	148	GLY	2.7
1	A	325	TYR	2.7
2	C	200	THR	2.7
2	E	1	ALA	2.7
2	C	195	SER	2.6
1	A	336	GLY	2.6
1	A	84	MET	2.6
3	D	173	SER	2.6
1	A	182	VAL	2.6
1	A	90	SER	2.5
1	B	43	GLU	2.5
1	B	90	SER	2.5
1	B	309	TRP	2.5
2	C	194	PRO	2.5
1	A	245	ARG	2.5
1	B	314	PHE	2.5
1	A	296	LEU	2.4
1	B	282	ASP	2.4
1	B	12	ALA	2.4
1	B	86	GLY	2.4
1	B	177	SER	2.4
3	D	207	ARG	2.4
3	D	153	GLY	2.4
1	B	178	ASP	2.4
3	D	175	LEU	2.4
1	A	338	GLY	2.4
3	F	36	GLY	2.4
1	B	11	ASP	2.4
2	E	54	THR	2.4
3	D	152	SER	2.4
1	B	154	ILE	2.3
2	C	214	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	33	ALA	2.3
2	E	144	THR	2.3
1	A	377	TYR	2.3
2	C	55	GLY	2.3
2	C	133	LEU	2.3
3	F	129	VAL	2.2
2	C	1	ALA	2.2
1	B	337	ILE	2.2
1	A	144	LEU	2.2
1	B	279	VAL	2.1
1	B	136	PHE	2.1
1	A	31	MET	2.1
1	B	326	GLN	2.1
1	A	282	ASP	2.1
1	B	336	GLY	2.1
2	C	167	ALA	2.1
3	D	174	THR	2.1
3	D	206	ASN	2.0
1	A	143	LEU	2.0
1	B	89	ALA	2.0
1	B	379	TRP	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, 95^{th} 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
5	3PH	A	502	27/48	0.78	0.34	62,93,143,151	0
5	3PH	B	503	27/48	0.80	0.27	71,92,130,142	0

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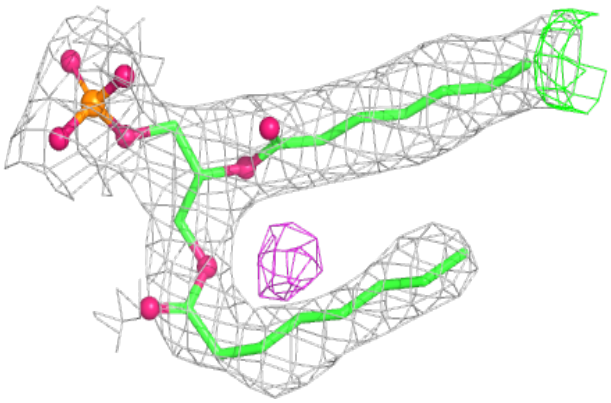
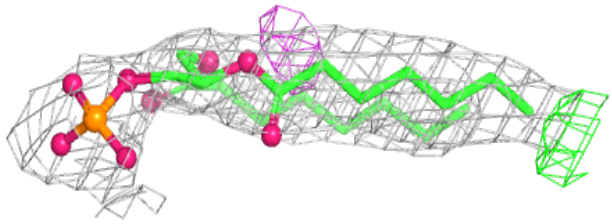
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	3PH	B	502	23/48	0.85	0.32	58,99,151,152	0
7	PG4	B	505	13/13	0.85	0.44	74,83,90,91	0
6	PO4	B	504	5/5	0.86	0.12	75,90,99,119	0
7	PG4	A	504	13/13	0.90	0.14	45,54,68,71	0
8	3PE	B	501	28/51	0.90	0.19	74,90,105,131	0
4	CDL	A	501	53/100	0.91	0.19	68,94,142,148	0
6	PO4	A	503	5/5	0.91	0.12	78,82,97,117	0
9	CL	C	302	1/1	0.91	0.18	73,73,73,73	0
9	CL	E	301	1/1	0.98	0.08	63,63,63,63	0
9	CL	C	303	1/1	0.99	0.07	48,48,48,48	0
9	CL	C	301	1/1	0.99	0.07	49,49,49,49	0

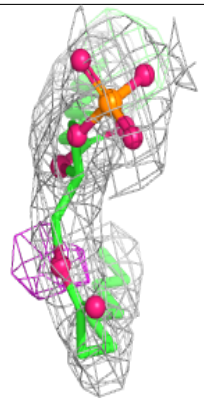
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3PH 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)

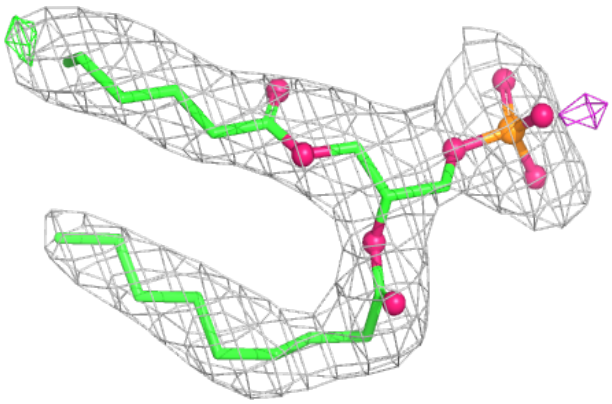


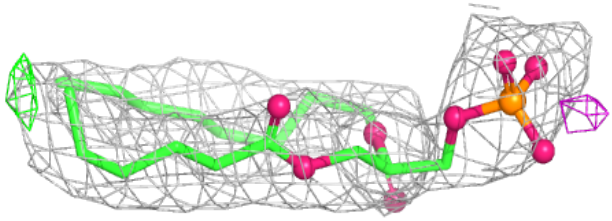


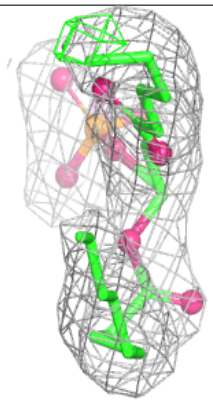


Electron density around 3PH B 503:

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

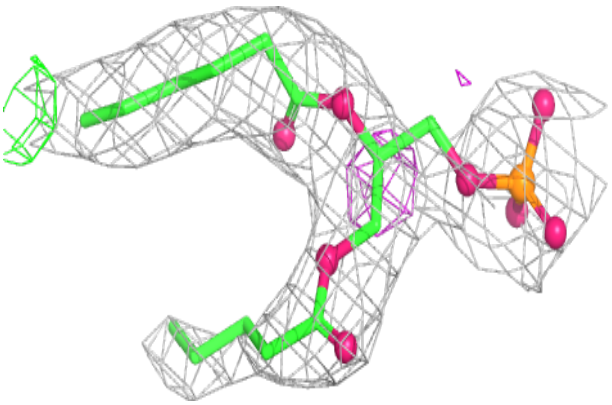


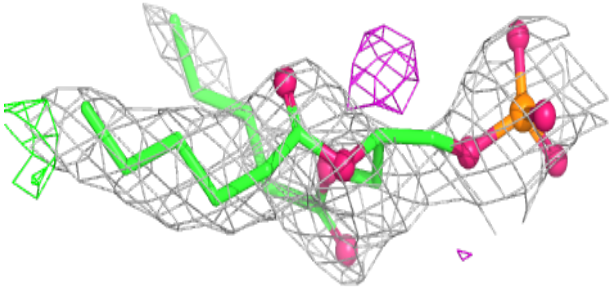


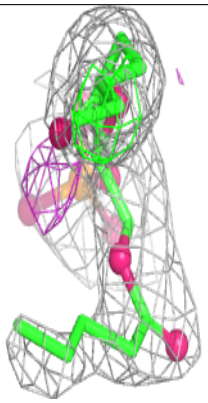


Electron density around 3PH B 502:

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

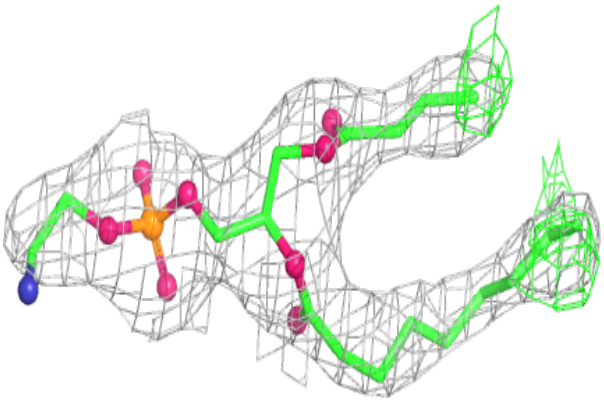


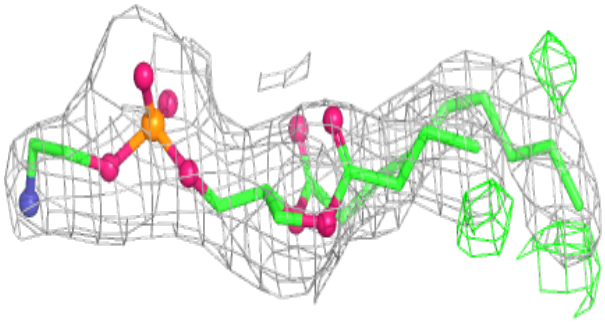


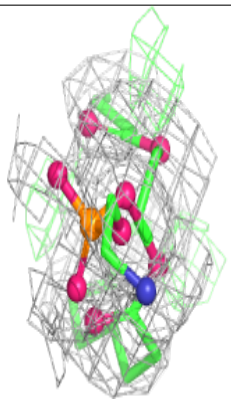


Electron density around 3PE B 501:

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

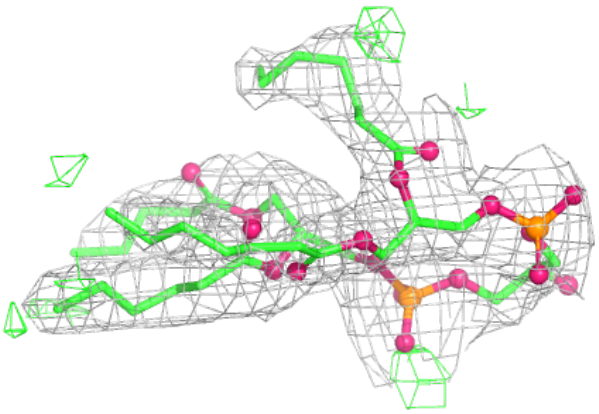






Electron density around CDL A 501:

$2mF_o$-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.