



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:35 AM UTC

PDB ID : 7A0W / pdb_00007a0w
Title : Structure of dimeric sodium proton antiporter NhaA, at pH 8.5, crystallized with chimeric Fab antibodies
Authors : Fippel, A.; Gross, N.M.; Mir, S.H.; Wirth, C.; Hunte, C.
Deposited on : 2020-08-11
Resolution : 2.04 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

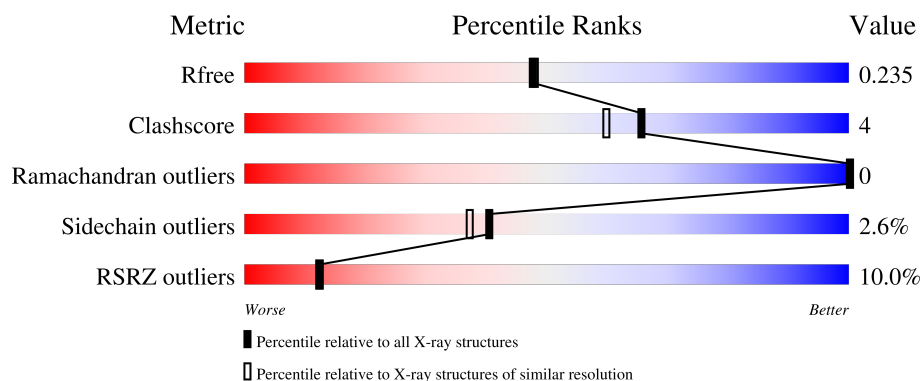
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	406	14% 79% 11% 9%
1	B	406	13% 78% 13% 8%
2	C	252	9% 79% 5% 15%
2	E	252	4% 83% 5% 12%
3	D	210	8% 89% 10%

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Mol	Chain	Length	Quality of chain
3	F	210	% 92% 7%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12332 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	368	Total	C	N	O	S	69	2	0
			2772	1851	448	459	14			
1	B	373	Total	C	N	O	S	80	3	0
			2815	1880	456	465	14			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

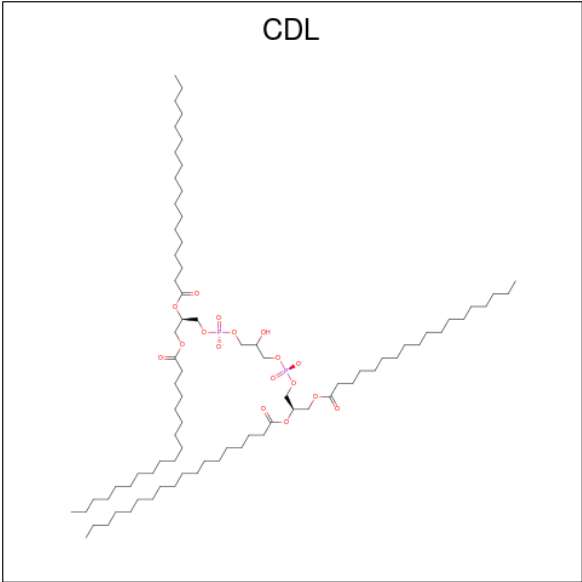
- Molecule 2 is a protein called chimeric antibody Fab-F6, heavy chain, chimeric antibody Fab-F6, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	213	Total	C	N	O	S	28	0	0
			1565	982	268	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.

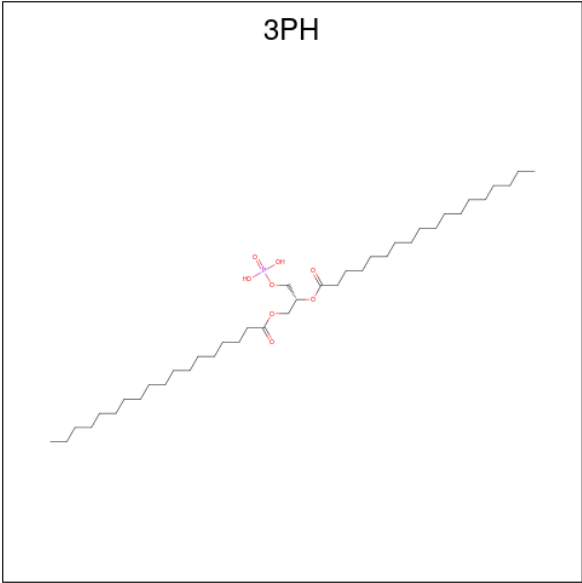
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	207	Total	C	N	O	S	27	0	0
			1555	972	263	316	4			
3	F	209	Total	C	N	O	S	4	0	0
			1568	979	265	320	4			

- Molecule 4 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	A	1	52	33	17	2	0	0

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



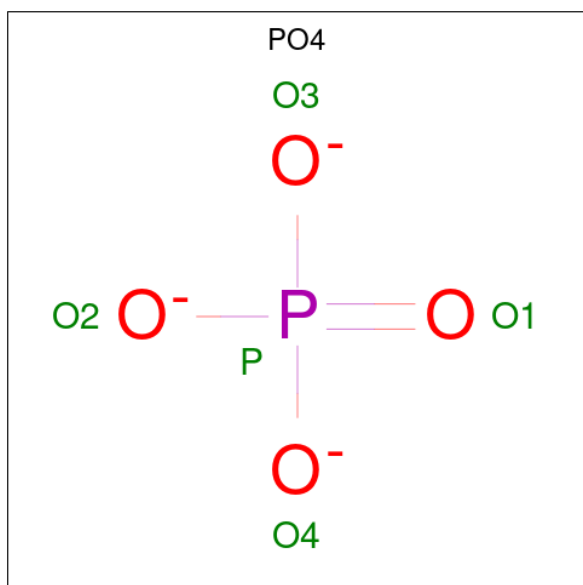
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
5	A	1	27	18	8	1	0	0
5	B	1	21	12	8	1	0	0

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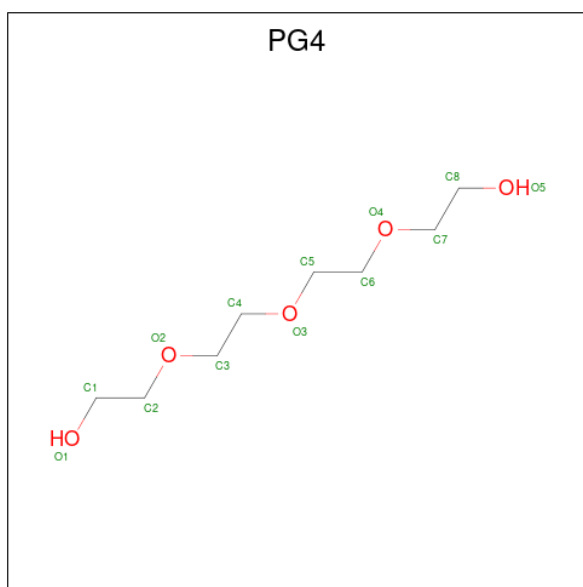
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			27	18	8	1		
5	B	1	Total	C	O	P	0	0
			19	10	8	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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: C₈H₁₈O₅).



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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	3	Total	Cl	0	0
			3	3		

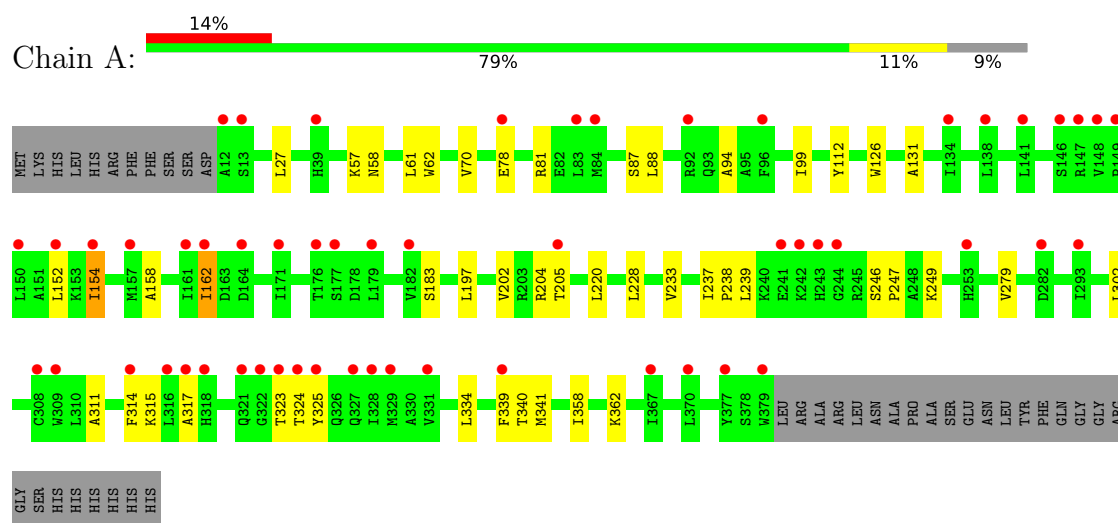
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	8	Total	O	0	0
			8	8		
9	B	4	Total	O	0	0
			4	4		
9	C	45	Total	O	0	0
			45	45		
9	D	51	Total	O	0	0
			51	51		
9	E	70	Total	O	0	0
			70	70		
9	F	61	Total	O	0	0
			61	61		

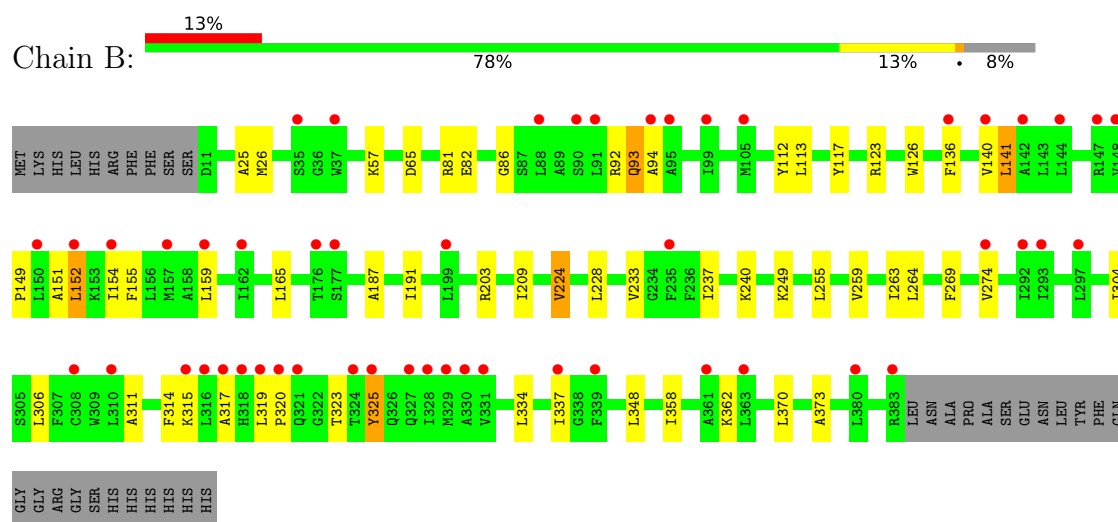
3 Residue-property plots [i](#)

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.

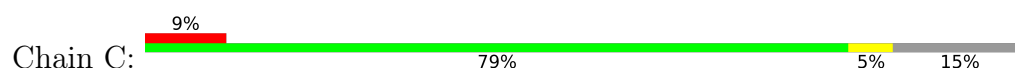
- Molecule 1: Na(+)/H(+) antiporter NhaA

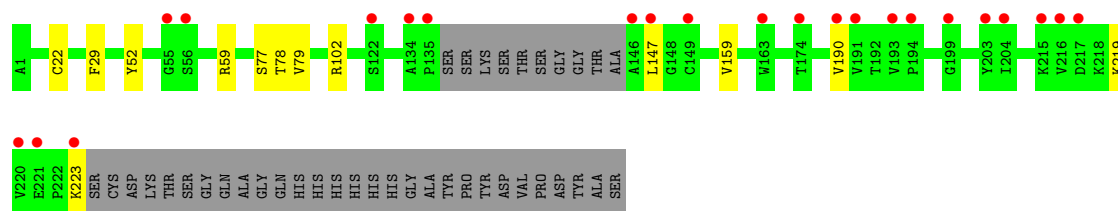


- Molecule 1: Na(+)/H(+) antiporter NhaA

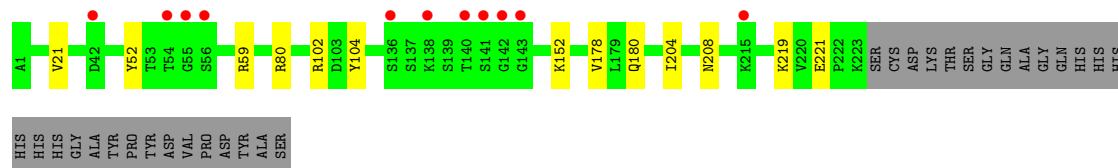
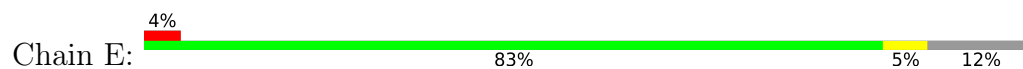


- Molecule 2: chimeric antibody Fab-F6, heavy chain, chimeric antibody Fab-F6, heavy chain

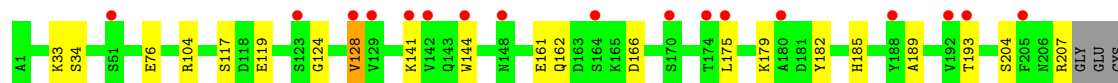
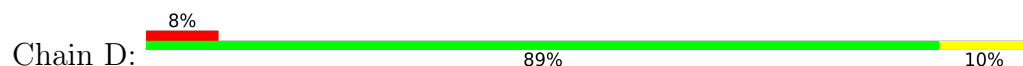




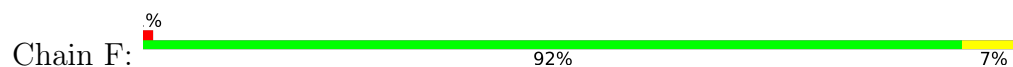
- Molecule 2: chimeric antibody Fab-F6, heavy chain, chimeric antibody Fab-F6, heavy chain



- 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	112.79Å 92.16Å 139.10Å 90.00° 109.89° 90.00°	Depositor
Resolution (Å)	24.86 – 2.04 24.86 – 2.04	Depositor EDS
% Data completeness (in resolution range)	56.1 (24.86-2.04) 56.1 (24.86-2.04)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.04Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.198 , 0.235 0.200 , 0.235	Depositor DCC
R_{free} test set	2414 reflections (1.43%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12332	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PH, PG4, CL, PO4, 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	0.14	0/2839	0.33	0/3873
1	B	0.13	0/2887	0.33	0/3937
2	C	0.20	0/1600	0.41	0/2177
2	E	0.23	0/1672	0.45	0/2274
3	D	0.19	0/1590	0.40	0/2165
3	F	0.22	0/1603	0.43	0/2182
All	All	0.18	0/12191	0.38	0/16608

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	2772	0	2942	31	0
1	B	2815	0	3004	31	0
2	C	1565	0	1528	4	0
2	E	1633	0	1600	5	0
3	D	1555	0	1511	12	0
3	F	1568	0	1520	8	0
4	A	52	0	48	2	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	67	0	53	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	13	0	18	1	0
7	B	13	0	18	0	0
8	C	3	0	0	1	0
9	A	8	0	0	0	0
9	B	4	0	0	0	0
9	C	45	0	0	0	0
9	D	51	0	0	0	0
9	E	70	0	0	0	0
9	F	61	0	0	0	0
All	All	12332	0	12269	91	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 (91) 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:C:52:TYR:OH	2:C:102:ARG:NH1	2.23	0.72
1:A:204:ARG:NH1	4:A:501:CDL:OB4	2.23	0.71
1:B:203:ARG:HH12	1:B:240:LYS:HB2	1.56	0.69
1:B:82:GLU:HA	1:B:86:GLY:HA3	1.76	0.67
1:A:323:THR:HG22	1:A:325:TYR:H	1.63	0.64
3:D:182:TYR:O	3:D:207:ARG:NH2	2.32	0.62
3:D:141:LYS:HB3	3:D:193:THR:HB	1.83	0.61
3:D:128:VAL:HG13	3:D:175:LEU:HB3	1.83	0.60
1:A:58:ASN:HD21	1:A:61:LEU:HD23	1.66	0.60
3:D:104:ARG:NH1	3:D:166:ASP:O	2.35	0.59
2:E:52:TYR:OH	2:E:102:ARG:NH1	2.36	0.59
1:B:358:ILE:HG13	1:B:362:LYS:HE3	1.86	0.58
3:F:104:ARG:NH1	3:F:167:SER:OG	2.37	0.57
2:C:59:ARG:HD3	8:C:302:CL:CL	2.41	0.57
3:D:117:SER:OG	3:D:119:GLU:OE1	2.23	0.57
3:F:85:SER:OG	3:F:86:ALA:N	2.36	0.57
1:B:224:VAL:HG13	1:B:348:LEU:HD13	1.86	0.56
1:B:323:THR:HG22	1:B:325:TYR:H	1.68	0.56
1:A:87:SER:HB3	1:A:154:ILE:HD11	1.87	0.56
1:A:358:ILE:HG13	1:A:362:LYS:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:PHE:HD2	1:B:337:ILE:HG21	1.73	0.53
1:A:239:LEU:HD11	1:A:249:LYS:HE2	1.91	0.52
1:A:205:THR:HG22	1:A:247:PRO:HB3	1.91	0.51
1:A:81:ARG:HD2	1:A:249:LYS:HZ3	1.75	0.51
2:E:219:LYS:NZ	2:E:221:GLU:OE2	2.42	0.50
1:A:238:PRO:HG2	1:A:247:PRO:HG2	1.94	0.50
1:B:311:ALA:HB1	1:B:317:ALA:HB2	1.93	0.50
1:A:88:LEU:HA	1:A:94:ALA:HB2	1.94	0.50
2:C:22:CYS:O	2:C:78:THR:HA	2.12	0.49
3:D:128:VAL:HG22	3:D:144:TRP:CH2	2.48	0.49
1:B:151:ALA:HA	1:B:154:ILE:HG22	1.95	0.49
1:A:311:ALA:O	1:A:317:ALA:HB2	2.13	0.49
1:B:337:ILE:HD11	1:B:373:ALA:HB2	1.94	0.49
2:E:59:ARG:HG3	2:E:104:TYR:OH	2.12	0.49
1:B:259:VAL:HA	1:B:263:ILE:HB	1.95	0.48
1:B:149:PRO:HG2	1:B:152:LEU:HB2	1.94	0.48
1:B:323:THR:C	1:B:325:TYR:H	2.20	0.48
3:D:185:HIS:O	3:D:207:ARG:NH2	2.47	0.48
1:B:187:ALA:O	1:B:191:ILE:HG12	2.13	0.48
1:B:320:PRO:O	1:B:323:THR:OG1	2.28	0.47
1:A:112:TYR:CD1	1:A:126:TRP:HA	2.50	0.47
3:F:56:ARG:HB2	3:F:71:THR:O	2.14	0.47
1:A:197:LEU:HG	1:A:202:VAL:HG21	1.94	0.47
1:B:81:ARG:HH21	1:B:249:LYS:HG2	1.78	0.47
2:E:21:VAL:HG22	2:E:80[B]:ARG:HG3	1.96	0.47
1:B:57:LYS:NZ	1:B:65:ASP:OD2	2.40	0.47
3:F:120:GLN:HG2	3:F:125:THR:O	2.15	0.47
1:B:323:THR:HG22	1:B:325:TYR:N	2.30	0.46
1:A:57:LYS:HB2	1:A:62:TRP:CD1	2.51	0.46
3:F:75:ALA:HA	3:F:102:VAL:HG21	1.97	0.46
1:A:246:SER:HB3	1:A:249:LYS:HB2	1.98	0.46
1:A:58:ASN:ND2	1:A:61:LEU:HD23	2.30	0.45
1:B:93:GLN:HG3	1:B:94:ALA:H	1.81	0.45
3:F:16:VAL:HG13	3:F:70:ILE:HB	1.98	0.45
1:A:323:THR:C	1:A:325:TYR:H	2.25	0.44
1:B:25:ALA:HB2	1:B:269:PHE:HA	1.99	0.44
3:D:33:LYS:HE3	3:D:162:GLN:HB3	1.99	0.44
2:E:152:LYS:NZ	2:E:180:GLN:OE1	2.50	0.44
1:A:99:ILE:HG21	1:A:311:ALA:HB2	1.99	0.44
1:A:131:ALA:HB1	1:A:341:MET:HB3	1.99	0.44
4:A:501:CDL:H142	1:B:209:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:TYR:CD2	1:B:126:TRP:HA	2.52	0.44
1:B:159:LEU:HD21	1:B:304:ILE:HD12	2.00	0.44
1:A:158:ALA:O	1:A:162:ILE:HG22	2.18	0.43
1:B:151:ALA:O	1:B:155:PHE:N	2.49	0.43
1:A:339:PHE:CD2	1:A:340:THR:HG23	2.53	0.43
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.91	0.43
1:B:233:VAL:O	1:B:237:ILE:HG13	2.19	0.43
1:A:314:PHE:O	1:A:315:LYS:HG2	2.17	0.43
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.92	0.43
3:D:189:ALA:HB2	3:D:204:SER:HB3	2.01	0.43
1:B:26:MET:HE1	1:B:274:VAL:HB	2.00	0.42
3:D:76:GLU:CD	3:D:76:GLU:H	2.27	0.42
3:D:124:GLY:HA2	3:D:179:LYS:HD2	2.02	0.42
1:A:279:VAL:HG22	7:A:504:PG4:H71	2.02	0.42
1:B:117:TYR:O	1:B:123:ARG:NH1	2.46	0.42
2:C:29:PHE:CD2	2:C:77:SER:HA	2.55	0.42
1:B:264:LEU:HD23	1:B:264:LEU:HA	1.90	0.42
1:A:323:THR:O	1:A:324:THR:OG1	2.33	0.42
1:B:314:PHE:O	1:B:315:LYS:HG2	2.20	0.42
1:A:233:VAL:O	1:A:237:ILE:HG12	2.20	0.41
1:A:311:ALA:C	1:A:317:ALA:HB2	2.45	0.41
3:F:186:LYS:HD2	3:F:186:LYS:HA	1.78	0.41
1:A:78:GLU:HA	1:A:81:ARG:HD3	2.01	0.41
3:F:162:GLN:HG2	3:F:167:SER:HA	2.01	0.41
1:B:141:LEU:HD23	1:B:141:LEU:HA	1.80	0.40
1:B:113:LEU:HD21	1:B:126:TRP:HB3	2.03	0.40
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.89	0.40
1:B:319:LEU:HD11	1:B:323:THR:HG21	2.03	0.40
1:A:99:ILE:HD13	1:A:99:ILE:HA	1.92	0.40
3:D:34:SER:OG	3:D:161:GLU:OE1	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	368/406 (91%)	352 (96%)	16 (4%)	0	100	100
1	B	374/406 (92%)	357 (96%)	17 (4%)	0	100	100
2	C	209/252 (83%)	205 (98%)	4 (2%)	0	100	100
2	E	222/252 (88%)	215 (97%)	7 (3%)	0	100	100
3	D	205/210 (98%)	196 (96%)	9 (4%)	0	100	100
3	F	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
All	All	1585/1736 (91%)	1521 (96%)	64 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	284/314 (90%)	277 (98%)	7 (2%)	42	39
1	B	289/314 (92%)	276 (96%)	13 (4%)	24	18
2	C	169/199 (85%)	163 (96%)	6 (4%)	31	26
2	E	177/199 (89%)	174 (98%)	3 (2%)	53	53
3	D	176/178 (99%)	175 (99%)	1 (1%)	78	83
3	F	177/178 (99%)	174 (98%)	3 (2%)	53	53
All	All	1272/1382 (92%)	1239 (97%)	33 (3%)	40	37

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	70	VAL
1	A	154	ILE
1	A	162	ILE

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Mol	Chain	Res	Type
1	A	183	SER
1	A	302	LEU
1	A	334	LEU
1	B	92	ARG
1	B	93	GLN
1	B	140	VAL
1	B	141	LEU
1	B	152	LEU
1	B	165	LEU
1	B	224	VAL
1	B	228	LEU
1	B	255	LEU
1	B	306	LEU
1	B	325	TYR
1	B	334	LEU
1	B	370	LEU
2	C	79	VAL
2	C	147	LEU
2	C	159	VAL
2	C	190	VAL
2	C	219	LYS
2	C	223	LYS
3	D	128	VAL
2	E	178	VAL
2	E	204	ILE
2	E	208	ASN
3	F	16	VAL
3	F	110	SER
3	F	150	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	HIS
2	C	82	GLN
2	C	173	HIS
3	D	11	ASN
3	D	134	ASN
3	D	143	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 3 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$
7	PG4	B	505	-	12,12,12	0.47	0	11,11,11	0.34	0
4	CDL	A	501	-	51,51,99	1.28	4 (7%)	57,63,111	1.22	6 (10%)
5	3PH	A	502	-	26,26,47	0.28	0	29,31,52	0.35	0
5	3PH	B	501	-	20,20,47	0.46	0	23,25,52	0.48	0
5	3PH	B	502	-	26,26,47	0.26	0	29,31,52	0.34	0
7	PG4	A	504	-	12,12,12	0.49	0	11,11,11	0.35	0
5	3PH	B	503	-	18,18,47	0.52	0	21,23,52	0.64	1 (4%)
6	PO4	A	503	-	4,4,4	0.91	0	6,6,6	0.49	0
6	PO4	B	504	-	4,4,4	0.94	0	6,6,6	0.40	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
4	CDL	A	501	-	-	18/62/62/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3PH	A	502	-	-	5/28/28/49	-
5	3PH	B	501	-	-	6/22/22/49	-
5	3PH	B	502	-	-	2/28/28/49	-
7	PG4	A	504	-	-	1/10/10/10	-
5	3PH	B	503	-	-	8/20/20/49	-
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	4.32	1.45	1.33
4	A	501	CDL	OB8-CB7	4.28	1.45	1.33
4	A	501	CDL	OA6-CA5	4.11	1.45	1.34
4	A	501	CDL	OB6-CB5	4.04	1.45	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	CDL	OA6-CA5-C11	3.89	119.89	111.48
4	A	501	CDL	OB6-CB5-C51	3.11	118.20	111.48
4	A	501	CDL	OA8-CA7-C31	2.96	120.87	111.83
4	A	501	CDL	OB8-CB7-C71	2.72	120.14	111.83
4	A	501	CDL	CA4-OA6-CA5	-2.64	111.48	117.80
5	B	503	3PH	O14-P-O11	2.13	112.23	106.67
4	A	501	CDL	OB8-CB7-OB9	-2.04	118.53	123.63

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	OA7-CA5-OA6-CA4
4	A	501	CDL	C11-CA5-OA6-CA4
4	A	501	CDL	CB3-OB5-PB2-OB2
4	A	501	CDL	CB3-OB5-PB2-OB3
4	A	501	CDL	CB3-OB5-PB2-OB4
5	A	502	3PH	C1-O11-P-O13
5	A	502	3PH	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
5	A	502	3PH	C1-O11-P-O12
5	B	503	3PH	C1-O11-P-O13
4	A	501	CDL	O1-C1-CB2-OB2
7	A	504	PG4	O2-C3-C4-O3
4	A	501	CDL	CA2-C1-CB2-OB2
5	B	503	3PH	C1-O11-P-O12
4	A	501	CDL	C31-C32-C33-C34
5	B	502	3PH	O11-C1-C2-C3
5	B	503	3PH	C1-O11-P-O14
5	A	502	3PH	C31-C32-C33-C34
4	A	501	CDL	CB7-C71-C72-C73
5	B	501	3PH	C1-C2-C3-O31
5	B	501	3PH	O21-C21-C22-C23
5	B	502	3PH	O11-C1-C2-O21
5	B	501	3PH	O21-C2-C3-O31
4	A	501	CDL	CA2-OA2-PA1-OA3
4	A	501	CDL	CA4-CA3-OA5-PA1
5	B	501	3PH	C1-O11-P-O12
5	B	501	3PH	O22-C21-C22-C23
4	A	501	CDL	C1-CB2-OB2-PB2
5	B	503	3PH	O21-C2-C3-O31
4	A	501	CDL	CA7-C31-C32-C33
4	A	501	CDL	CB5-C51-C52-C53
5	B	501	3PH	C1-O11-P-O13
7	B	505	PG4	O2-C3-C4-O3
5	B	503	3PH	O31-C31-C32-C33
4	A	501	CDL	CA5-C11-C12-C13
5	B	503	3PH	O21-C21-C22-C23
5	A	502	3PH	O31-C31-C32-C33
5	B	503	3PH	C2-C1-O11-P
5	B	503	3PH	C22-C21-O21-C2

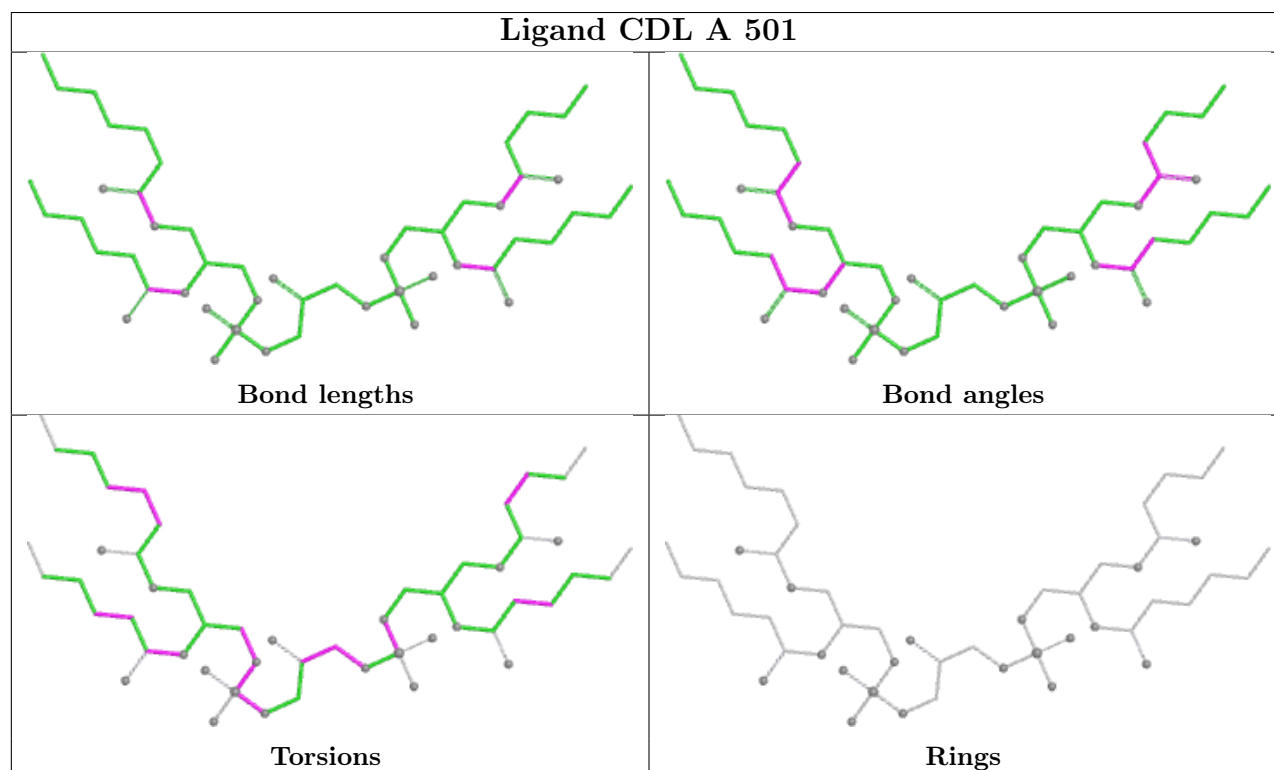
There are no ring outliers.

2 monomers are involved in 3 short contacts:

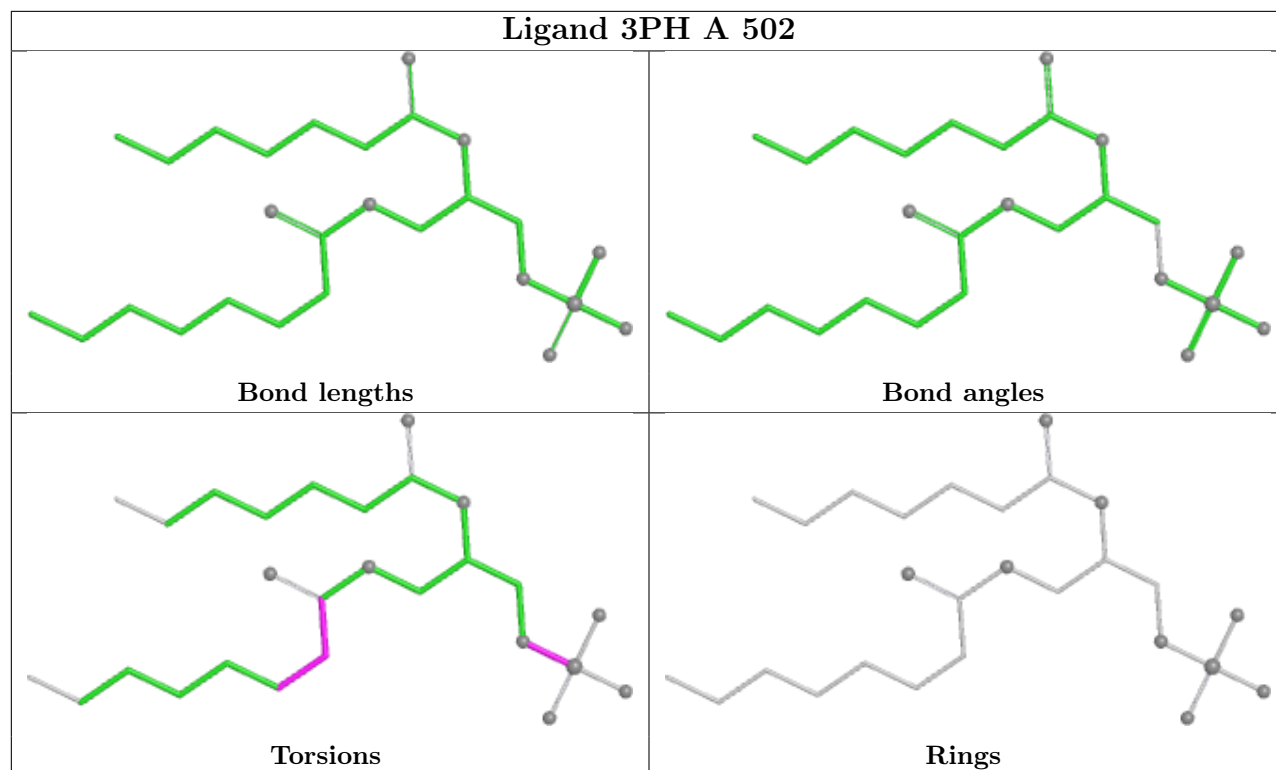
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	CDL	2	0
7	A	504	PG4	1	0

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

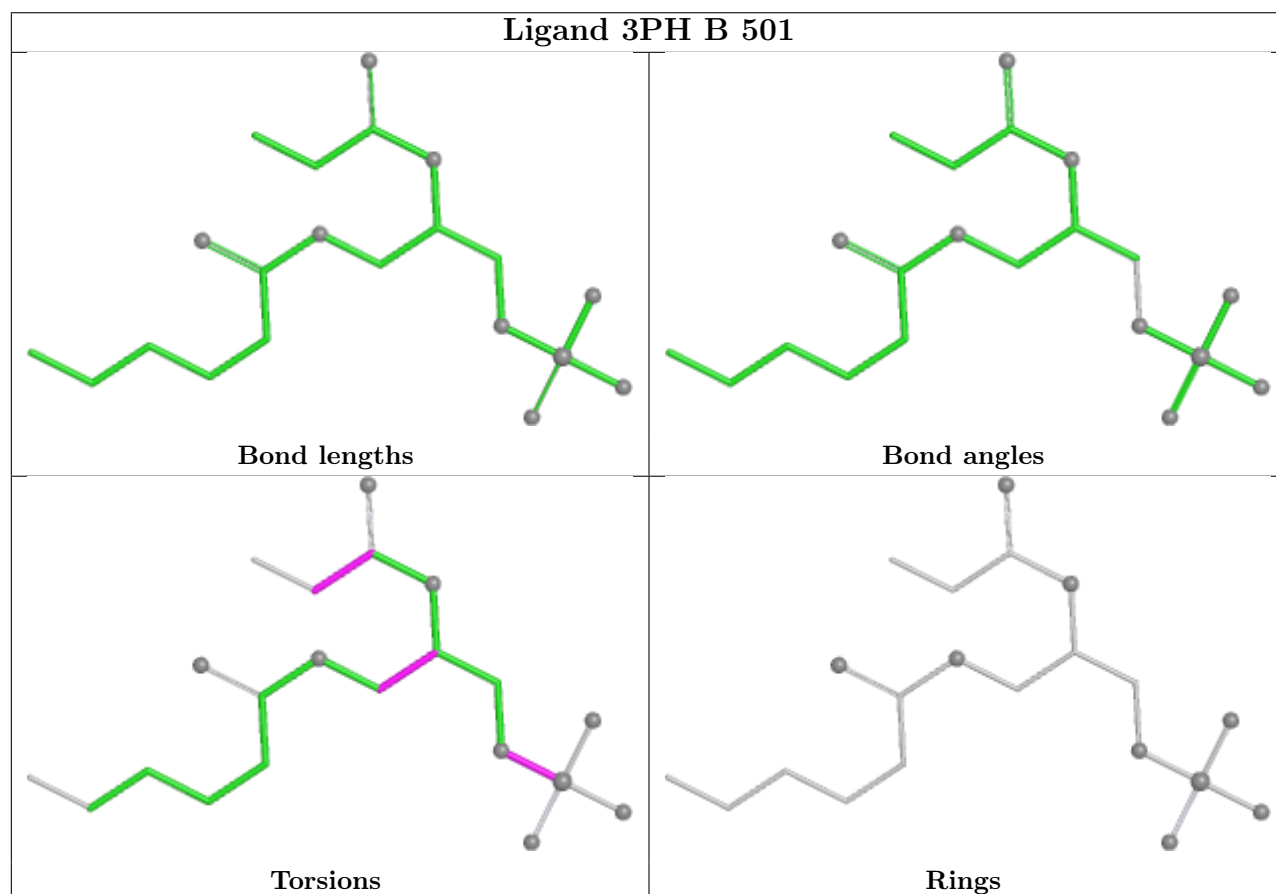
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

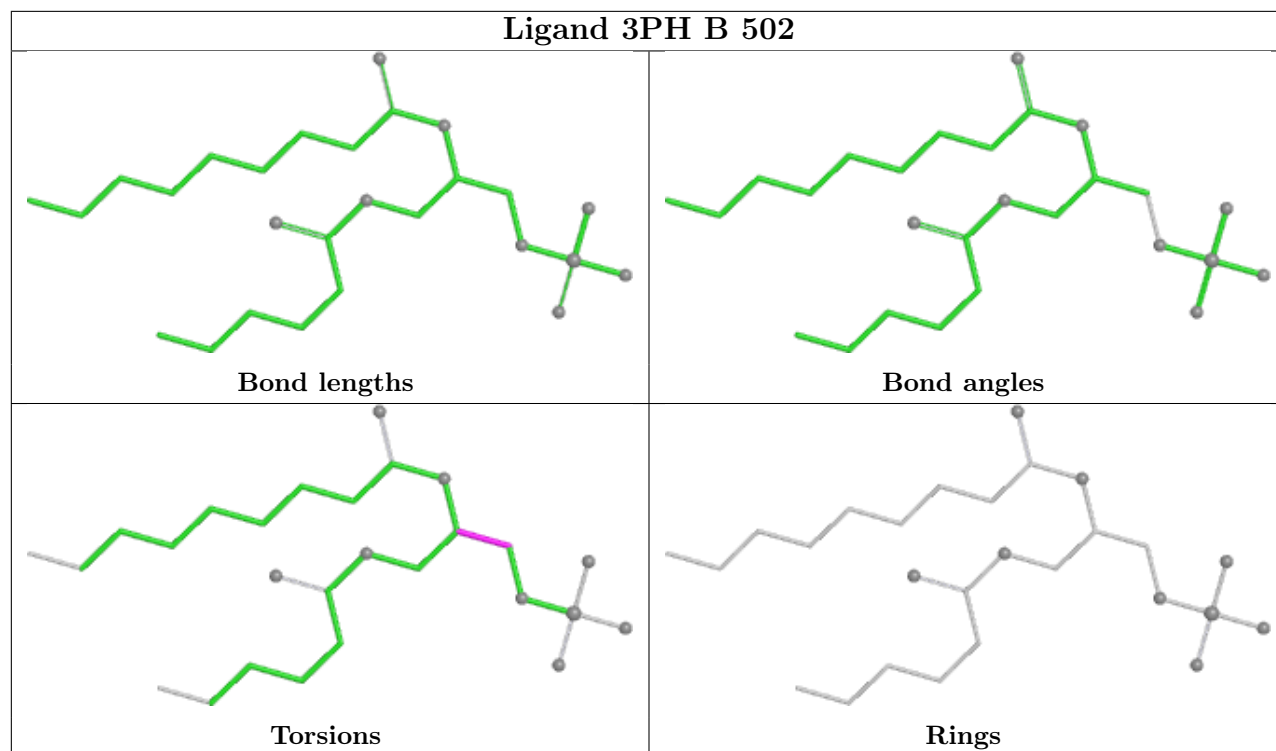


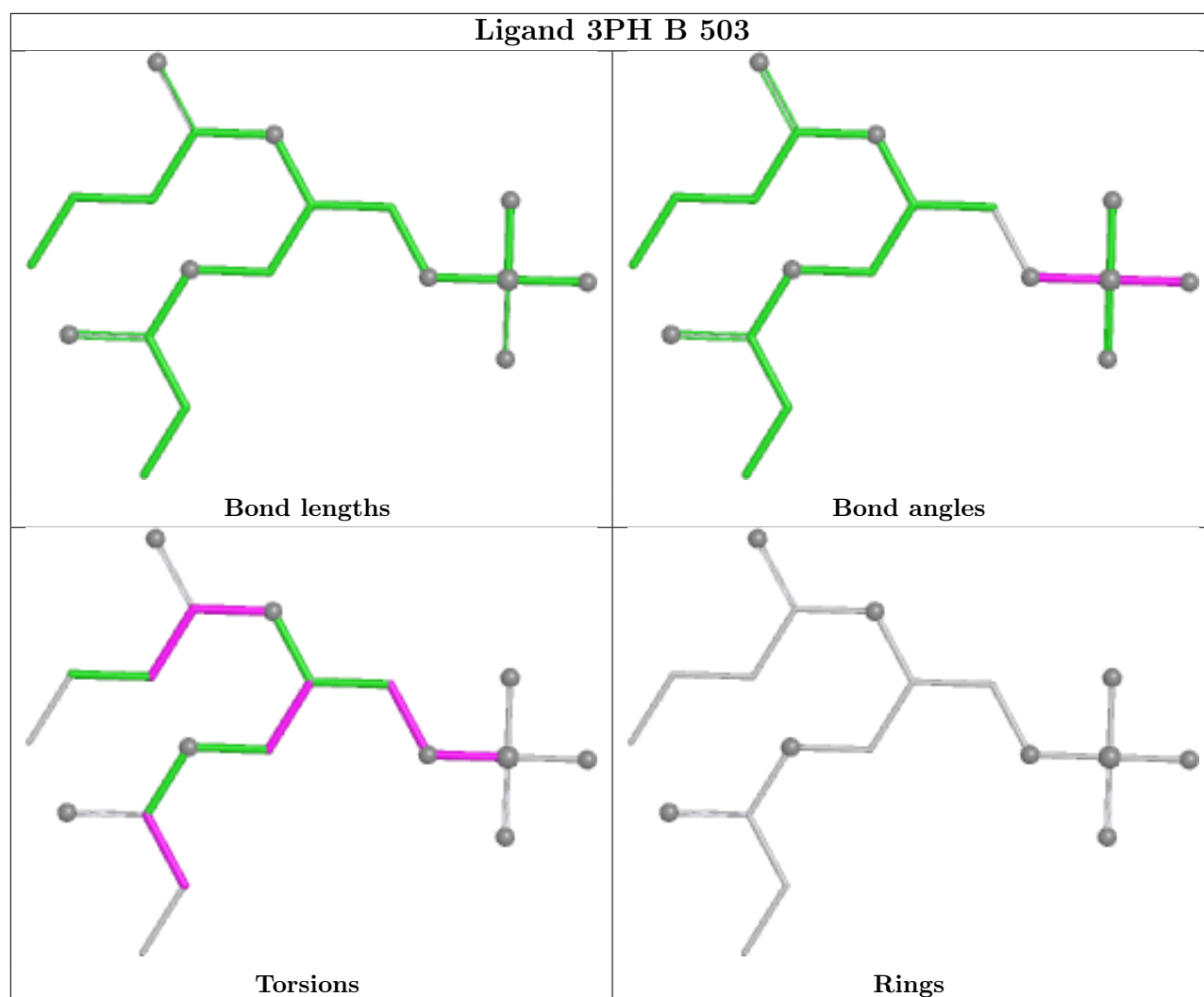
Ligand 3PH A 502



Ligand 3PH B 501







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	368/406 (90%)	0.90	55 (14%)	5 5	28, 81, 134, 168	17 (4%)
1	B	371/406 (91%)	1.02	51 (13%)	6 6	45, 91, 145, 177	19 (5%)
2	C	210/252 (83%)	0.47	23 (10%)	10 10	31, 58, 123, 172	2 (0%)
2	E	223/252 (88%)	0.09	11 (4%)	35 35	30, 49, 93, 146	3 (1%)
3	D	206/210 (98%)	0.51	17 (8%)	17 17	32, 68, 136, 160	6 (2%)
3	F	209/210 (99%)	0.03	2 (0%)	79 81	32, 52, 80, 103	1 (0%)
All	All	1587/1736 (91%)	0.59	159 (10%)	12 12	28, 72, 135, 177	48 (3%)

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309[A]	TRP	6.3
2	E	140	THR	6.0
1	B	37[A]	TRP	5.3
1	A	325	TYR	5.0
1	A	327	GLN	5.0
3	D	142	VAL	4.8
1	A	164	ASP	4.7
1	B	320	PRO	4.7
2	C	55	GLY	4.7
3	F	1	ALA	4.7
2	C	146	ALA	4.6
1	B	94	ALA	4.6
1	A	322	GLY	4.6
1	A	141	LEU	4.5
1	A	161	ILE	4.4
1	A	324	THR	4.3
1	B	157	MET	4.0
1	B	316	LEU	4.0
2	E	56	SER	3.9

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Mol	Chain	Res	Type	RSRZ
3	D	164	SER	3.9
1	A	253	HIS	3.8
1	B	361	ALA	3.8
2	C	56	SER	3.8
2	E	141	SER	3.7
2	E	142	GLY	3.7
1	A	379	TRP	3.6
1	B	140	VAL	3.6
2	C	147	LEU	3.6
1	A	157	MET	3.5
1	B	324	THR	3.5
1	A	328	ILE	3.5
2	E	55	GLY	3.5
1	A	134	ILE	3.4
3	D	128	VAL	3.3
1	B	95	ALA	3.3
1	B	144	LEU	3.3
1	B	318	HIS	3.3
2	E	42	ASP	3.3
1	B	99	ILE	3.3
1	B	310	LEU	3.3
1	A	241	GLU	3.3
1	B	325	TYR	3.3
1	A	92	ARG	3.3
1	B	176	THR	3.2
1	B	152	LEU	3.2
1	A	242	LYS	3.2
1	B	339	PHE	3.2
1	B	150	LEU	3.2
2	C	220	VAL	3.2
1	A	150	LEU	3.2
1	B	91	LEU	3.1
1	A	339	PHE	3.1
2	E	138	LYS	3.1
1	B	337	ILE	3.1
3	D	123	SER	3.1
3	D	141	LYS	3.0
1	B	317	ALA	3.0
1	A	316	LEU	3.0
1	B	136	PHE	3.0
1	A	39[A]	HIS	3.0
1	A	370	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	159	LEU	3.0
1	B	177	SER	3.0
1	B	319	LEU	3.0
1	B	154	ILE	3.0
3	D	174	THR	3.0
1	A	318	HIS	3.0
2	C	191	VAL	2.9
1	B	383	ARG	2.9
2	C	221	GLU	2.9
1	B	105	MET	2.8
2	E	215	LYS	2.8
1	B	148	VAL	2.8
1	A	323	THR	2.8
1	A	149	PRO	2.8
1	A	84	MET	2.7
1	A	179	LEU	2.7
1	B	327	GLN	2.7
2	E	136	SER	2.7
1	B	88	LEU	2.7
2	C	203	TYR	2.7
2	C	149	CYS	2.7
1	A	12	ALA	2.6
1	A	317	ALA	2.6
1	A	182	VAL	2.6
1	A	293	ILE	2.6
2	E	143	GLY	2.6
2	C	163	TRP	2.6
2	C	174	THR	2.6
2	E	54	THR	2.6
1	B	297	LEU	2.6
1	A	377	TYR	2.6
2	C	216	VAL	2.6
3	D	129	VAL	2.6
2	C	194	PRO	2.6
1	B	235	PHE	2.5
1	A	244	GLY	2.5
3	D	188	TYR	2.5
1	A	243	HIS	2.5
3	D	148	ASN	2.5
1	A	154	ILE	2.5
3	D	193	THR	2.5
2	C	134	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	152	LEU	2.5
1	B	308	CYS	2.4
1	B	90	SER	2.4
2	C	122	SER	2.4
3	D	192	VAL	2.4
2	C	215	LYS	2.4
2	C	135	PRO	2.4
1	A	321	GLN	2.4
1	B	162	ILE	2.4
1	B	274	VAL	2.4
1	B	142	ALA	2.3
1	A	138	LEU	2.3
1	B	328	ILE	2.3
2	C	193	VAL	2.3
1	A	308	CYS	2.3
1	B	147	ARG	2.3
1	B	321	GLN	2.3
2	C	204	ILE	2.3
1	A	148	VAL	2.3
2	C	223	LYS	2.3
1	B	363	LEU	2.3
1	A	83	LEU	2.2
3	D	175	LEU	2.2
1	A	162	ILE	2.2
1	A	367	ILE	2.2
1	B	293[A]	ILE	2.2
1	B	380	LEU	2.2
1	A	177	SER	2.2
1	B	35	SER	2.2
3	D	51	SER	2.2
3	D	170	SER	2.2
1	A	314	PHE	2.2
1	B	330	ALA	2.2
3	D	180	ALA	2.2
1	A	13	SER	2.2
1	B	315	LYS	2.2
1	A	329	MET	2.2
1	B	329	MET	2.2
3	D	144	TRP	2.2
1	A	171	ILE	2.1
2	C	190	VAL	2.1
1	B	199	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	146	SER	2.1
1	A	282	ASP	2.1
1	A	176	THR	2.1
1	A	205	THR	2.1
1	A	147	ARG	2.1
1	A	78	GLU	2.1
1	B	292	ILE	2.1
1	A	331	VAL	2.1
2	C	199	GLY	2.1
1	A	96	PHE	2.1
1	B	331	VAL	2.1
3	D	205	PHE	2.1
3	F	137	PRO	2.0
2	C	217	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
6	PO4	B	504	5/5	0.65	0.12	102,118,120,136	0
5	3PH	A	502	27/48	0.68	0.18	78,97,145,154	0
5	3PH	B	501	21/48	0.77	0.19	69,123,151,153	0
5	3PH	B	502	27/48	0.79	0.15	78,103,128,135	0
6	PO4	A	503	5/5	0.81	0.11	99,105,111,126	0
4	CDL	A	501	52/100	0.82	0.16	61,95,149,153	0
7	PG4	B	505	13/13	0.84	0.18	78,90,94,99	0
5	3PH	B	503	19/48	0.88	0.14	75,92,112,127	0
7	PG4	A	504	13/13	0.93	0.10	44,59,76,76	0

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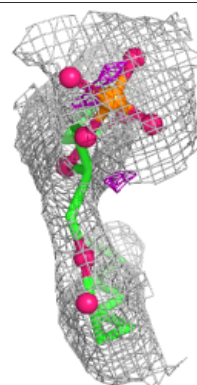
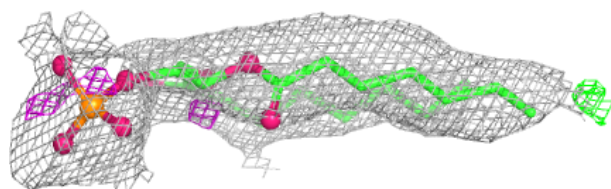
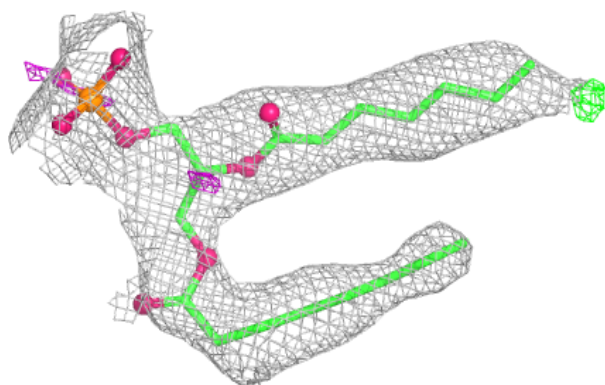
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CL	C	302	1/1	0.97	0.16	65,65,65,65	0
8	CL	C	303	1/1	0.98	0.09	53,53,53,53	0
8	CL	C	301	1/1	0.99	0.07	50,50,50,50	0

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.

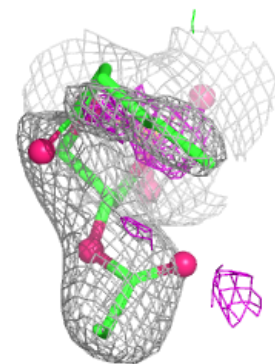
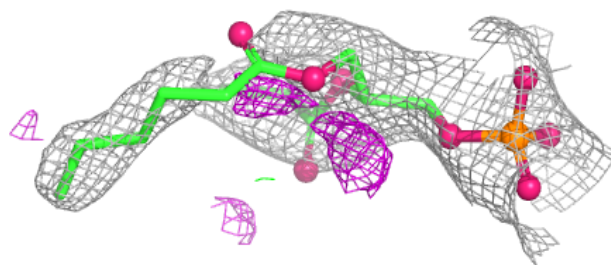
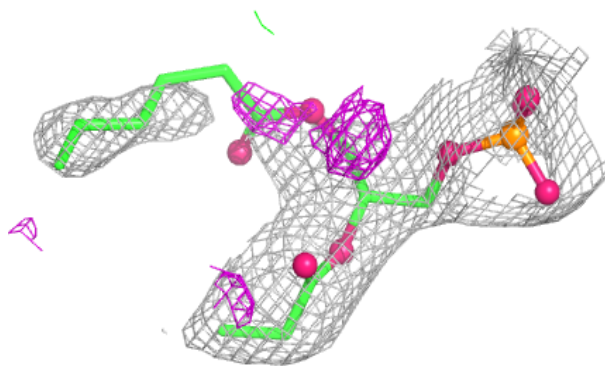
Electron density around 3PH A 502:

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

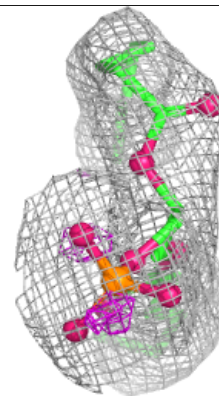
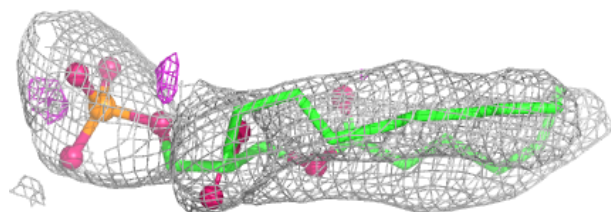
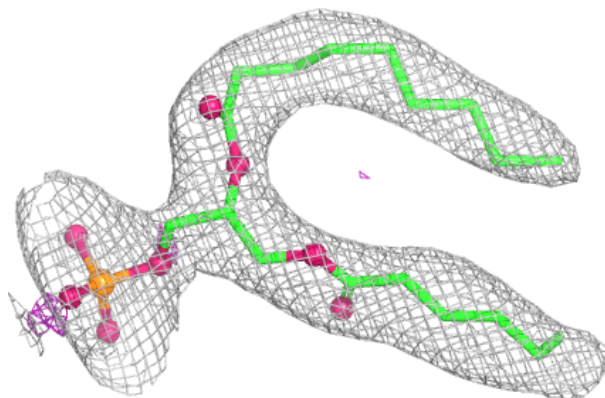


Electron density around 3PH B 501:

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

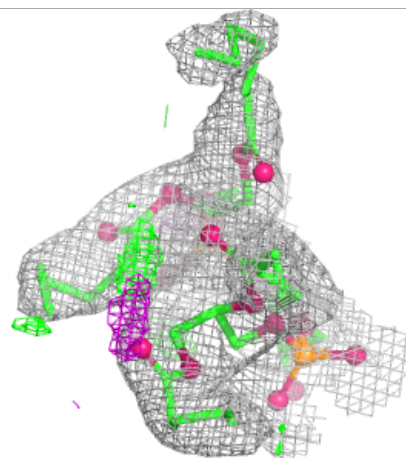
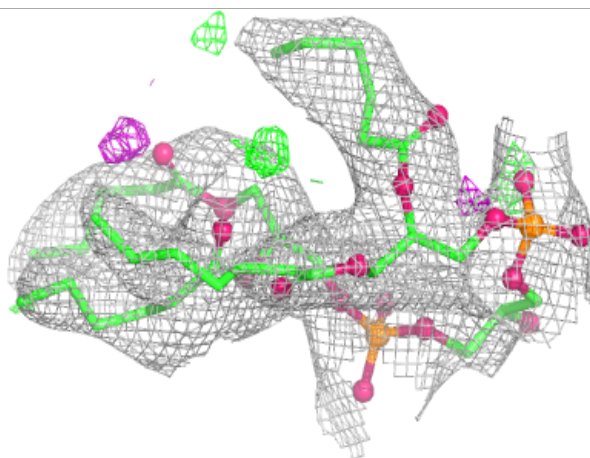
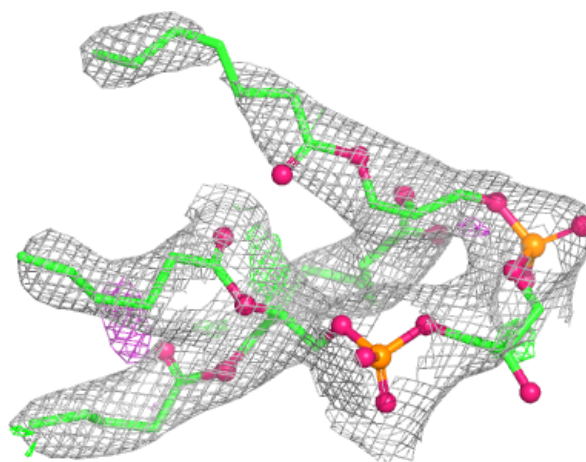
**Electron density around 3PH B 502:**

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



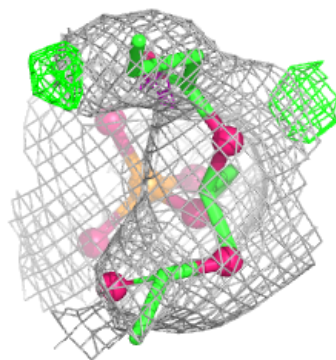
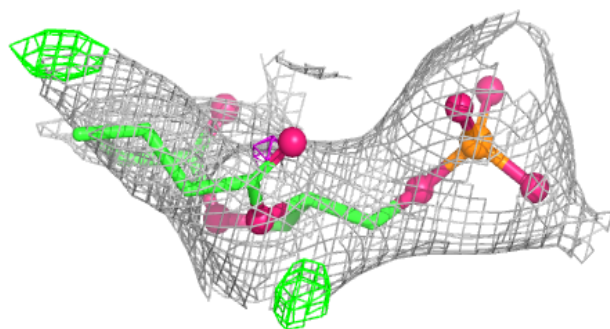
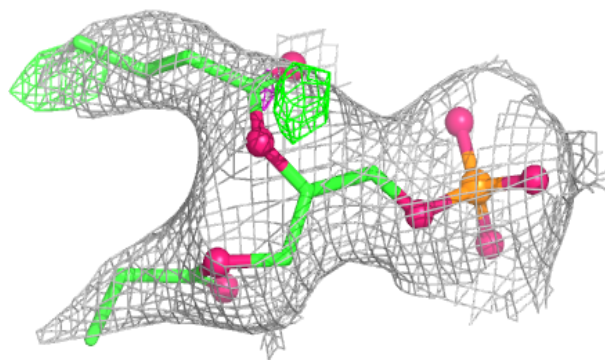
Electron density around CDL A 501:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.