



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:39 PM UTC

PDB ID : 7A0X / pdb_00007a0x
Title : Structure of dimeric sodium proton antiporter NhaA, at pH 6.0, crystallized with chimeric Fab antibodies
Authors : Fippel, A.; Lentes, C.J.; Mir, S.H.; Wirth, C.; Hunte, C.
Deposited on : 2020-08-11
Resolution : 2.37 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

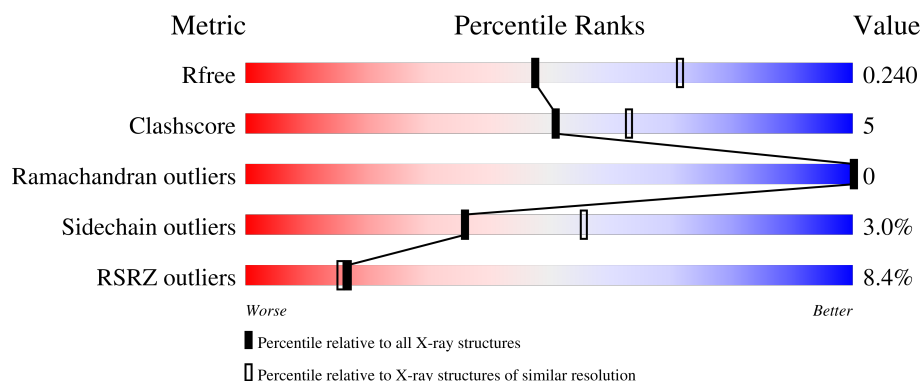
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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.



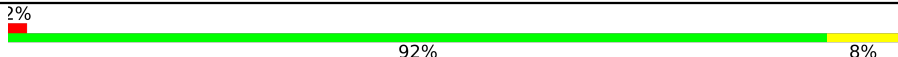
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	9% 76% 15% 9%
1	B	406	7% 75% 16% 8%
2	C	252	13% 71% 12% 17%
2	E	252	2% 76% 12% 12%
3	D	210	11% 89% 9% ..

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Mol	Chain	Length	Quality of chain
3	F	210	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '92%', and a small yellow segment at the end labeled '8%'.

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 12318 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	370	Total	C	N	O	S	55	2	0
			2783	1855	449	465	14			
1	B	373	Total	C	N	O	S	58	4	0
			2826	1890	457	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

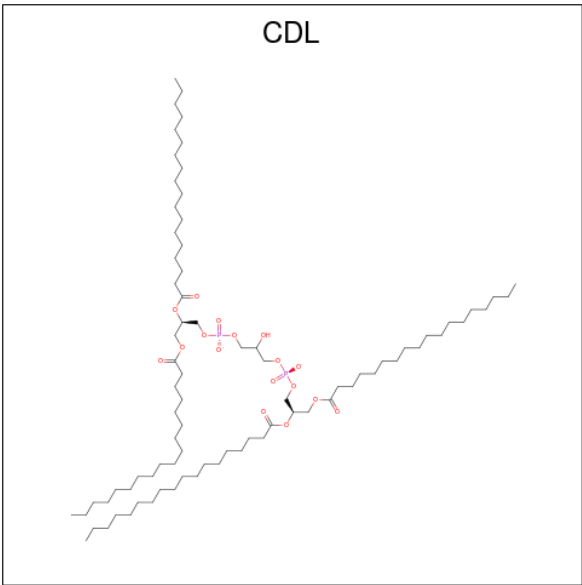
- Molecule 2 is a protein called chimeric antibody Fab-F6, heavy chain,chimeric antibody Fab-F6, heavy chain,chimeric antibody Fab-F6, heavy chain,chimeric antibody Fab-F6, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	210	Total	C	N	O	S	42	2	0
			1556	977	268	306	5			
2	E	223	Total	C	N	O	S	5	1	0
			1631	1019	280	327	5			

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

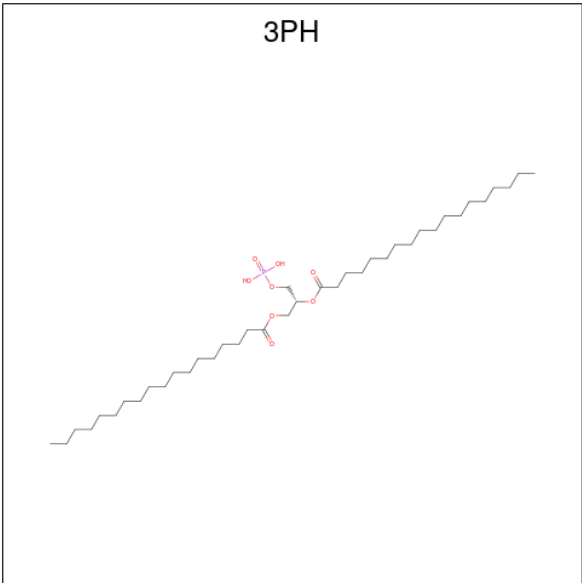
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	207	Total	C	N	O	S	20	0	0
			1555	972	263	316	4			
3	F	209	Total	C	N	O	S	4	0	0
			1568	979	265	320	4			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	A	1	54	35	17	2	0	0

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



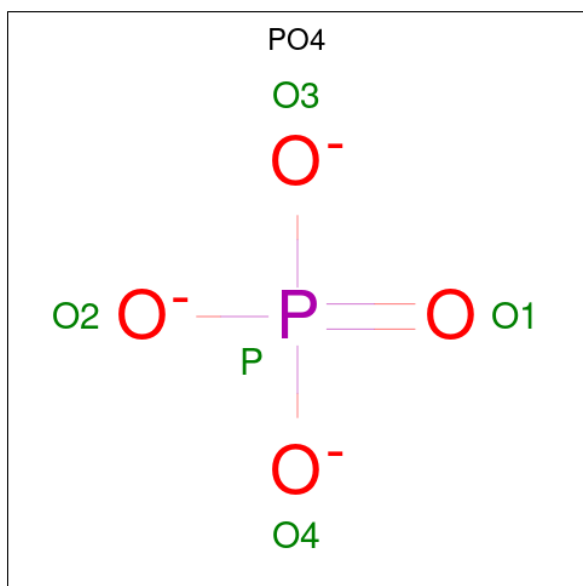
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
5	A	1	27	18	8	1	0	0
5	B	1	27	18	8	1	0	0

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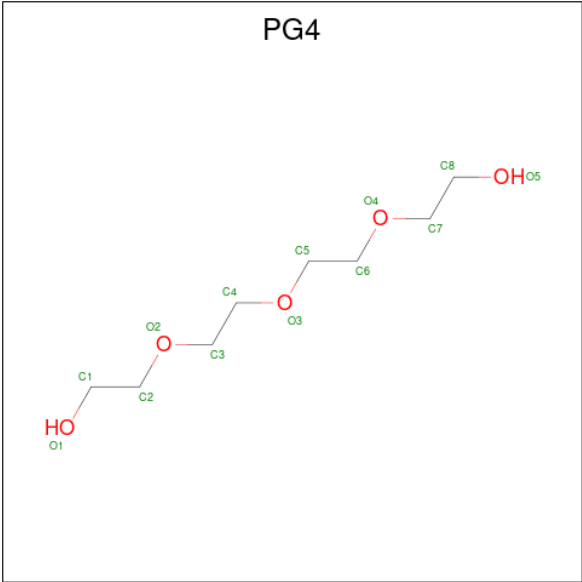
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			22	13	8	1		

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



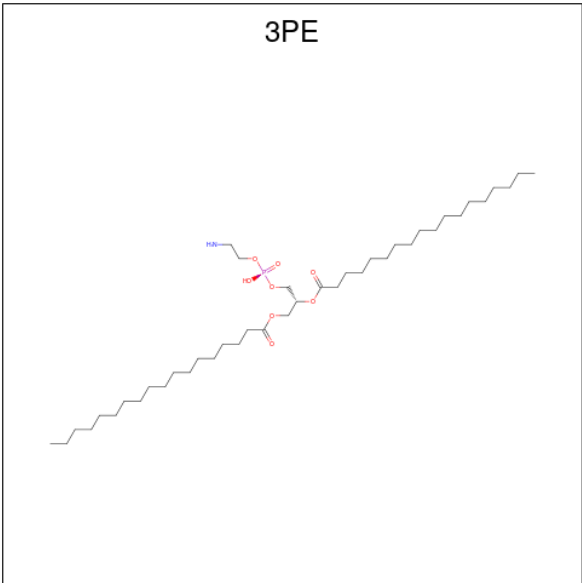
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

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



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		
7	E	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			26	16	1	8	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	2	Total	Cl	0	0
			2	2		
9	F	1	Total	Cl	0	0
			1	1		

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	F	1	Total	Ca	0	0
			1	1		

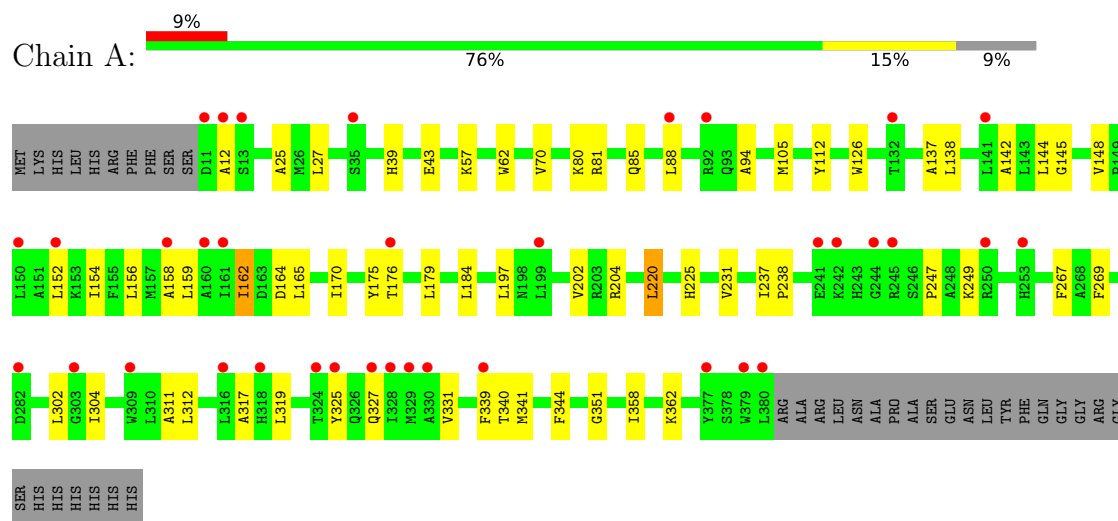
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	8	Total	O	0	0
			8	8		
11	B	3	Total	O	0	0
			3	3		
11	C	29	Total	O	0	0
			29	29		
11	D	34	Total	O	0	0
			34	34		
11	E	51	Total	O	0	0
			51	51		
11	F	52	Total	O	0	0
			52	52		

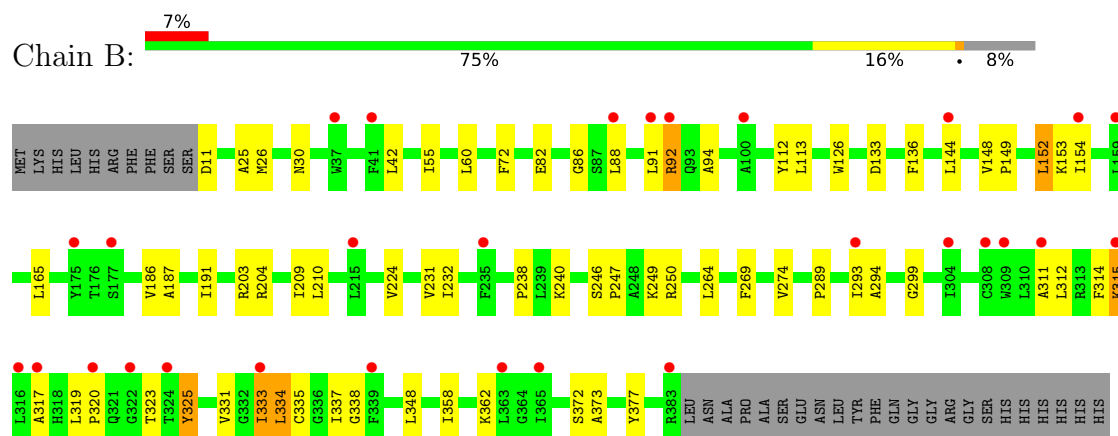
3 Residue-property plots [i](#)

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

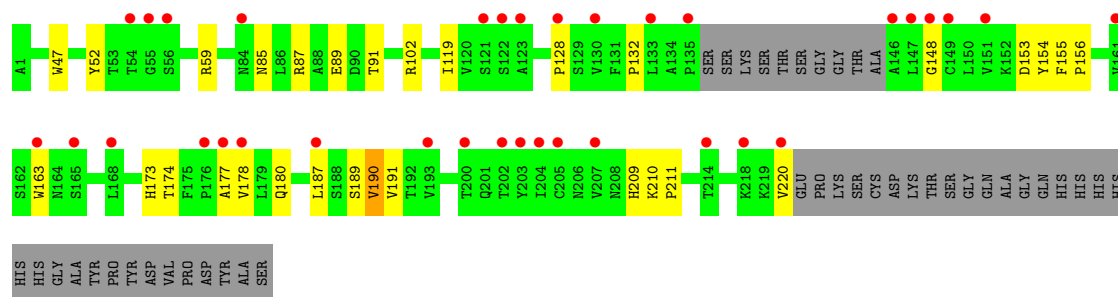


- Molecule 1: Na(+)/H(+) antiporter NhaA

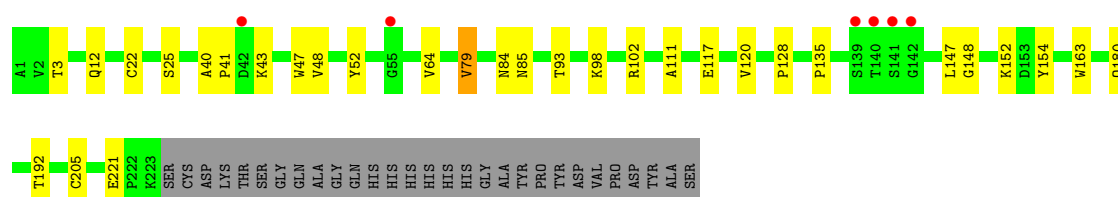
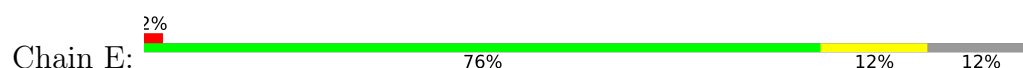


- Molecule 2: chimeric antibody Fab-F6, heavy chain, chimeric antibody Fab-F6, heavy chain, chimeric antibody Fab-F6, heavy chain, chimeric antibody Fab-F6, heavy chain

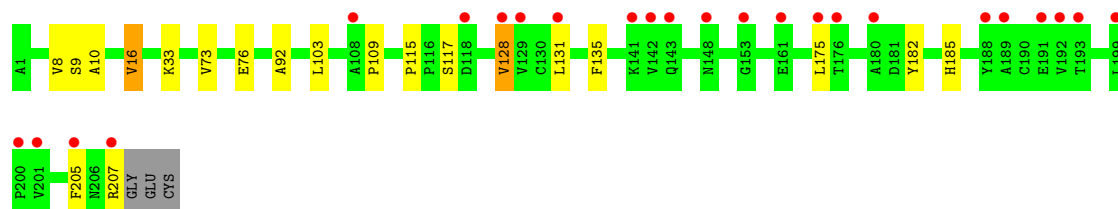
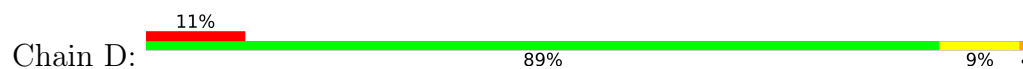




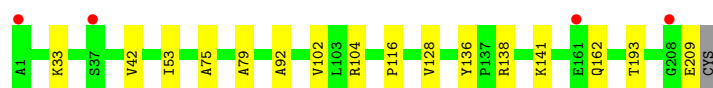
- Molecule 2: chimeric antibody Fab-F6, heavy chain, chimeric antibody Fab-F6, heavy chain, chimeric antibody Fab-F6, heavy chain, chimeric antibody Fab-F6, heavy chain



- Molecule 3: chimeric antibody Fab-F6, light chain, chimeric antibody Fab-F6, light chain, 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, 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	113.01Å 91.71Å 140.00Å 90.00° 109.80° 90.00°	Depositor
Resolution (Å)	24.90 – 2.37 24.90 – 2.37	Depositor EDS
% Data completeness (in resolution range)	63.1 (24.90-2.37) 63.4 (24.90-2.37)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.36Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.205 , 0.241 0.204 , 0.240	Depositor DCC
R_{free} test set	2222 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12318	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: CL, CDL, PO4, CA, 3PE, 3PH, PG4

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	0.10	0/2848	0.29	0/3884
1	B	0.12	0/2903	0.31	0/3960
2	C	0.09	0/1593	0.28	0/2167
2	E	0.08	0/1670	0.27	0/2272
3	D	0.08	0/1590	0.25	0/2165
3	F	0.07	0/1603	0.27	0/2182
All	All	0.10	0/12207	0.28	0/16630

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	2783	0	2953	32	0
1	B	2826	0	3014	42	0
2	C	1556	0	1525	20	0
2	E	1631	0	1595	15	0
3	D	1555	0	1511	11	0
3	F	1568	0	1520	8	0
4	A	54	0	52	4	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	49	0	44	2	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
7	E	26	0	36	2	0
8	B	26	0	26	1	0
9	C	2	0	0	1	0
9	F	1	0	0	0	0
10	F	1	0	0	0	0
11	A	8	0	0	0	0
11	B	3	0	0	0	0
11	C	29	0	0	0	0
11	D	34	0	0	0	0
11	E	51	0	0	1	0
11	F	52	0	0	0	0
All	All	12318	0	12339	126	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 5.

All (126) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:10:ALA:HB2	3:D:16:VAL:HG23	1.72	0.72
2:C:52:TYR:OH	2:C:102:ARG:NH1	2.26	0.68
3:D:182:TYR:O	3:D:207:ARG:NH2	2.27	0.68
3:D:33:LYS:NZ	3:D:76:GLU:O	2.25	0.67
1:A:88:LEU:HA	1:A:94:ALA:HB2	1.79	0.65
1:A:204:ARG:NH1	4:A:501:CDL:OB4	2.29	0.65
1:A:39[A]:HIS:NE2	1:A:43:GLU:OE1	2.30	0.65
1:A:85:GLN:OE1	1:A:249:LYS:NZ	2.31	0.63
1:A:57:LYS:NZ	1:A:220:LEU:O	2.31	0.63
2:E:135:PRO:HG3	2:E:147:LEU:HB3	1.81	0.63
3:D:185:HIS:O	3:D:207:ARG:NH2	2.32	0.63
1:B:88:LEU:HA	1:B:94:ALA:HB3	1.79	0.62
1:B:186:VAL:HG11	8:B:503:3PE:H231	1.80	0.62
3:F:141:LYS:HB3	3:F:193:THR:HB	1.82	0.62
2:C:173:HIS:HB2	2:C:190:VAL:HG12	1.82	0.61
2:C:153:ASP:OD1	2:C:180:GLN:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:MET:O	1:B:30:ASN:ND2	2.30	0.59
1:B:191:ILE:HD12	1:B:232:ILE:HG21	1.84	0.59
1:B:320:PRO:O	1:B:323:THR:OG1	2.21	0.58
1:B:203:ARG:HH12	1:B:240:LYS:HB2	1.69	0.58
4:A:501:CDL:H162	1:B:209:ILE:HD13	1.86	0.58
1:A:358:ILE:HG13	1:A:362:LYS:HE3	1.86	0.57
2:E:98:LYS:HB3	2:E:111:ALA:HB3	1.86	0.57
1:B:165:LEU:HD11	1:B:231:VAL:HG11	1.86	0.57
3:D:128:VAL:HG13	3:D:175:LEU:HB3	1.85	0.57
1:A:25:ALA:HB2	1:A:269:PHE:HA	1.88	0.56
1:A:152:LEU:HD11	1:A:327:GLN:HB3	1.86	0.56
2:E:40:ALA:HB3	2:E:43:LYS:HB2	1.87	0.56
4:A:501:CDL:H732	4:A:501:CDL:H522	1.86	0.56
1:B:149:PRO:HB2	1:B:152:LEU:HB2	1.86	0.56
1:B:337:ILE:HD11	1:B:373:ALA:HB2	1.88	0.56
1:A:156:LEU:HD13	1:A:331:VAL:HB	1.88	0.55
1:B:25:ALA:HB2	1:B:269:PHE:HA	1.88	0.55
1:B:42:LEU:HD22	1:B:60:LEU:HD13	1.88	0.55
1:B:238:PRO:HG2	1:B:247:PRO:HG2	1.89	0.55
2:C:132:PRO:O	3:D:117:SER:OG	2.26	0.54
1:B:11:ASP:N	1:B:11:ASP:OD1	2.41	0.54
7:E:301:PG4:H72	7:E:302:PG4:H12	1.90	0.54
3:F:75:ALA:HA	3:F:102:VAL:HG21	1.88	0.54
3:F:116:PRO:HD3	3:F:128:VAL:HG22	1.90	0.53
1:A:311:ALA:C	1:A:317:ALA:HB2	2.34	0.53
2:E:22:CYS:HB3	2:E:79:VAL:HG13	1.90	0.53
1:B:331:VAL:O	1:B:335:CYS:N	2.42	0.53
1:B:204:ARG:HD3	5:B:501:3PH:H222	1.91	0.52
2:E:128:PRO:HB3	2:E:154:TYR:HB3	1.91	0.52
2:C:177:ALA:HA	2:C:187:LEU:HB3	1.91	0.52
2:C:148:GLY:HA2	2:C:163:TRP:HH2	1.76	0.51
1:A:138:LEU:HD23	1:A:156:LEU:HD23	1.92	0.51
1:A:105:MET:HE1	1:A:170:ILE:HD12	1.91	0.51
2:C:190:VAL:HG21	3:D:131:LEU:HD22	1.93	0.51
1:B:187:ALA:O	1:B:191:ILE:HG12	2.11	0.50
1:A:80:LYS:NZ	1:A:237:ILE:O	2.40	0.50
2:C:89:GLU:N	2:C:89:GLU:OE1	2.45	0.49
4:A:501:CDL:H342	5:B:502:3PH:H221	1.94	0.49
1:B:331:VAL:HA	1:B:334:LEU:HB2	1.94	0.49
2:C:177:ALA:HB2	2:C:187:LEU:HD23	1.95	0.48
2:E:52:TYR:OH	2:E:102:ARG:NH1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3:THR:OG1	2:E:25:SER:OG	2.31	0.48
3:F:42:VAL:HA	3:F:53:ILE:HG13	1.94	0.48
1:A:145:GLY:HA2	1:A:148:VAL:HG13	1.95	0.48
1:A:176:THR:HG21	1:A:225:HIS:HE1	1.79	0.48
2:E:152:LYS:NZ	2:E:180:GLN:OE1	2.47	0.48
1:A:159:LEU:HD21	1:A:304:ILE:HD13	1.96	0.47
1:B:246:SER:HB3	1:B:249:LYS:HB2	1.95	0.47
2:C:85:ASN:OD1	2:C:87[B]:ARG:NH1	2.48	0.47
2:E:84:ASN:ND2	11:E:401:HOH:O	2.40	0.47
1:B:312:LEU:HD21	1:B:319:LEU:HD13	1.96	0.46
1:A:179:LEU:HD13	1:A:184:LEU:HD21	1.98	0.46
1:B:133:ASP:HB3	1:B:337:ILE:HG22	1.97	0.46
2:C:47:TRP:CD2	3:D:92:ALA:HB3	2.50	0.46
1:B:148:VAL:HG21	1:B:153:LYS:HE3	1.97	0.46
1:B:224:VAL:HG22	1:B:348:LEU:HD13	1.97	0.46
2:E:48:VAL:HG13	2:E:64:VAL:HG21	1.98	0.46
1:B:136:PHE:HB3	1:B:337:ILE:HG21	1.98	0.45
1:B:144:LEU:HD23	1:B:377:TYR:CE1	2.51	0.45
1:A:112:TYR:CD1	1:A:126:TRP:HA	2.51	0.45
1:A:126:TRP:HE1	1:A:175:TYR:HE2	1.65	0.45
1:B:144:LEU:HD23	1:B:377:TYR:CD1	2.52	0.45
2:C:128:PRO:HB3	2:C:154:TYR:HB3	1.99	0.44
1:A:57:LYS:HG3	1:A:62:TRP:NE1	2.32	0.44
3:F:138:ARG:O	3:F:138:ARG:NH1	2.37	0.44
1:B:72:PHE:HB3	1:B:231:VAL:HG13	1.99	0.44
3:D:109:PRO:HB3	3:D:135:PHE:HB3	1.98	0.44
1:A:238:PRO:HG2	1:A:247:PRO:HG2	1.99	0.44
1:B:289:PRO:O	1:B:293[B]:ILE:HG12	2.17	0.44
2:C:209:HIS:CE1	2:C:211:PRO:HD2	2.52	0.44
2:E:41:PRO:HG3	7:E:302:PG4:H11	2.00	0.44
1:B:333:ILE:O	1:B:372:SER:HB3	2.18	0.44
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.85	0.44
1:A:311:ALA:O	1:A:317:ALA:HB2	2.18	0.44
2:C:148:GLY:HA2	2:C:163:TRP:CH2	2.53	0.43
3:D:9:SER:HB3	3:D:103:LEU:HD21	2.00	0.43
1:B:113:LEU:HD21	1:B:126:TRP:HB3	2.00	0.43
1:B:314:PHE:O	1:B:315:LYS:HG2	2.18	0.43
1:A:137:ALA:HB1	1:A:156:LEU:HD21	2.00	0.43
1:B:26:MET:HE1	1:B:274:VAL:HB	1.99	0.43
1:B:294:ALA:O	1:B:299:GLY:N	2.46	0.43
1:B:82:GLU:HA	1:B:86:GLY:HA3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ALA:HB1	1:B:317:ALA:HB2	1.99	0.43
3:F:33:LYS:HG2	3:F:79:ALA:HB2	2.00	0.42
2:C:174:THR:HA	2:C:189:SER:HA	2.01	0.42
1:A:164:ASP:HB3	1:A:341:MET:HE2	2.01	0.42
1:B:112:TYR:CD1	1:B:126:TRP:HA	2.54	0.42
1:B:312:LEU:HD23	1:B:312:LEU:HA	1.89	0.42
1:A:351:GLY:O	2:C:102:ARG:NH2	2.51	0.42
1:B:165:LEU:HD12	1:B:165:LEU:HA	1.86	0.42
2:C:59:ARG:HD3	9:C:302:CL:CL	2.57	0.42
2:E:47:TRP:CD2	3:F:92:ALA:HB3	2.55	0.42
1:B:358:ILE:HG13	1:B:362:LYS:HE3	2.01	0.42
1:A:339:PHE:CD2	1:A:340:THR:HG23	2.55	0.42
1:A:165:LEU:HD11	1:A:231:VAL:HG11	2.02	0.41
2:C:210:LYS:HB2	2:C:211:PRO:HD3	2.02	0.41
3:F:104:ARG:HH21	3:F:136:TYR:HE2	1.68	0.41
2:E:93:THR:OG1	2:E:117:GLU:OE1	2.35	0.41
2:E:148:GLY:HA2	2:E:163:TRP:CZ2	2.56	0.41
1:B:323:THR:C	1:B:325:TYR:H	2.29	0.41
1:A:12:ALA:HB2	1:A:142:ALA:HB3	2.02	0.41
1:A:158:ALA:O	1:A:162:ILE:HG22	2.21	0.41
1:A:267:PHE:CZ	1:A:344:PHE:HB2	2.56	0.41
2:C:91:THR:HG23	2:C:119:ILE:HA	2.03	0.41
1:A:312:LEU:HD23	1:A:317:ALA:HB1	2.03	0.40
1:B:133:ASP:HB2	1:B:338:GLY:O	2.21	0.40
3:D:115:PRO:HB3	3:D:205:PHE:CE2	2.57	0.40
1:B:91:LEU:HA	1:B:92:ARG:NH2	2.37	0.40
2:E:12:GLN:O	2:E:120:VAL:HA	2.22	0.40
2:C:155:PHE:HA	2:C:156:PRO:HA	1.87	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	370/406 (91%)	345 (93%)	25 (7%)	0	100	100
1	B	375/406 (92%)	348 (93%)	27 (7%)	0	100	100
2	C	208/252 (82%)	200 (96%)	8 (4%)	0	100	100
2	E	222/252 (88%)	214 (96%)	8 (4%)	0	100	100
3	D	205/210 (98%)	194 (95%)	11 (5%)	0	100	100
3	F	207/210 (99%)	198 (96%)	9 (4%)	0	100	100
All	All	1587/1736 (91%)	1499 (94%)	88 (6%)	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	286/314 (91%)	274 (96%)	12 (4%)	26	42
1	B	290/314 (92%)	279 (96%)	11 (4%)	29	46
2	C	168/199 (84%)	164 (98%)	4 (2%)	43	63
2	E	177/199 (89%)	172 (97%)	5 (3%)	38	58
3	D	176/178 (99%)	172 (98%)	4 (2%)	44	64
3	F	177/178 (99%)	175 (99%)	2 (1%)	65	81
All	All	1274/1382 (92%)	1236 (97%)	38 (3%)	36	56

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	70	VAL
1	A	81	ARG
1	A	144	LEU
1	A	154	ILE
1	A	162	ILE
1	A	197	LEU

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Mol	Chain	Res	Type
1	A	202	VAL
1	A	220	LEU
1	A	302	LEU
1	A	319	LEU
1	A	325	TYR
1	B	55	ILE
1	B	92	ARG
1	B	152	LEU
1	B	154	ILE
1	B	210	LEU
1	B	250	ARG
1	B	264	LEU
1	B	315	LYS
1	B	325	TYR
1	B	333	ILE
1	B	334	LEU
2	C	178	VAL
2	C	190	VAL
2	C	191	VAL
2	C	220	VAL
3	D	8	VAL
3	D	16	VAL
3	D	73	VAL
3	D	128	VAL
2	E	79	VAL
2	E	85	ASN
2	E	192	THR
2	E	205	CYS
2	E	221	GLU
3	F	162	GLN
3	F	209	GLU

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

Mol	Chain	Res	Type
1	A	56	ASN
1	A	253	HIS
1	B	47	GLN
1	B	56	ASN
2	C	84	ASN

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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	501	-	26,26,47	0.27	0	29,31,52	0.38	0
7	PG4	E	302	-	12,12,12	0.44	0	11,11,11	0.42	0
6	PO4	A	503	-	4,4,4	0.96	0	6,6,6	0.46	0
6	PO4	B	504	-	4,4,4	0.96	0	6,6,6	0.45	0
7	PG4	A	504	-	12,12,12	0.46	0	11,11,11	0.29	0
5	3PH	A	502	-	26,26,47	0.25	0	29,31,52	0.37	0
7	PG4	E	301	-	12,12,12	0.45	0	11,11,11	0.35	0
4	CDL	A	501	-	53,53,99	1.27	4 (7%)	59,65,111	1.25	7 (11%)
8	3PE	B	503	-	25,25,50	0.41	0	28,30,55	0.40	0
5	3PH	B	502	-	21,21,47	0.28	0	24,26,52	0.57	1 (4%)
7	PG4	B	505	-	12,12,12	0.45	0	11,11,11	0.28	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	501	-	-	2/28/28/49	-
7	PG4	E	302	-	-	1/10/10/10	-
7	PG4	A	504	-	-	1/10/10/10	-
5	3PH	A	502	-	-	6/28/28/49	-
7	PG4	E	301	-	-	2/10/10/10	-
4	CDL	A	501	-	-	23/64/64/110	-
8	3PE	B	503	-	-	8/29/29/54	-
5	3PH	B	502	-	-	4/23/23/49	-
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	4.39	1.46	1.33
4	A	501	CDL	OB8-CB7	4.25	1.45	1.33
4	A	501	CDL	OA6-CA5	4.17	1.46	1.34
4	A	501	CDL	OB6-CB5	4.12	1.45	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	CDL	OB6-CB5-C51	4.15	120.45	111.48
4	A	501	CDL	OA6-CA5-C11	3.53	119.12	111.48
4	A	501	CDL	OA8-CA7-C31	2.89	120.66	111.83
4	A	501	CDL	CA4-OA6-CA5	-2.67	111.40	117.80
4	A	501	CDL	OB8-CB7-C71	2.57	119.67	111.83
4	A	501	CDL	CB4-OB6-CB5	-2.21	112.50	117.80
5	B	502	3PH	O11-P-O12	2.01	111.88	106.44
4	A	501	CDL	OA6-CA5-OA7	-2.00	119.03	123.70

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	CDL	CB2-C1-CA2-OA2
4	A	501	CDL	C1-CA2-OA2-PA1
4	A	501	CDL	CA2-OA2-PA1-OA4
4	A	501	CDL	CA3-OA5-PA1-OA3
4	A	501	CDL	CB2-OB2-PB2-OB4
4	A	501	CDL	CB2-OB2-PB2-OB5
4	A	501	CDL	CB3-OB5-PB2-OB4

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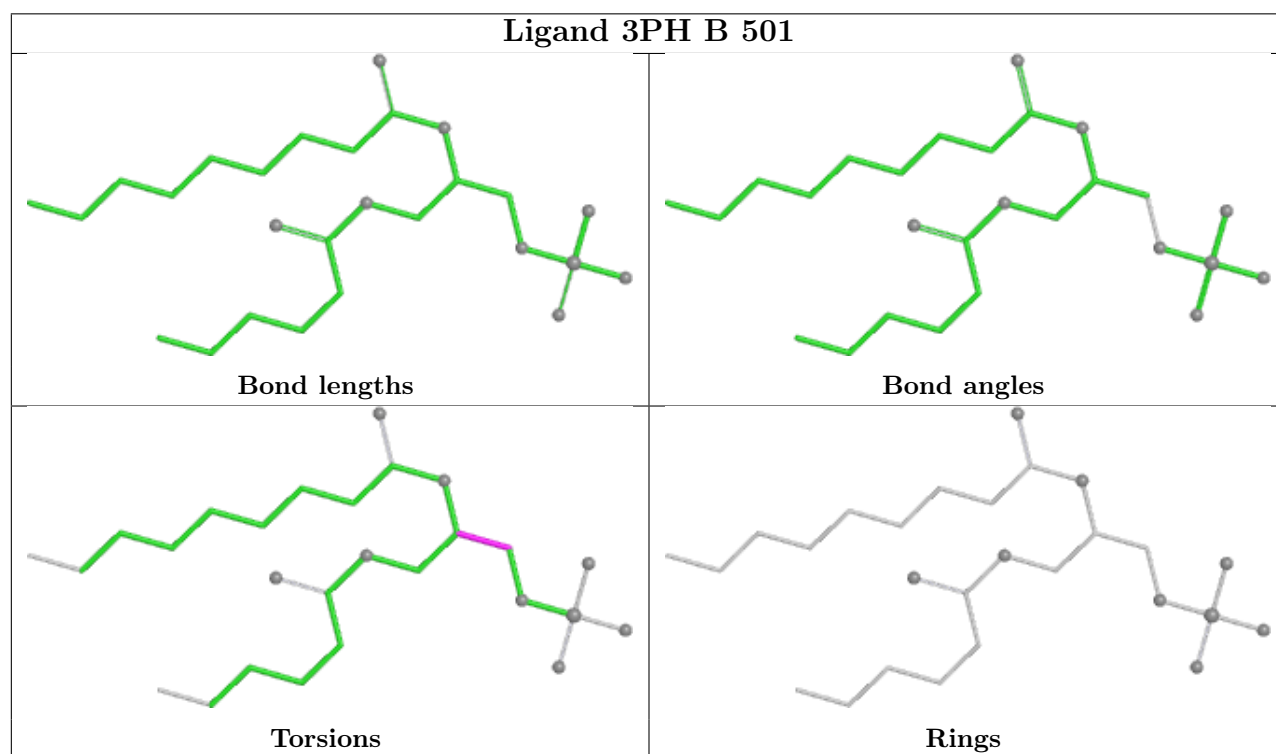
Mol	Chain	Res	Type	Atoms
5	A	502	3PH	C1-O11-P-O13
5	A	502	3PH	C1-O11-P-O14
5	B	502	3PH	C1-O11-P-O13
5	B	502	3PH	C1-O11-P-O14
8	B	503	3PE	C1-O11-P-O12
8	B	503	3PE	C1-O11-P-O14
8	B	503	3PE	C11-O13-P-O11
4	A	501	CDL	O1-C1-CA2-OA2
7	E	301	PG4	O2-C3-C4-O3
4	A	501	CDL	O1-C1-CB2-OB2
4	A	501	CDL	CA2-C1-CB2-OB2
4	A	501	CDL	C51-C52-C53-C54
5	B	502	3PH	C22-C23-C24-C25
4	A	501	CDL	OA5-CA3-CA4-CA6
5	B	501	3PH	O11-C1-C2-C3
4	A	501	CDL	C31-C32-C33-C34
5	A	502	3PH	O11-C1-C2-O21
4	A	501	CDL	C12-C13-C14-C15
4	A	501	CDL	OA5-CA3-CA4-OA6
5	B	501	3PH	O11-C1-C2-O21
7	A	504	PG4	O2-C3-C4-O3
7	E	301	PG4	C6-C5-O3-C4
5	A	502	3PH	O11-C1-C2-C3
8	B	503	3PE	O11-C1-C2-C3
8	B	503	3PE	O11-C1-C2-O21
4	A	501	CDL	CA2-OA2-PA1-OA5
4	A	501	CDL	CA3-OA5-PA1-OA2
4	A	501	CDL	CA3-OA5-PA1-OA4
8	B	503	3PE	C1-O11-P-O13
8	B	503	3PE	C11-O13-P-O14
4	A	501	CDL	CA4-CA3-OA5-PA1
4	A	501	CDL	CA7-C31-C32-C33
5	A	502	3PH	C31-C32-C33-C34
5	B	502	3PH	O21-C2-C3-O31
5	A	502	3PH	C1-O11-P-O12
8	B	503	3PE	O31-C31-C32-C33
4	A	501	CDL	CB7-C71-C72-C73
7	B	505	PG4	O2-C3-C4-O3
7	E	302	PG4	C5-C6-O4-C7
4	A	501	CDL	C52-C51-CB5-OB6
4	A	501	CDL	C52-C51-CB5-OB7

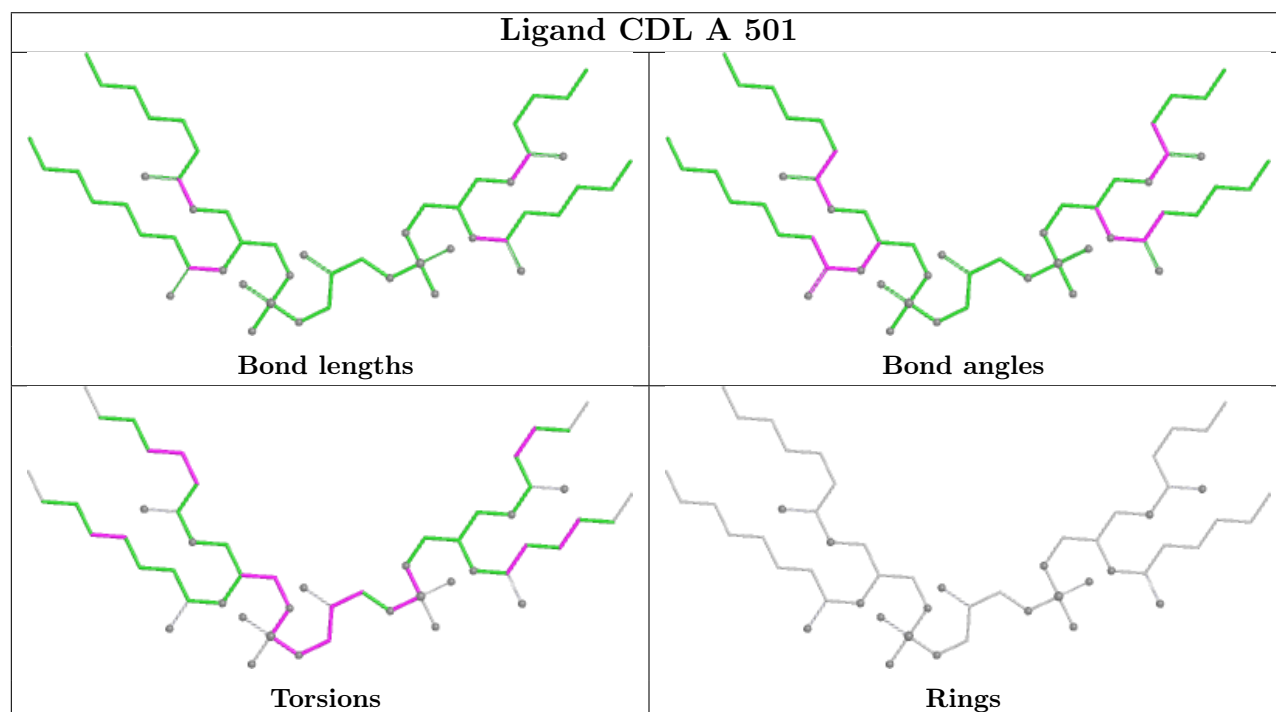
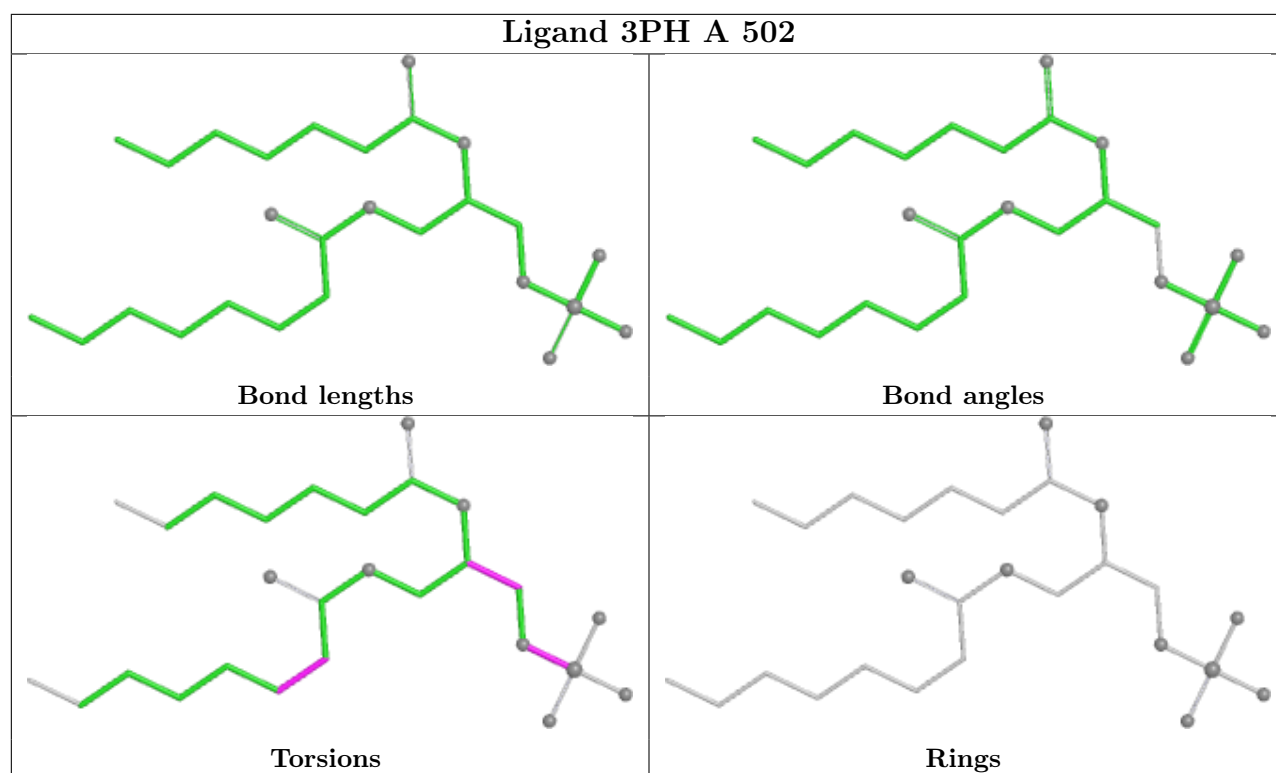
There are no ring outliers.

6 monomers are involved in 8 short contacts:

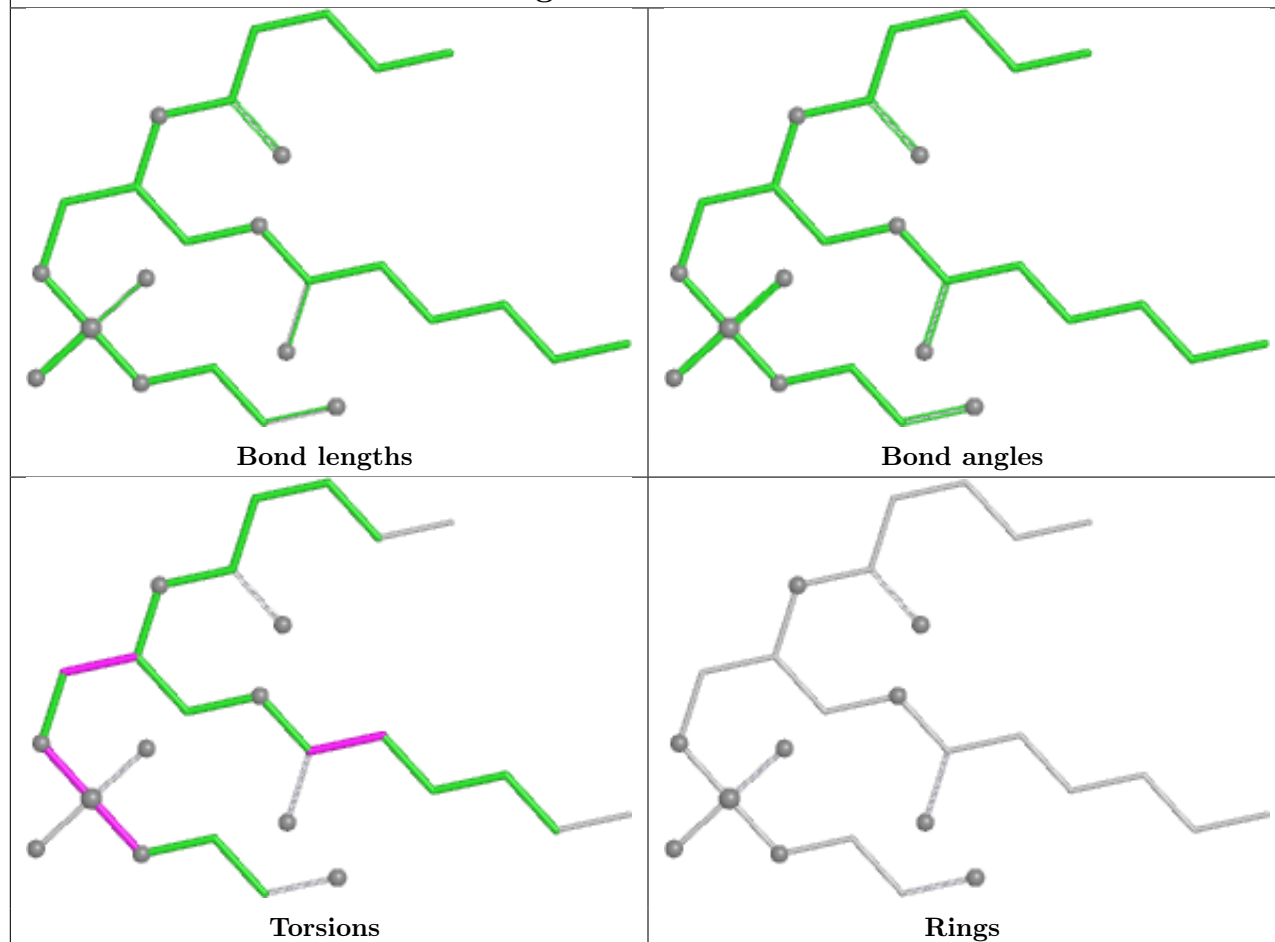
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	3PH	1	0
7	E	302	PG4	2	0
7	E	301	PG4	1	0
4	A	501	CDL	4	0
8	B	503	3PE	1	0
5	B	502	3PH	1	0

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.

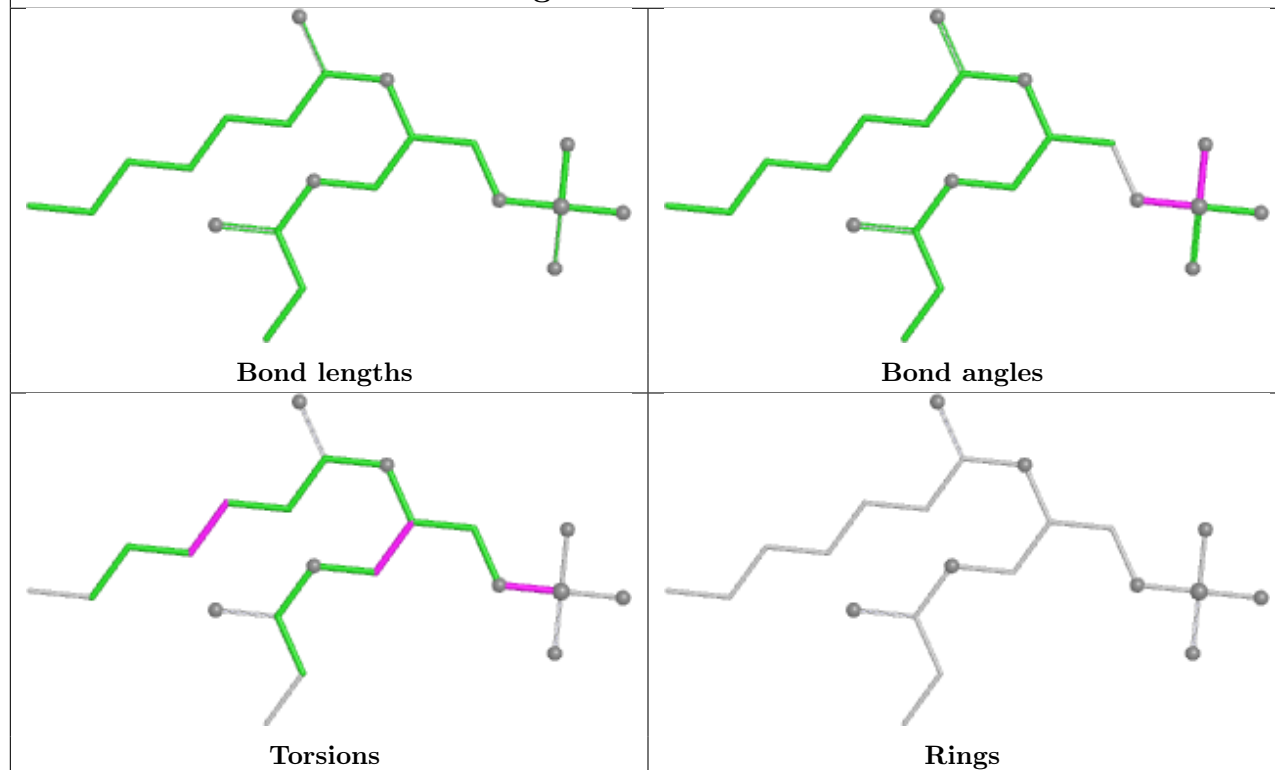




Ligand 3PE B 503



Ligand 3PH B 502



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	370/406 (91%)	0.70	36 (9%)	13 12	27, 76, 128, 204	15 (4%)
1	B	373/406 (91%)	0.69	29 (7%)	19 17	42, 86, 139, 184	18 (4%)
2	C	207/252 (82%)	0.84	34 (16%)	4 4	26, 62, 129, 156	8 (3%)
2	E	223/252 (88%)	0.11	6 (2%)	56 56	31, 54, 93, 149	3 (1%)
3	D	207/210 (98%)	0.60	24 (11%)	9 8	36, 68, 142, 165	6 (2%)
3	F	209/210 (99%)	-0.01	4 (1%)	66 65	34, 52, 78, 107	1 (0%)
All	All	1589/1736 (91%)	0.53	133 (8%)	17 15	26, 71, 131, 204	51 (3%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	TYR	7.5
2	C	55	GLY	6.8
2	C	177	ALA	5.5
1	B	309[A]	TRP	5.4
1	A	327	GLN	5.1
1	A	380	LEU	5.1
1	A	152	LEU	5.0
1	A	324	THR	4.7
2	C	203	TYR	4.6
2	E	42	ASP	4.5
2	C	204	ILE	4.5
1	B	304	ILE	4.5
1	A	244	GLY	4.4
2	C	202	THR	4.3
2	C	220	VAL	4.2
3	D	193	THR	4.2
1	B	37[A]	TRP	4.2
1	B	91	LEU	4.2
1	A	150	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	E	139	SER	4.1
2	C	149	CYS	4.1
2	C	151	VAL	4.0
3	D	141	LYS	3.7
2	C	56	SER	3.7
2	C	54	THR	3.6
3	D	161	GLU	3.6
1	B	88	LEU	3.5
1	B	320	PRO	3.4
2	C	163	TRP	3.4
2	E	141	SER	3.4
1	B	316	LEU	3.4
3	D	201	VAL	3.4
2	C	122	SER	3.4
2	E	140	THR	3.3
3	D	142	VAL	3.3
1	B	159	LEU	3.3
1	B	154	ILE	3.2
1	A	88	LEU	3.2
1	A	330	ALA	3.2
2	C	147	LEU	3.1
1	A	242	LYS	3.1
1	A	318	HIS	3.0
1	B	339	PHE	3.0
1	A	241	GLU	3.0
1	A	11	ASP	2.9
2	C	130	VAL	2.9
1	B	383	ARG	2.9
1	B	144	LEU	2.9
1	A	13	SER	2.8
1	A	92	ARG	2.8
1	B	324	THR	2.8
1	A	160	ALA	2.8
2	C	128	PRO	2.8
1	A	161	ILE	2.8
1	A	158	ALA	2.8
1	A	250	ARG	2.8
3	D	192	VAL	2.8
2	C	205	CYS	2.7
1	A	339	PHE	2.7
1	A	35	SER	2.7
3	D	180	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	176	THR	2.7
2	C	135	PRO	2.6
1	B	308	CYS	2.6
1	B	317	ALA	2.6
3	F	37	SER	2.6
3	D	118	ASP	2.6
3	D	176	THR	2.6
1	A	282	ASP	2.6
3	D	199	LEU	2.5
1	A	245	ARG	2.5
2	C	146	ALA	2.5
1	A	379	TRP	2.5
1	B	363	LEU	2.5
1	A	12	ALA	2.5
2	C	176	PRO	2.5
3	D	200	PRO	2.5
1	A	329	MET	2.5
1	A	253	HIS	2.5
2	E	142	GLY	2.5
3	F	208	GLY	2.5
2	C	165	SER	2.4
2	C	148	GLY	2.4
1	B	293[A]	ILE	2.4
2	C	178	VAL	2.4
1	B	92	ARG	2.4
2	E	55	GLY	2.4
2	C	161	VAL	2.4
3	D	128	VAL	2.4
1	A	316	LEU	2.4
1	B	100	ALA	2.3
1	B	315	LYS	2.3
2	C	214	THR	2.3
2	C	121	SER	2.3
1	B	175	TYR	2.3
1	B	365	ILE	2.3
1	B	333	ILE	2.3
2	C	193	VAL	2.3
1	A	199	LEU	2.3
2	C	168	LEU	2.3
2	C	123	ALA	2.3
2	C	207	VAL	2.3
3	D	188	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	1	ALA	2.2
3	D	148	ASN	2.2
3	D	191	GLU	2.2
1	A	309	TRP	2.2
3	D	143	GLN	2.2
1	B	311	ALA	2.2
1	A	377	TYR	2.2
1	A	141	LEU	2.2
3	D	129	VAL	2.2
1	A	303	GLY	2.2
1	B	215	LEU	2.1
3	D	153	GLY	2.1
1	A	132	THR	2.1
3	D	189	ALA	2.1
1	A	328	ILE	2.1
2	C	133	LEU	2.1
2	C	187	LEU	2.1
2	C	218	LYS	2.1
1	B	41	PHE	2.1
3	D	175	LEU	2.1
1	B	235	PHE	2.1
1	B	322	GLY	2.1
2	C	200	THR	2.1
2	C	84	ASN	2.1
3	D	207	ARG	2.1
1	B	177	SER	2.0
3	D	108	ALA	2.0
3	D	205	PHE	2.0
3	F	161	GLU	2.0
3	D	131	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

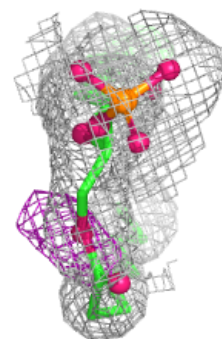
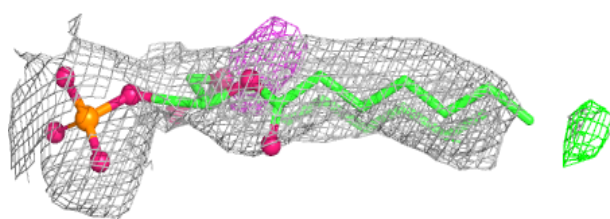
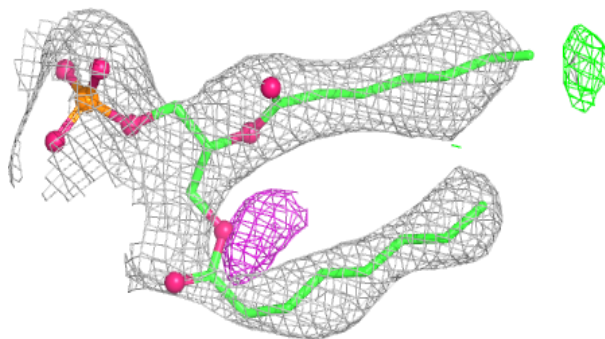
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	0.65	0.19	67,97,137,147	0
8	3PE	B	503	26/51	0.69	0.20	60,112,142,143	0
7	PG4	E	302	13/13	0.73	0.24	88,99,112,112	0
5	3PH	B	501	27/48	0.74	0.16	75,95,146,157	0
6	PO4	B	504	5/5	0.77	0.12	85,95,105,128	0
6	PO4	A	503	5/5	0.81	0.10	85,91,100,116	0
4	CDL	A	501	54/100	0.83	0.17	68,94,155,156	0
7	PG4	E	301	13/13	0.83	0.17	67,78,90,93	0
5	3PH	B	502	22/48	0.85	0.14	76,93,106,121	0
7	PG4	B	505	13/13	0.90	0.11	56,70,83,87	0
7	PG4	A	504	13/13	0.94	0.10	44,54,80,82	0
9	CL	C	302	1/1	0.95	0.11	76,76,76,76	0
10	CA	F	302	1/1	0.97	0.10	97,97,97,97	0
9	CL	F	301	1/1	0.98	0.07	59,59,59,59	0
9	CL	C	301	1/1	0.98	0.08	59,59,59,59	0

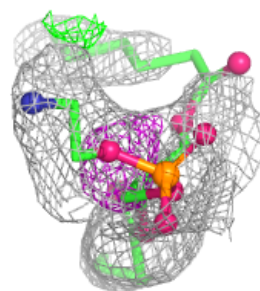
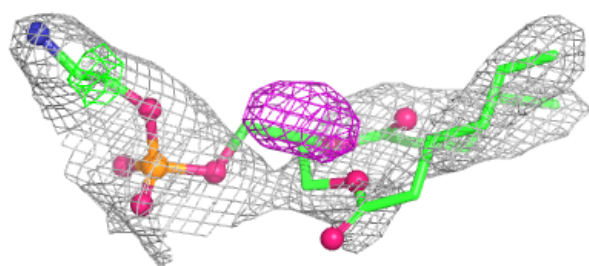
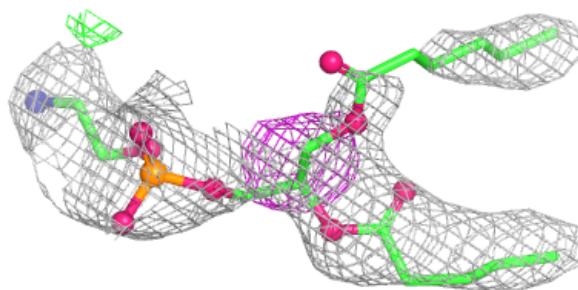
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

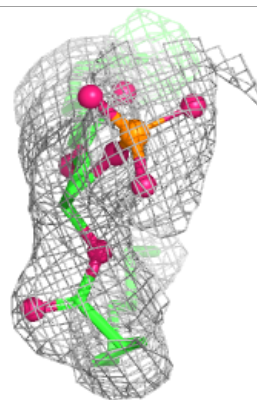
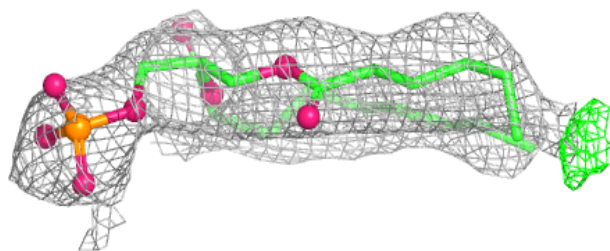
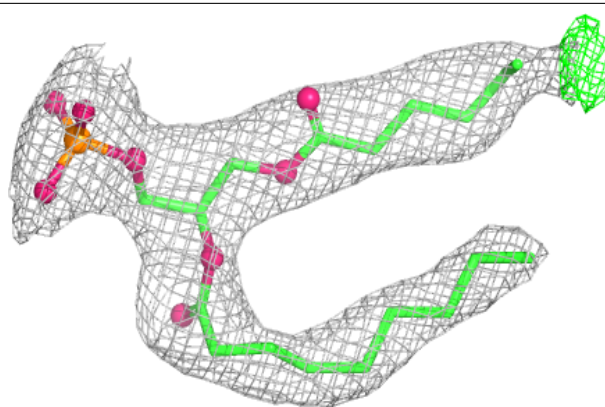
**Electron density around 3PE B 503:**

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

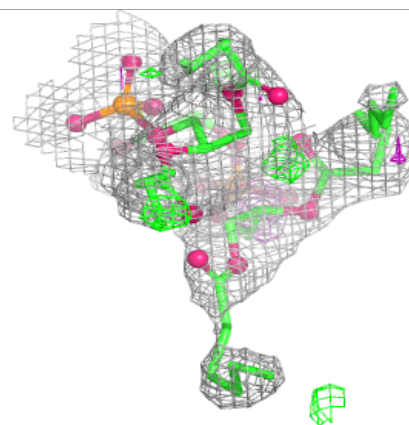
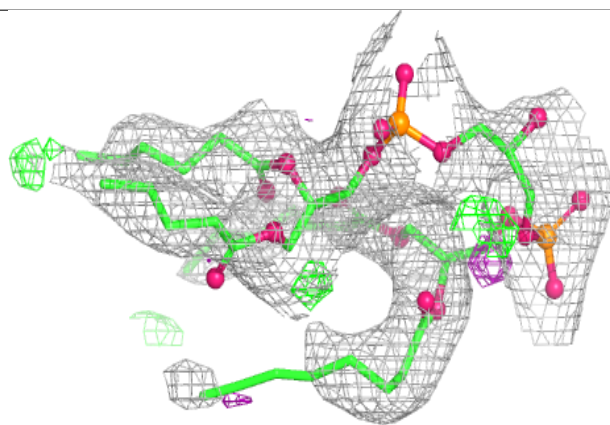
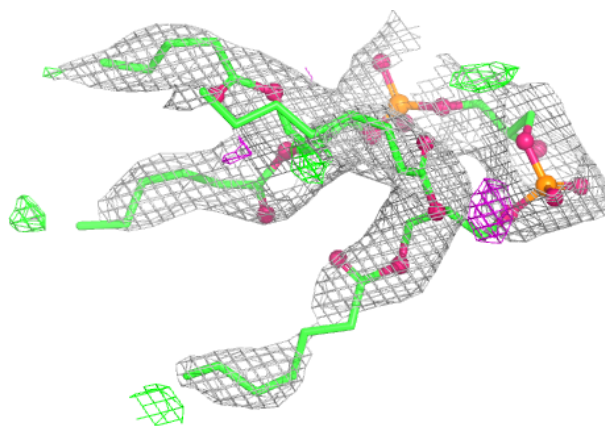


Electron density around 3PH B 501:

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

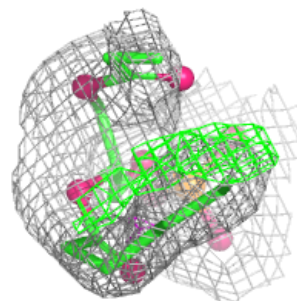
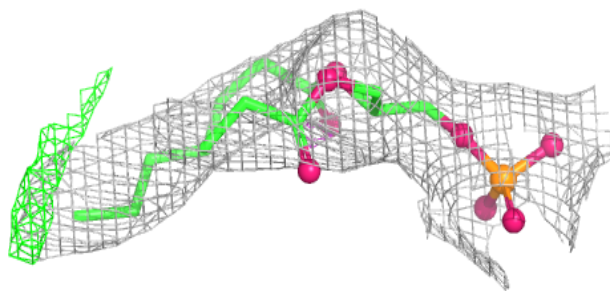
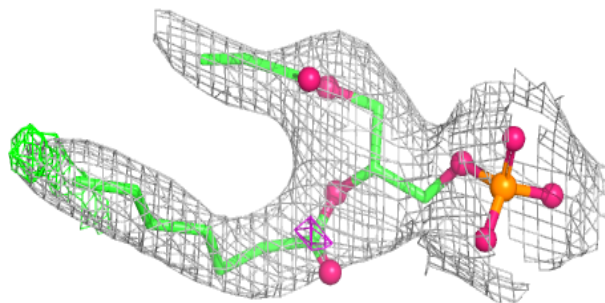
**Electron density around CDL A 501:**

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.