



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:35 AM UTC

PDB ID : 7A0Y / pdb_00007a0y
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

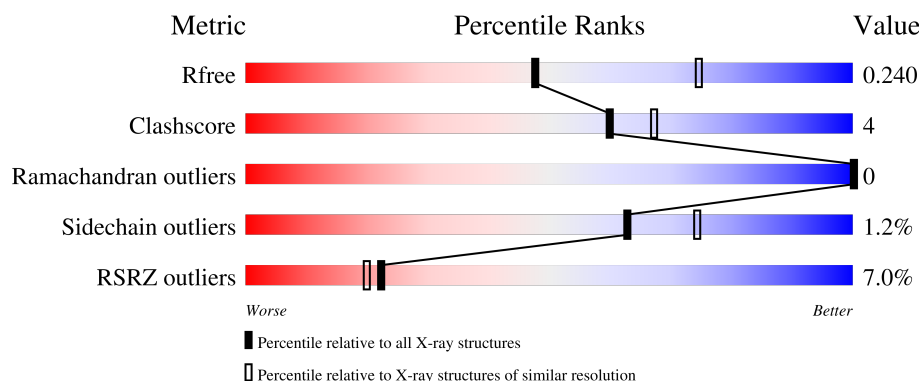
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	411	8% 77% 13% 9%
1	B	411	8% 77% 14% 9%
2	C	252	8% 79% 5% 15%
2	E	252	3% 78% 10% 12%
3	D	210	9% 89% 10% .

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Mol	Chain	Length	Quality of chain
3	F	210	2% 95% 5%

2 Entry composition

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.

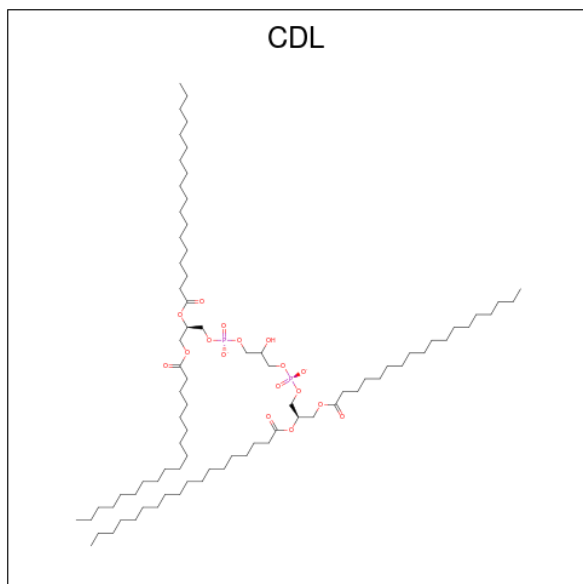
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	207	Total	C	N	O	S	27	1	0
			1561	976	263	318	4			

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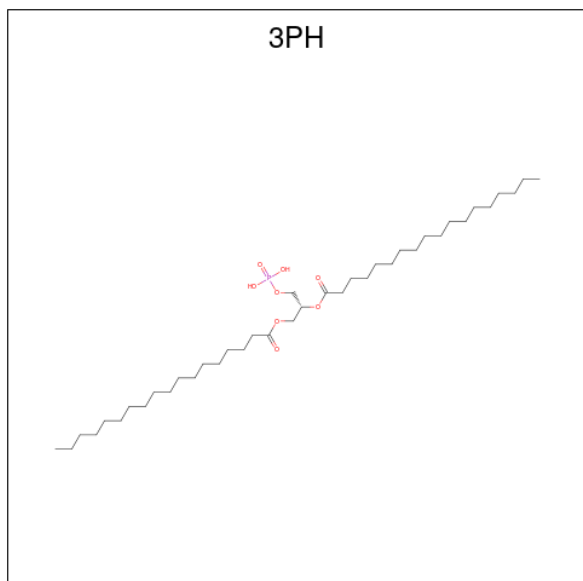
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	209	Total	C	N	O	S	4	0	0
			1568	979	265	320	4			

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



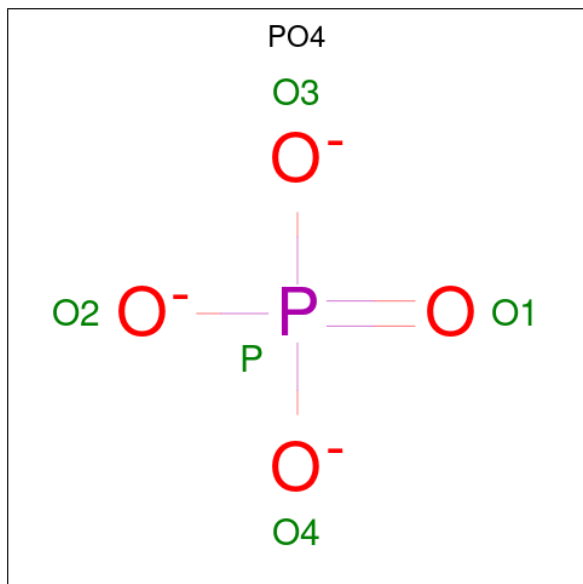
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			53	34	17	2		

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



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

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

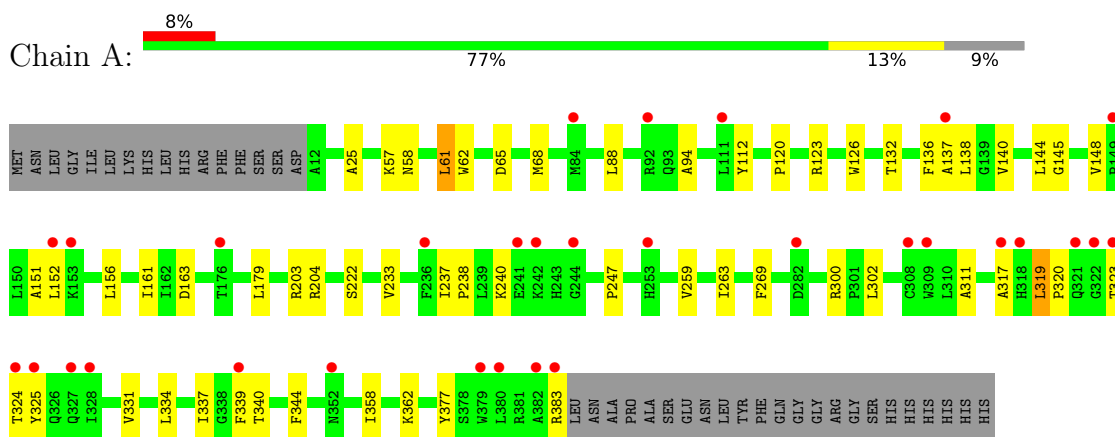
- Molecule 10 is water.

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

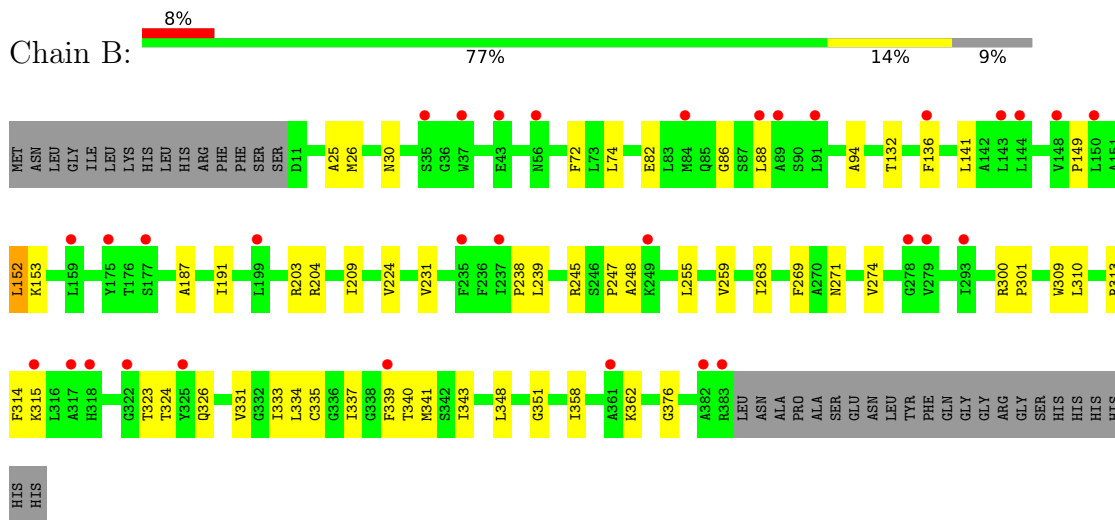
3 Residue-property plots [i](#)

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.

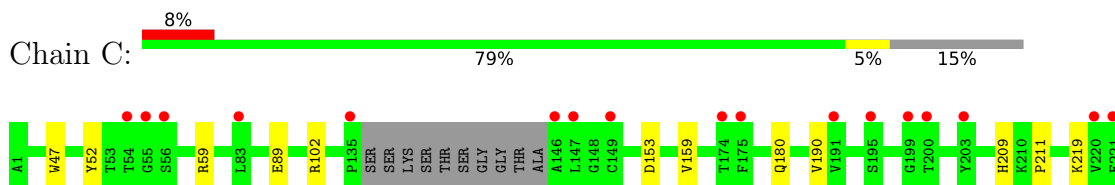
- Molecule 1: Na(+)/H(+) antiporter NhaA



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

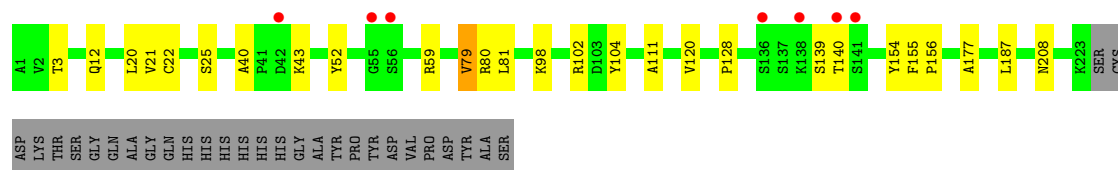
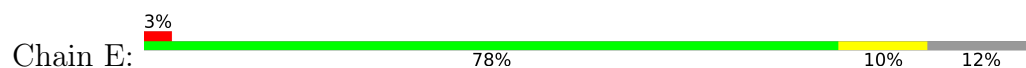


- Molecule 2: chimeric antibody Fab-F6, heavy chain, chimeric antibody Fab-F6, heavy chain

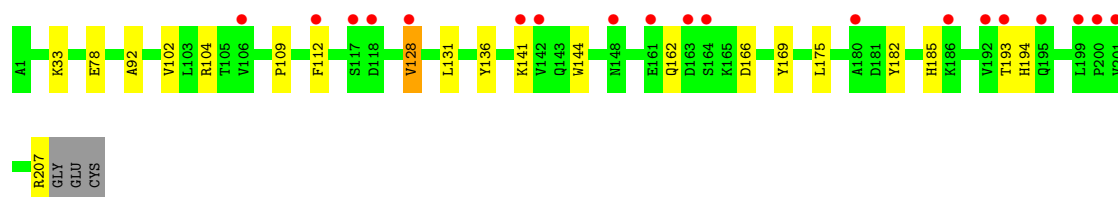
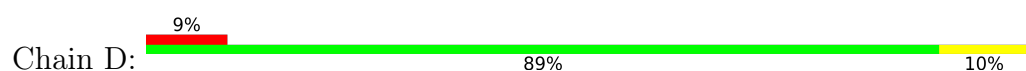




- Molecule 2: chimeric antibody Fab-F6, heavy chain, chimeric antibody Fab-F6, heavy chain



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



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



4 Data and refinement statistics

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) 59.6 (24.74-2.45)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.44Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.203 , 0.241 0.204 , 0.240	Depositor DCC
R_{free} test set	1746 reflections (1.80%)	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)	0.25 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.08	0/2884	0.26	0/3933
1	B	0.08	0/2873	0.24	0/3917
2	C	0.08	0/1611	0.25	0/2191
2	E	0.08	0/1672	0.26	0/2274
3	D	0.07	0/1599	0.23	0/2177
3	F	0.08	0/1603	0.25	0/2182
All	All	0.08	0/12242	0.25	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 [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	2814	0	2995	32	0
1	B	2806	0	2994	34	0
2	C	1573	0	1541	7	0
2	E	1633	0	1600	16	0
3	D	1561	0	1517	13	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	104	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:323:THR:O	1:A:324:THR:OG1	2.30	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
1:A:323:THR:C	1:A:325:TYR:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:72:PHE:HZ	1:B:341:MET:HE1	1.81	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
3:D:78:GLU:OE2	3:D:169:TYR:OH	2.35	0.42
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
2:E:139:SER:C	2:E:140:THR:HG1	2.26	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:B:26:MET:HE1	1:B:274:VAL:HB	2.02	0.41
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:311:ALA:C	1:A:317:ALA:HB2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	53	67
1	B	288/318 (91%)	284 (99%)	4 (1%)	59	72
2	C	170/199 (85%)	167 (98%)	3 (2%)	51	65
2	E	177/199 (89%)	175 (99%)	2 (1%)	65	76
3	D	177/178 (99%)	176 (99%)	1 (1%)	78	86
3	F	177/178 (99%)	177 (100%)	0	100	100
All	All	1277/1390 (92%)	1262 (99%)	15 (1%)	63	74

All (15) 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	323	THR
1	B	324	THR
1	B	326	GLN
2	C	159	VAL
2	C	219	LYS
2	C	223	LYS
3	D	128	VAL
2	E	79	VAL
2	E	208	ASN

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

Mol	Chain	Res	Type
1	B	39	HIS
1	B	225	HIS
2	E	173	HIS
3	F	133	ASN
3	F	162	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	$\# Z > 2$
6	PO4	B	504	-	4,4,4	0.96	0	6,6,6	0.45	0
5	3PH	A	502	-	26,26,47	0.26	0	29,31,52	0.33	0
5	3PH	B	502	-	22,22,47	0.28	0	25,27,52	0.37	0
7	PG4	B	505	-	12,12,12	0.45	0	11,11,11	0.29	0
7	PG4	A	504	-	12,12,12	0.46	0	11,11,11	0.27	0
5	3PH	B	503	-	26,26,47	0.25	0	29,31,52	0.32	0
6	PO4	A	503	-	4,4,4	0.96	0	6,6,6	0.46	0
4	CDL	A	501	-	52,52,99	1.27	4 (7%)	58,64,111	1.28	5 (8%)
8	3PE	B	501	-	27,27,50	0.39	0	30,32,55	0.35	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	A	502	-	-	3/28/28/49	-
5	3PH	B	502	-	-	4/24/24/49	-
7	PG4	B	505	-	-	1/10/10/10	-
7	PG4	A	504	-	-	1/10/10/10	-
5	3PH	B	503	-	-	1/28/28/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CDL	A	501	-	-	16/63/63/110	-
8	3PE	B	501	-	-	5/31/31/54	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	CDL	OA8-CA7	4.28	1.45	1.33
4	A	501	CDL	OB8-CB7	4.28	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(°)	Ideal(°)
4	A	501	CDL	OA6-CA5-C11	4.13	120.42	111.48
4	A	501	CDL	OB6-CB5-C51	3.72	119.52	111.48
4	A	501	CDL	CA4-OA6-CA5	-3.02	110.58	117.80
4	A	501	CDL	OA8-CA7-C31	2.92	120.75	111.83
4	A	501	CDL	OB8-CB7-C71	2.66	119.95	111.83

There are no chirality outliers.

All (31) 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-OA2
4	A	501	CDL	CA3-OA5-PA1-OA3
4	A	501	CDL	CA3-OA5-PA1-OA4
4	A	501	CDL	CB3-OB5-PB2-OB2
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-O11
8	B	501	3PE	C11-O13-P-O12
8	B	501	3PE	C11-O13-P-O14
4	A	501	CDL	C11-CA5-OA6-CA4
4	A	501	CDL	CA5-C11-C12-C13
4	A	501	CDL	OA7-CA5-OA6-CA4
5	A	502	3PH	C1-O11-P-O12
5	B	502	3PH	O11-C1-C2-O21

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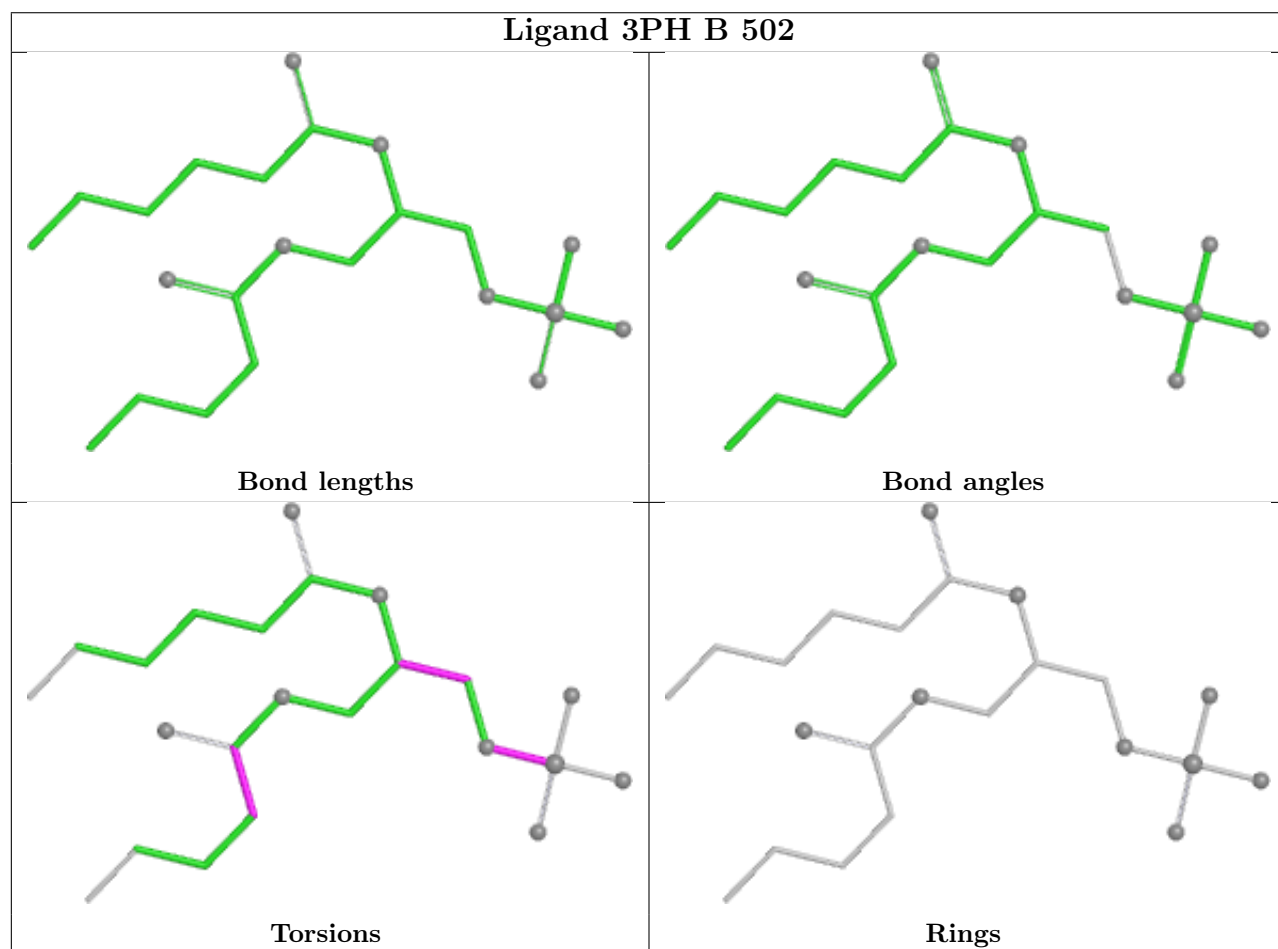
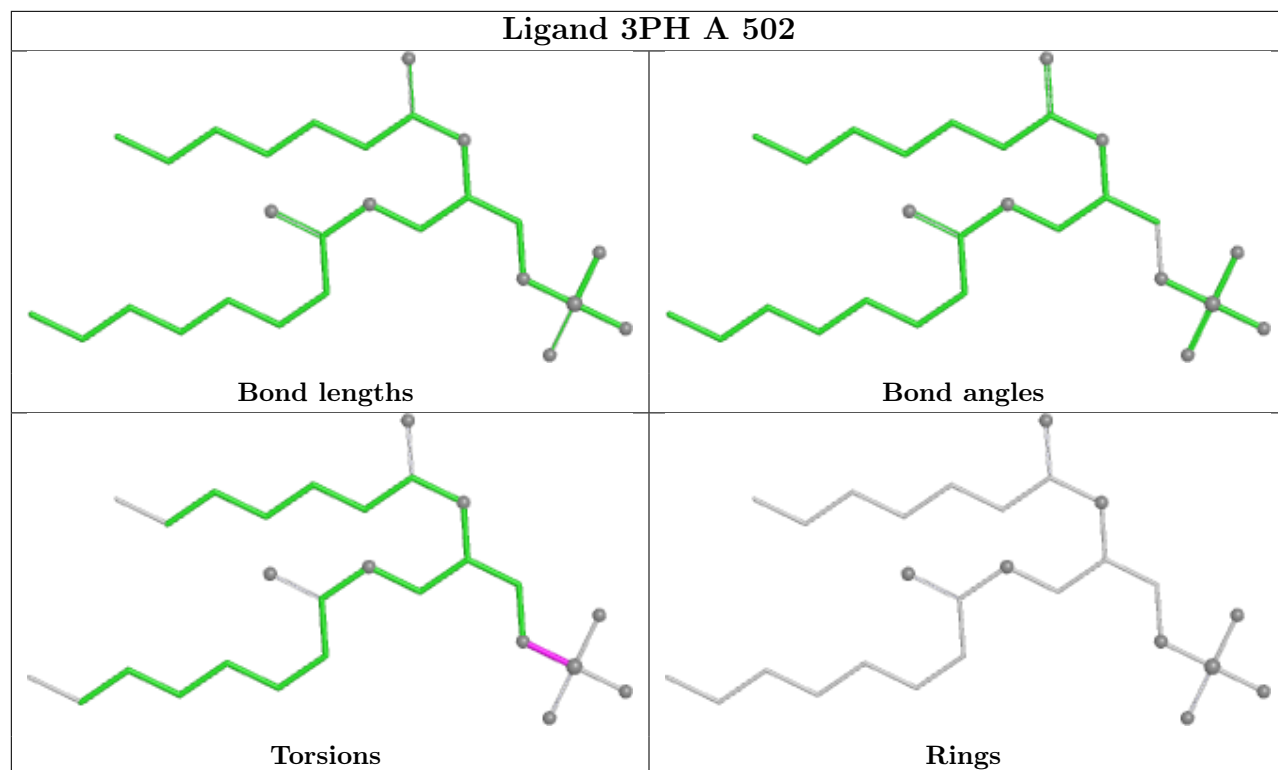
Mol	Chain	Res	Type	Atoms
4	A	501	CDL	OB5-CB3-CB4-CB6
4	A	501	CDL	OA6-CA4-CA6-OA8
4	A	501	CDL	C31-C32-C33-C34
5	B	502	3PH	O11-C1-C2-C3
4	A	501	CDL	OB5-CB3-CB4-OB6
4	A	501	CDL	CB2-OB2-PB2-OB3
4	A	501	CDL	CB3-OB5-PB2-OB3
5	B	502	3PH	C1-O11-P-O12
7	A	504	PG4	O2-C3-C4-O3
5	B	502	3PH	O31-C31-C32-C33
8	B	501	3PE	O21-C2-C3-O31
4	A	501	CDL	CA3-CA4-CA6-OA8
5	B	503	3PH	O11-C1-C2-C3
7	B	505	PG4	O2-C3-C4-O3

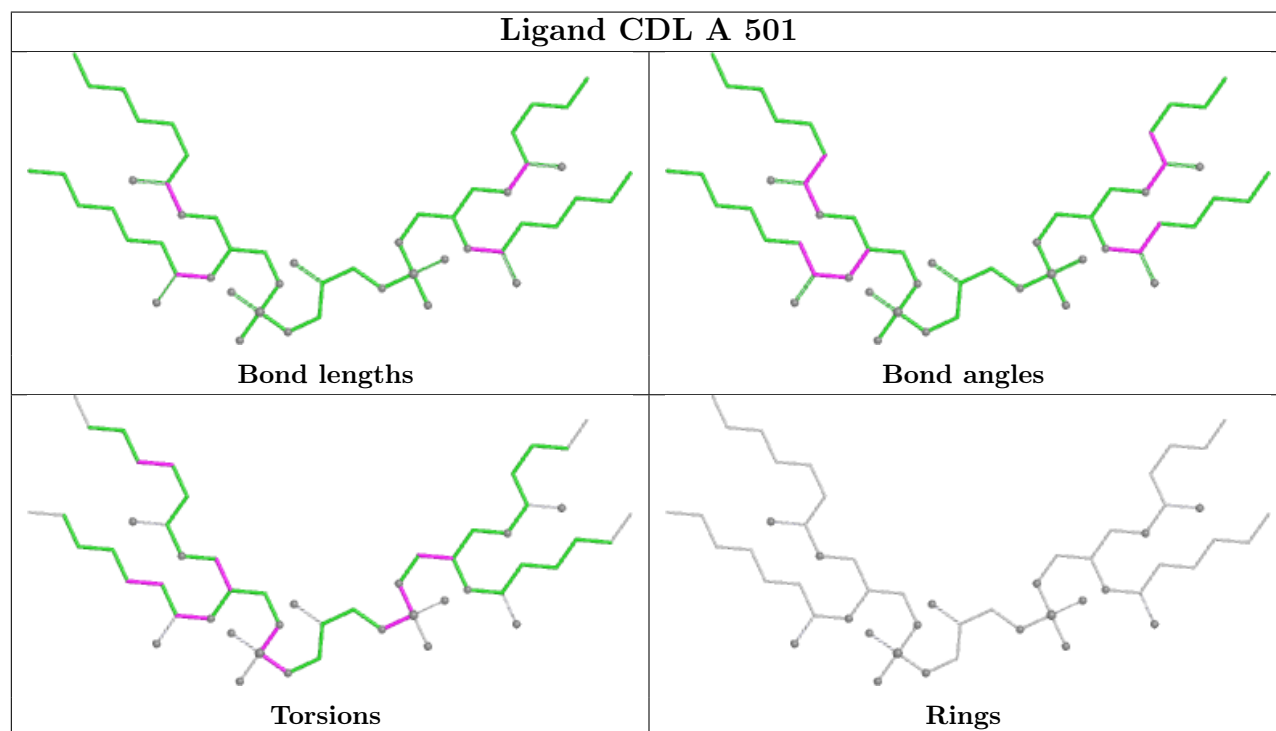
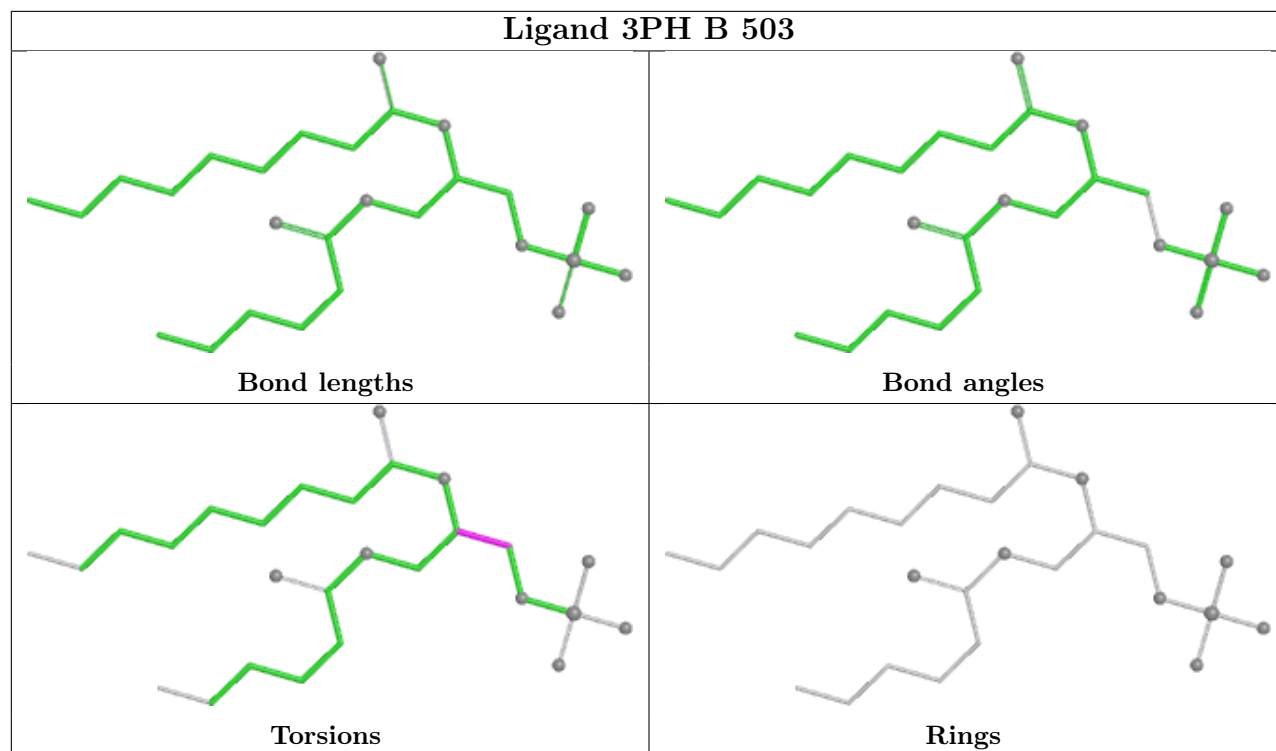
There are no ring outliers.

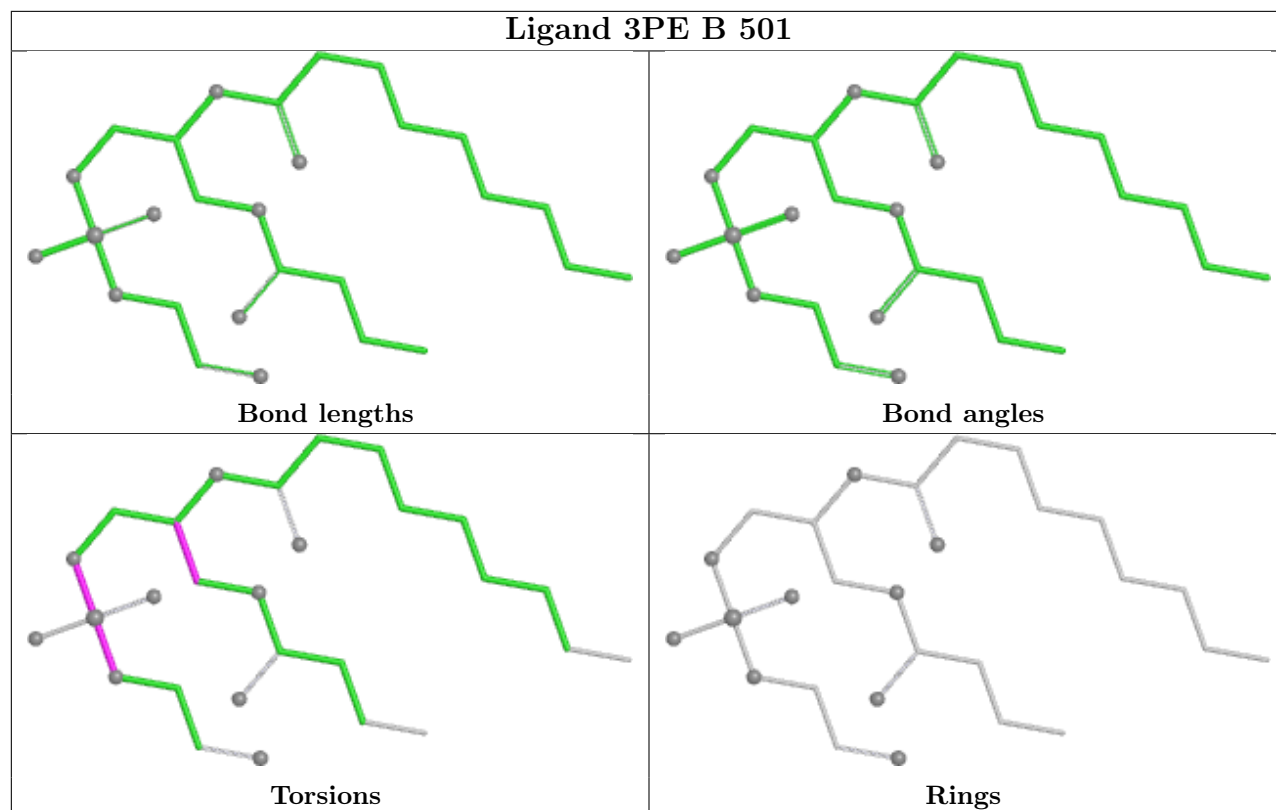
2 monomers are involved in 4 short contacts:

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	372/411 (90%)	0.64	31 (8%)	17 15	24, 72, 132, 170	16 (4%)
1	B	370/411 (90%)	0.70	32 (8%)	16 14	42, 84, 135, 157	15 (4%)
2	C	210/252 (83%)	0.43	19 (9%)	15 13	24, 54, 136, 172	3 (1%)
2	E	223/252 (88%)	-0.11	7 (3%)	51 52	26, 45, 87, 136	3 (1%)
3	D	206/210 (98%)	0.56	19 (9%)	14 12	28, 68, 144, 167	7 (3%)
3	F	209/210 (99%)	-0.05	4 (1%)	66 67	29, 51, 79, 106	1 (0%)
All	All	1590/1746 (91%)	0.42	112 (7%)	22 20	24, 67, 131, 172	45 (2%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	164	SER	5.9
2	C	146	ALA	5.9
3	D	193	THR	5.0
2	C	147	LEU	4.7
2	C	55	GLY	4.7
1	A	325	TYR	4.7
3	F	1	ALA	4.7
1	A	327	GLN	4.6
1	A	309[A]	TRP	4.5
1	A	324	THR	4.4
2	E	42	ASP	4.3
3	D	148	ASN	4.3
2	C	149	CYS	4.1
3	D	142	VAL	4.0
1	B	150	LEU	4.0
2	C	135	PRO	4.0
2	C	56	SER	3.9
1	B	325	TYR	3.8
1	B	91	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	221	GLU	3.7
1	B	37	TRP	3.6
2	E	140	THR	3.5
1	B	235	PHE	3.5
3	D	201	VAL	3.4
3	D	141	LYS	3.4
1	B	144	LEU	3.4
1	B	159	LEU	3.3
1	B	293[A]	ILE	3.3
2	E	138	LYS	3.3
3	D	128	VAL	3.3
1	A	380	LEU	3.2
3	D	163	ASP	3.2
1	A	382	ALA	3.1
1	A	322	GLY	3.1
1	A	244	GLY	3.0
1	A	352	ASN	3.0
1	B	43	GLU	2.9
2	C	54	THR	2.9
1	B	339	PHE	2.9
1	B	177	SER	2.8
1	A	152	LEU	2.8
1	A	379	TRP	2.8
1	A	176	THR	2.8
1	B	88	LEU	2.7
1	A	253	HIS	2.7
1	B	322	GLY	2.7
1	A	318	HIS	2.7
1	A	149	PRO	2.7
1	B	143	LEU	2.7
3	D	195	GLN	2.7
3	D	186	LYS	2.6
1	A	242	LYS	2.6
3	D	199	LEU	2.6
2	C	203	TYR	2.6
1	A	383	ARG	2.6
1	B	317	ALA	2.6
3	D	200	PRO	2.5
1	A	137	ALA	2.5
1	B	361	ALA	2.5
1	B	148	VAL	2.5
2	C	191	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	92	ARG	2.5
1	A	241	GLU	2.4
1	B	278	GLY	2.4
1	B	175	TYR	2.4
3	F	73	VAL	2.4
1	A	308	CYS	2.4
3	D	118	ASP	2.4
2	C	83	LEU	2.4
1	B	136	PHE	2.4
1	A	323	THR	2.3
1	A	111	LEU	2.3
2	C	175	PHE	2.3
2	C	220	VAL	2.3
3	D	192	VAL	2.3
1	B	56	ASN	2.3
1	B	318	HIS	2.3
3	D	117	SER	2.3
1	A	339	PHE	2.3
1	A	317	ALA	2.2
2	C	223	LYS	2.2
2	E	136	SER	2.2
1	B	382	ALA	2.2
1	B	249	LYS	2.2
1	B	315	LYS	2.2
1	A	236	PHE	2.2
2	E	56	SER	2.2
2	E	141	SER	2.2
1	A	321	GLN	2.1
2	C	200	THR	2.1
3	F	36	GLY	2.1
1	B	237	ILE	2.1
2	C	199	GLY	2.1
1	B	383	ARG	2.1
3	D	161	GLU	2.1
1	B	84	MET	2.1
1	B	89	ALA	2.1
2	C	174	THR	2.1
3	F	209	GLU	2.1
2	C	222	PRO	2.1
3	D	112	PHE	2.1
3	D	180	ALA	2.1
2	E	55	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	328	ILE	2.1
1	A	153	LYS	2.1
3	D	106	VAL	2.0
1	B	199	LEU	2.0
1	A	84	MET	2.0
1	B	35	SER	2.0
2	C	195	SER	2.0
1	B	279	VAL	2.0
1	A	282	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

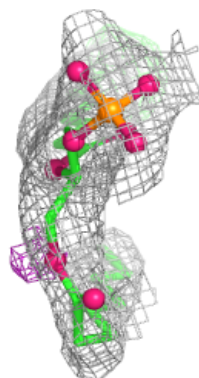
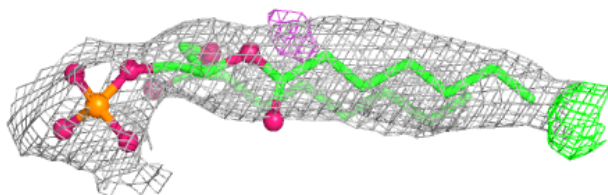
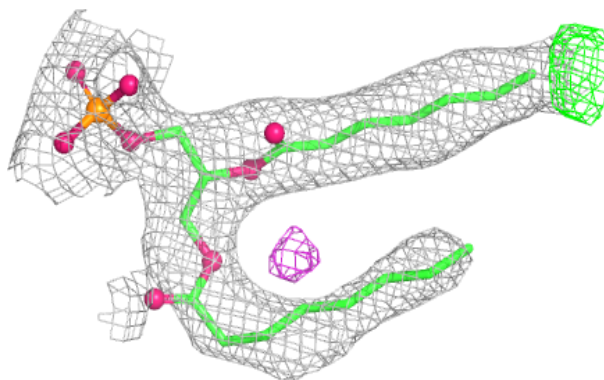
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	3PH	A	502	27/48	0.66	0.16	62,93,143,151	0
6	PO4	B	504	5/5	0.72	0.13	75,90,99,119	0
5	3PH	B	503	27/48	0.77	0.16	71,92,130,142	0
5	3PH	B	502	23/48	0.79	0.16	58,99,151,152	0
7	PG4	B	505	13/13	0.81	0.15	74,83,90,91	0
8	3PE	B	501	28/51	0.83	0.16	74,90,105,131	0
6	PO4	A	503	5/5	0.84	0.14	78,82,97,117	0
4	CDL	A	501	53/100	0.86	0.15	68,94,142,148	0
9	CL	C	302	1/1	0.91	0.15	73,73,73,73	0
7	PG4	A	504	13/13	0.93	0.10	45,54,68,71	0
9	CL	C	301	1/1	0.96	0.08	49,49,49,49	0
9	CL	C	303	1/1	0.99	0.05	48,48,48,48	0
9	CL	E	301	1/1	0.99	0.11	63,63,63,63	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.

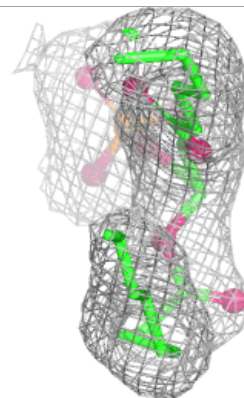
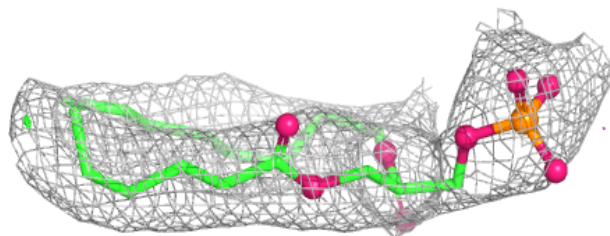
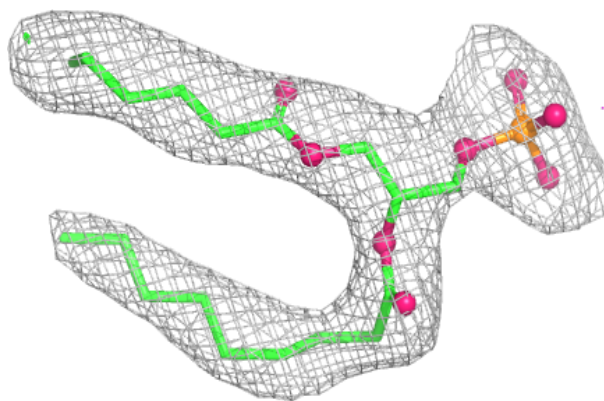
Electron density around 3PH A 502:

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

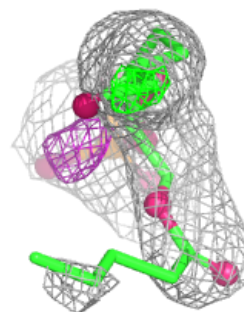
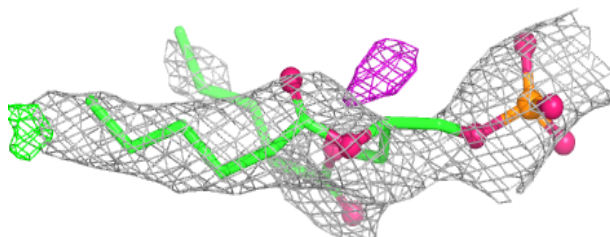
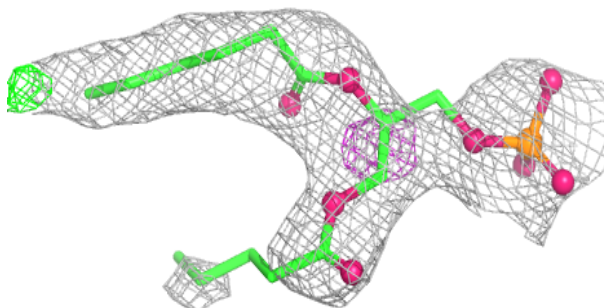


Electron density around 3PH B 503:

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

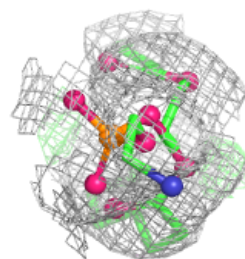
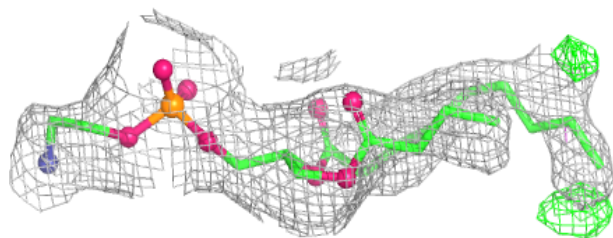
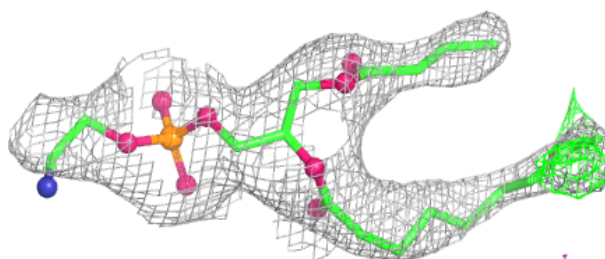
**Electron density around 3PH B 502:**

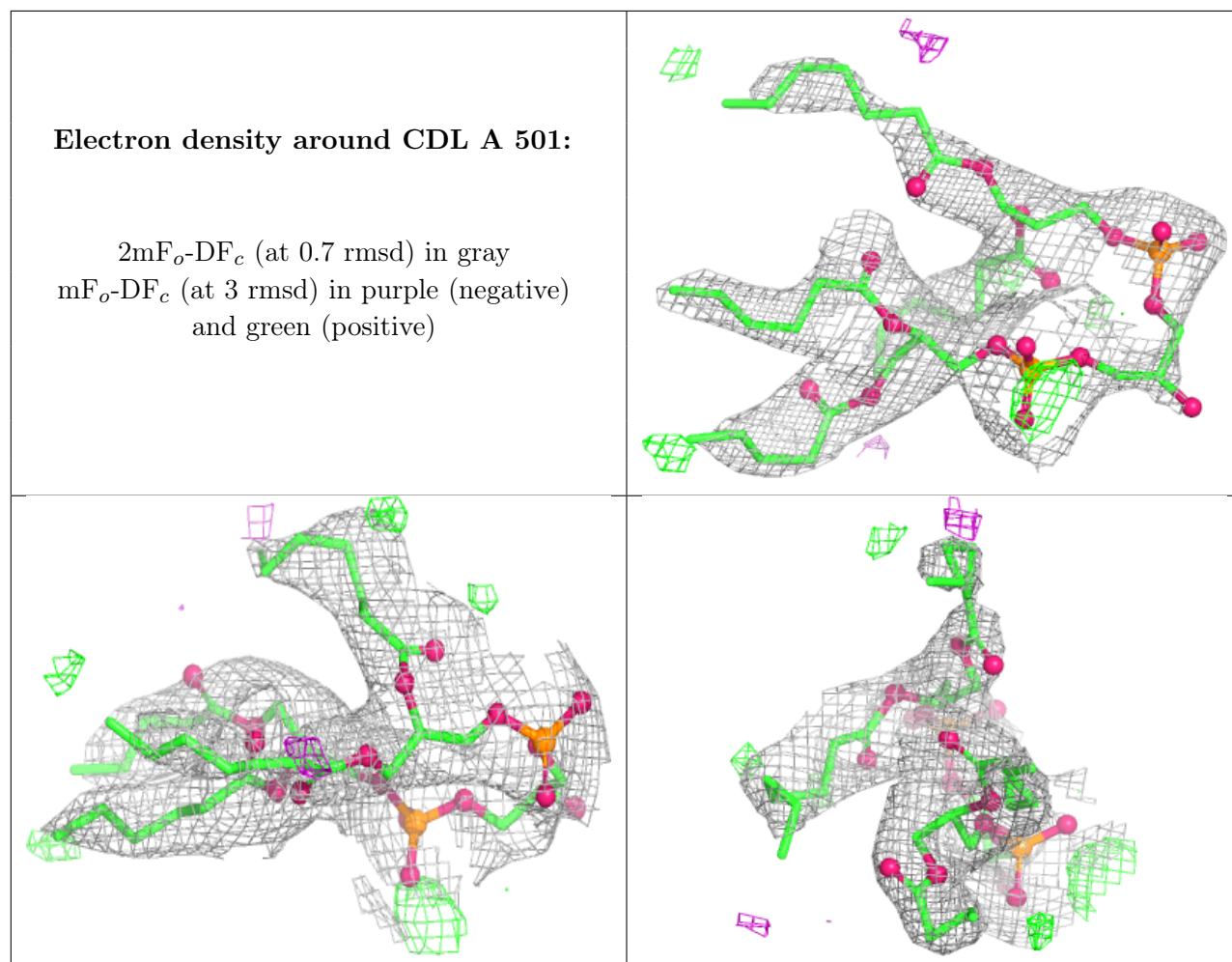
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.