



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:13 PM UTC

PDB ID : 6J8W / pdb_00006j8w
Title : Structure of MOEN5-SSO7D fusion protein in complex with lig 1
Authors : Ko, T.P.; Zhang, L.L.; Chen, C.C.; Guo, R.T.
Deposited on : 2019-01-21
Resolution : 2.35 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

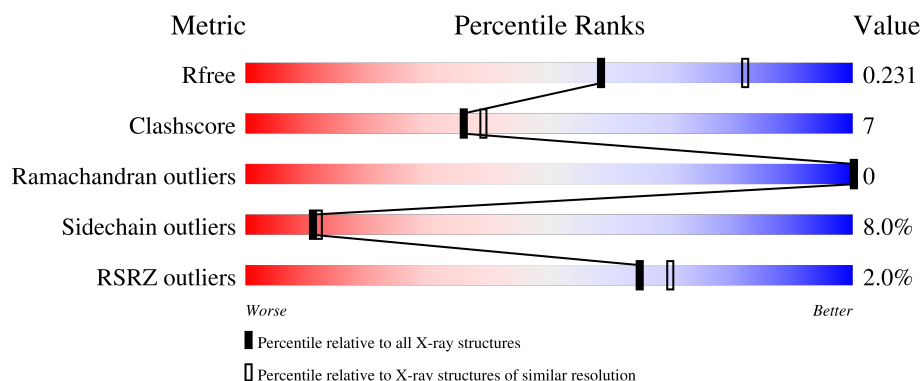
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	343	2% 65% 9% 24%
1	B	343	2% 82% 13% 3%
1	C	343	0% 64% 10% 24%
1	D	343	2% 71% 15% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9412 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 MoeN5,DNA-binding protein 7d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	1	0
			1990	1231	368	380	11			
1	B	333	Total	C	N	O	S	0	0	0
			2540	1576	464	486	14			
1	C	262	Total	C	N	O	S	0	0	0
			1994	1232	372	379	11			
1	D	304	Total	C	N	O	S	0	0	0
			2341	1455	430	443	13			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A010
A	-12	ALA	-	expression tag	UNP A0A010
A	-11	HIS	-	expression tag	UNP A0A010
A	-10	HIS	-	expression tag	UNP A0A010
A	-9	HIS	-	expression tag	UNP A0A010
A	-8	HIS	-	expression tag	UNP A0A010
A	-7	HIS	-	expression tag	UNP A0A010
A	-6	HIS	-	expression tag	UNP A0A010
A	-5	VAL	-	expression tag	UNP A0A010
A	-4	ASP	-	expression tag	UNP A0A010
A	-3	ASP	-	expression tag	UNP A0A010
A	-2	ASP	-	expression tag	UNP A0A010
A	-1	ASP	-	expression tag	UNP A0A010
A	0	LYS	-	expression tag	UNP A0A010
A	261	ALA	-	linker	UNP A0A010
A	262	GLY	-	linker	UNP A0A010
A	263	ALA	-	linker	UNP A0A010
A	264	GLY	-	linker	UNP A0A010
A	265	ALA	-	linker	UNP A0A010
B	-13	MET	-	expression tag	UNP A0A010
B	-12	ALA	-	expression tag	UNP A0A010

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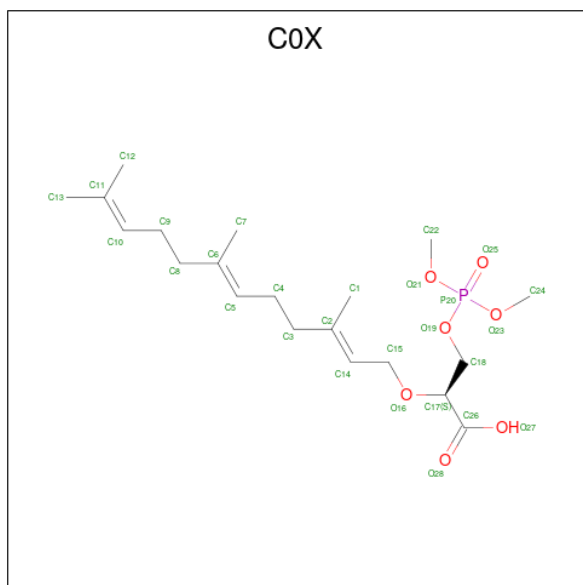
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0A010
B	-10	HIS	-	expression tag	UNP A0A010
B	-9	HIS	-	expression tag	UNP A0A010
B	-8	HIS	-	expression tag	UNP A0A010
B	-7	HIS	-	expression tag	UNP A0A010
B	-6	HIS	-	expression tag	UNP A0A010
B	-5	VAL	-	expression tag	UNP A0A010
B	-4	ASP	-	expression tag	UNP A0A010
B	-3	ASP	-	expression tag	UNP A0A010
B	-2	ASP	-	expression tag	UNP A0A010
B	-1	ASP	-	expression tag	UNP A0A010
B	0	LYS	-	expression tag	UNP A0A010
B	261	ALA	-	linker	UNP A0A010
B	262	GLY	-	linker	UNP A0A010
B	263	ALA	-	linker	UNP A0A010
B	264	GLY	-	linker	UNP A0A010
B	265	ALA	-	linker	UNP A0A010
C	-13	MET	-	expression tag	UNP A0A010
C	-12	ALA	-	expression tag	UNP A0A010
C	-11	HIS	-	expression tag	UNP A0A010
C	-10	HIS	-	expression tag	UNP A0A010
C	-9	HIS	-	expression tag	UNP A0A010
C	-8	HIS	-	expression tag	UNP A0A010
C	-7	HIS	-	expression tag	UNP A0A010
C	-6	HIS	-	expression tag	UNP A0A010
C	-5	VAL	-	expression tag	UNP A0A010
C	-4	ASP	-	expression tag	UNP A0A010
C	-3	ASP	-	expression tag	UNP A0A010
C	-2	ASP	-	expression tag	UNP A0A010
C	-1	ASP	-	expression tag	UNP A0A010
C	0	LYS	-	expression tag	UNP A0A010
C	261	ALA	-	linker	UNP A0A010
C	262	GLY	-	linker	UNP A0A010
C	263	ALA	-	linker	UNP A0A010
C	264	GLY	-	linker	UNP A0A010
C	265	ALA	-	linker	UNP A0A010
D	-13	MET	-	expression tag	UNP A0A010
D	-12	ALA	-	expression tag	UNP A0A010
D	-11	HIS	-	expression tag	UNP A0A010
D	-10	HIS	-	expression tag	UNP A0A010
D	-9	HIS	-	expression tag	UNP A0A010
D	-8	HIS	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	HIS	-	expression tag	UNP A0A010
D	-6	HIS	-	expression tag	UNP A0A010
D	-5	VAL	-	expression tag	UNP A0A010
D	-4	ASP	-	expression tag	UNP A0A010
D	-3	ASP	-	expression tag	UNP A0A010
D	-2	ASP	-	expression tag	UNP A0A010
D	-1	ASP	-	expression tag	UNP A0A010
D	0	LYS	-	expression tag	UNP A0A010
D	261	ALA	-	linker	UNP A0A010
D	262	GLY	-	linker	UNP A0A010
D	263	ALA	-	linker	UNP A0A010
D	264	GLY	-	linker	UNP A0A010
D	265	ALA	-	linker	UNP A0A010

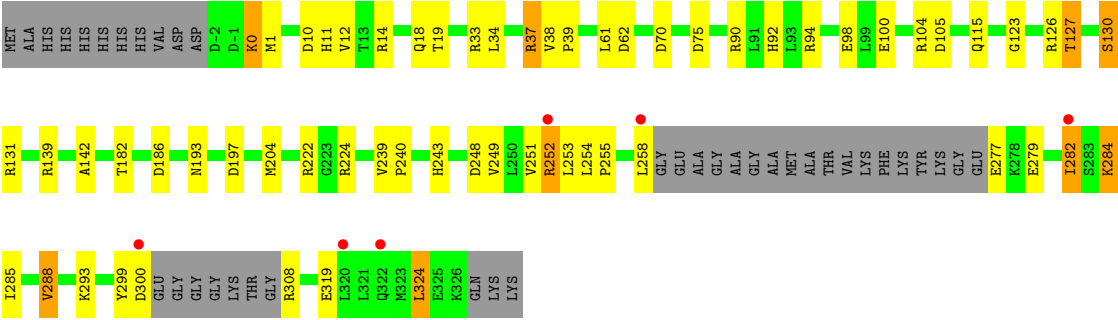
- Molecule 2 is (2S)-3-dimethoxyphosphoryloxy-2-[(2E,6E)-3,7,11-trimethyldodeca-2,6,10-trienoxy]propanoic acid (CCD ID: C0X) (formula: C₂₀H₃₅O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	O	P	0	0
			28	20	7	1		
2	D	1	Total	C	O	P	0	0
			18	10	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total 116	O 116	0	0
3	B	136	Total 136	O 136	0	0
3	C	105	Total 105	O 105	0	0
3	D	144	Total 144	O 144	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.78Å 217.67Å 104.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.35 25.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-2.35) 99.7 (25.00-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.175 , 0.225 0.184 , 0.231	Depositor DCC
R_{free} test set	3301 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.2	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	0.96	EDS
Total number of atoms	9412	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: C0X

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	1.13	0/2021	1.53	4/2747 (0.1%)
1	B	1.12	1/2579 (0.0%)	1.44	4/3488 (0.1%)
1	C	1.09	1/2026 (0.0%)	1.51	1/2753 (0.0%)
1	D	1.12	1/2376 (0.0%)	1.50	5/3216 (0.2%)
All	All	1.11	3/9002 (0.0%)	1.49	14/12204 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	202	HIS	CE1-NE2	5.53	1.38	1.32
1	B	222	ARG	C-O	5.19	1.30	1.24
1	D	70	ASP	C-O	5.14	1.30	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	105	ASP	CB-CA-C	7.91	120.02	108.87
1	D	105	ASP	CA-CB-CG	7.15	119.75	112.60
1	D	0	LYS	CA-C-N	6.46	128.84	120.44
1	D	0	LYS	C-N-CA	6.46	128.84	120.44
1	A	28	HIS	CA-C-N	6.39	129.36	120.29
1	A	28	HIS	C-N-CA	6.39	129.36	120.29
1	A	17	ALA	CA-C-O	-5.61	115.11	121.00
1	C	29	THR	CB-CA-C	5.52	119.55	110.88
1	A	111	ASP	CA-CB-CG	5.48	118.08	112.60
1	D	11	HIS	N-CA-C	-5.30	105.58	111.36
1	B	324	LEU	CA-C-N	5.25	127.32	120.28
1	B	324	LEU	C-N-CA	5.25	127.32	120.28
1	B	19	THR	CA-CB-OG1	5.11	117.26	109.60
1	B	19	THR	N-CA-CB	5.03	118.14	110.44

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	1990	0	1974	18	0
1	B	2540	0	2541	38	0
1	C	1994	0	1982	24	0
1	D	2341	0	2350	55	0
2	D	46	0	0	8	0
3	A	116	0	0	3	0
3	B	136	0	0	3	0
3	C	105	0	0	3	0
3	D	144	0	0	0	0
All	All	9412	0	8847	129	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 7.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LYS:HD3	1:D:300:ASP:HB3	1.27	1.12
1:C:139:ARG:HD3	1:C:179:MET:HE1	1.44	0.97
1:B:266:MET:HA	1:B:266:MET:HE3	1.45	0.96
1:B:187:LEU:HD21	1:B:204:MET:HE1	1.53	0.90
1:D:33:ARG:NH1	2:D:402:C0X:C24	2.38	0.86
1:A:192:ARG:HA	3:A:461:HOH:O	1.75	0.86
1:D:123:GLY:O	1:D:127:THR:HG23	1.82	0.80
1:B:258:LEU:HB3	1:B:262:GLY:HA3	1.65	0.79
1:D:37:ARG:HD2	2:D:402:C0X:O27	1.83	0.77
1:C:145:TYR:HB2	3:C:416:HOH:O	1.90	0.71
1:B:266:MET:HA	1:B:266:MET:CE	2.20	0.71
1:D:204:MET:HE1	1:D:254:LEU:HD11	1.74	0.70
1:D:251:VAL:HG23	1:D:252:ARG:N	2.09	0.68
1:D:222:ARG:HH11	1:D:243:HIS:HD2	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ARG:CZ	2:D:402:C0X:C24	2.73	0.66
1:D:299:TYR:O	1:D:308:ARG:NH2	2.30	0.64
1:C:189:ASP:OD1	1:C:192:ARG:NH1	2.32	0.62
1:B:179:MET:HE3	1:B:217:LEU:HD11	1.81	0.62
1:A:94:ARG:HD2	1:A:98:GLU:OE2	1.99	0.62
1:D:284:LYS:HE3	1:D:300:ASP:OD2	2.01	0.61
1:C:140:ALA:O	1:C:144:THR:HG23	2.00	0.61
1:D:34:LEU:CD1	2:D:402:C0X:O28	2.50	0.60
1:B:200:LEU:HG	1:B:204:MET:HE2	1.82	0.60
1:B:124:GLN:HE21	1:B:124:GLN:HA	1.67	0.59
1:D:224:ARG:HH21	1:D:224:ARG:HG2	1.67	0.59
1:A:179:MET:HE2	1:A:221:LEU:HD21	1.83	0.59
1:C:57:ARG:HD3	3:C:453:HOH:O	2.04	0.58
1:A:232:PRO:HA	1:A:233:PRO:C	2.28	0.57
1:D:288:VAL:HG13	1:D:324:LEU:HD13	1.85	0.57
1:A:139:ARG:HD3	1:A:179:MET:HE1	1.86	0.57
1:A:192:ARG:HB2	3:A:405:HOH:O	2.04	0.57
1:D:34:LEU:HD13	2:D:402:C0X:O28	2.04	0.57
1:B:200:LEU:HG	1:B:204:MET:CE	2.35	0.56
1:D:10:ASP:O	1:D:14:ARG:HG2	2.05	0.56
1:D:10:ASP:O	1:D:14:ARG:CG	2.54	0.56
1:D:284:LYS:HD3	1:D:300:ASP:CB	2.19	0.56
1:D:252:ARG:NE	1:D:252:ARG:O	2.38	0.56
1:D:222:ARG:NH1	1:D:243:HIS:HD2	2.04	0.56
1:D:251:VAL:O	1:D:255:PRO:CD	2.53	0.55
1:D:251:VAL:HG23	1:D:252:ARG:H	1.69	0.55
1:C:215:VAL:O	1:C:219:GLU:HG3	2.08	0.54
1:D:142:ALA:HB1	1:D:182:THR:HG21	1.89	0.54
1:D:37:ARG:HD2	2:D:402:C0X:C26	2.37	0.53
1:A:200:LEU:HG	1:A:204:MET:HE2	1.90	0.53
1:B:258:LEU:HD13	1:B:262:GLY:HA3	1.89	0.53
1:C:254:LEU:N	1:C:255:PRO:CD	2.72	0.53
1:B:179:MET:CE	1:B:217:LEU:HD11	2.39	0.52
1:B:266:MET:CE	1:B:266:MET:CA	2.85	0.52
1:C:179:MET:HG2	1:C:221:LEU:HD11	1.92	0.51
1:D:61:LEU:HD13	1:D:94:ARG:HG3	1.92	0.51
1:B:222:ARG:HH11	1:B:243:HIS:HD2	1.58	0.51
1:B:19:THR:CG2	1:B:90:ARG:HG3	2.40	0.51
1:D:75:ASP:CG	1:D:75:ASP:O	2.49	0.51
1:A:116:ASP:HA	3:A:468:HOH:O	2.11	0.50
1:D:94:ARG:HD2	1:D:98:GLU:OE2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:VAL:O	1:D:255:PRO:HG2	2.11	0.50
1:C:127:THR:HG21	1:C:145:TYR:CD2	2.46	0.50
1:C:187:LEU:HD21	1:C:204:MET:HE1	1.94	0.50
1:C:44:GLU:HG2	1:C:238:LEU:HG	1.94	0.49
1:D:299:TYR:CE2	1:D:308:ARG:HB3	2.47	0.49
1:D:222:ARG:HH11	1:D:243:HIS:CD2	2.27	0.49
1:D:204:MET:HE1	1:D:254:LEU:CD1	2.41	0.49
1:D:251:VAL:CG2	1:D:252:ARG:N	2.75	0.49
1:D:38:VAL:HG12	1:D:39:PRO:HD3	1.94	0.49
1:D:12:VAL:HG22	1:D:61:LEU:HD23	1.95	0.48
1:D:239:VAL:N	1:D:240:PRO:HD2	2.29	0.48
1:C:15:CYS:O	1:C:19:THR:HG22	2.13	0.48
1:C:187:LEU:HD21	1:C:204:MET:CE	2.44	0.48
1:D:90:ARG:C	1:D:90:ARG:HD3	2.39	0.47
1:D:288:VAL:CG1	1:D:324:LEU:HD13	2.44	0.47
1:B:179:MET:HE2	1:B:221:LEU:HD21	1.96	0.47
1:B:224:ARG:HD2	3:B:485:HOH:O	2.14	0.47
1:D:282:ILE:O	1:D:282:ILE:HG23	2.14	0.47
1:B:266:MET:HE2	1:B:267:ALA:H	1.80	0.47
1:D:34:LEU:HD13	2:D:402:C0X:C26	2.44	0.47
1:A:100:GLU:OE1	1:B:100:GLU:OE1	2.33	0.46
1:D:251:VAL:O	1:D:255:PRO:HD2	2.14	0.46
1:B:266:MET:HE2	1:B:267:ALA:N	2.30	0.46
1:C:38:VAL:N	1:C:39:PRO:CD	2.79	0.46
1:A:81:ARG:NH2	1:B:72:LEU:O	2.48	0.46
1:A:90:ARG:C	1:A:90:ARG:HD3	2.41	0.46
1:C:25:LEU:HD22	1:C:83:GLU:HG3	1.98	0.46
1:D:94:ARG:HD3	1:D:98:GLU:HG3	1.98	0.45
1:B:205:ARG:NH1	1:C:131:ARG:HG2	2.32	0.45
1:D:293:LYS:HE3	1:D:293:LYS:HB2	1.85	0.45
1:D:1:MET:C	1:D:1:MET:HE3	2.41	0.45
1:C:239:VAL:HB	1:C:240:PRO:HD3	1.98	0.45
1:D:249:VAL:HA	1:D:253:LEU:HB2	1.98	0.45
1:C:10:ASP:OD2	1:C:14:ARG:NH2	2.40	0.45
1:D:248:ASP:OD1	1:D:252:ARG:HG2	2.17	0.44
1:D:37:ARG:CD	2:D:402:C0X:O27	2.59	0.44
1:D:251:VAL:CG2	1:D:252:ARG:H	2.29	0.44
1:B:222:ARG:O	1:B:226:LEU:HG	2.18	0.44
1:B:254:LEU:CB	1:B:255:PRO:HD3	2.48	0.44
1:C:254:LEU:N	1:C:255:PRO:HD3	2.33	0.44
1:B:187:LEU:HD21	1:B:204:MET:CE	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:MET:HA	1:C:209:VAL:O	2.18	0.44
1:D:126:ARG:O	1:D:130:SER:OG	2.32	0.43
1:B:254:LEU:HB2	1:B:255:PRO:HD3	1.99	0.43
1:D:38:VAL:N	1:D:39:PRO:CD	2.81	0.43
1:D:282:ILE:HG12	1:D:319:GLU:HB3	2.01	0.43
1:B:203:LEU:HB3	1:B:209:VAL:HG23	2.01	0.42
1:A:165:GLN:HE21	1:A:165:GLN:HB3	1.62	0.42
1:B:19:THR:HG23	1:B:90:ARG:HG3	2.01	0.42
1:B:38:VAL:HG11	1:B:150:LEU:HD11	2.01	0.42
1:D:62:ASP:OD1	1:D:92:HIS:ND1	2.52	0.42
1:C:13:THR:HG22	1:C:29:THR:HG22	2.00	0.42
1:D:308:ARG:HH21	1:D:308:ARG:HG3	1.83	0.42
1:B:254:LEU:N	1:B:255:PRO:CD	2.83	0.42
1:B:19:THR:HG21	1:B:90:ARG:HG3	2.01	0.42
1:C:172:GLU:HG2	3:C:469:HOH:O	2.20	0.42
1:A:166:PRO:HD3	1:A:233:PRO:HD2	2.01	0.42
1:B:138:TRP:CH2	1:B:183:MET:HG2	2.54	0.42
1:B:271:PHE:HB3	1:B:311:VAL:CG1	2.50	0.42
1:A:38:VAL:HG12	1:A:39:PRO:HD3	2.01	0.41
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.84	0.41
1:B:163:GLU:HA	3:B:443:HOH:O	2.20	0.41
1:A:186:ASP:OD2	1:A:200:LEU:N	2.48	0.41
1:B:26:VAL:HG11	1:D:193:ASN:HA	2.02	0.41
1:D:251:VAL:O	1:D:255:PRO:CG	2.68	0.41
1:C:203:LEU:HB3	1:C:209:VAL:HG23	2.03	0.41
1:A:104:ARG:NH1	1:A:158:ALA:O	2.53	0.41
1:D:131:ARG:HH11	1:D:131:ARG:HG2	1.85	0.40
1:A:254:LEU:N	1:A:255:PRO:CD	2.84	0.40
1:B:164:GLY:C	3:B:441:HOH:O	2.64	0.40
1:A:106:PRO:HB2	1:B:106:PRO:HB2	2.03	0.40
1:B:38:VAL:N	1:B:39:PRO:CD	2.85	0.40
1:B:90:ARG:C	1:B:90:ARG:HD3	2.47	0.40
1:C:100:GLU:OE1	1:D:100:GLU:OE1	2.40	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	257/343 (75%)	248 (96%)	9 (4%)	0	100	100
1	B	331/343 (96%)	318 (96%)	13 (4%)	0	100	100
1	C	260/343 (76%)	256 (98%)	4 (2%)	0	100	100
1	D	298/343 (87%)	288 (97%)	10 (3%)	0	100	100
All	All	1146/1372 (84%)	1110 (97%)	36 (3%)	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	206/270 (76%)	189 (92%)	17 (8%)	10	11
1	B	261/270 (97%)	237 (91%)	24 (9%)	8	9
1	C	205/270 (76%)	193 (94%)	12 (6%)	18	22
1	D	244/270 (90%)	224 (92%)	20 (8%)	10	11
All	All	916/1080 (85%)	843 (92%)	73 (8%)	11	12

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	18	GLN

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Mol	Chain	Res	Type
1	A	29	THR
1	A	94	ARG
1	A	107	LYS
1	A	128	LYS
1	A	131	ARG
1	A	139	ARG
1	A	163	GLU
1	A	165	GLN
1	A	186	ASP
1	A	189	ASP
1	A	191	ASP
1	A	192	ARG
1	A	197	ASP
1	A	199	ASN
1	A	254	LEU
1	B	18	GLN
1	B	19	THR
1	B	38	VAL
1	B	67	LYS
1	B	115	GLN
1	B	124	GLN
1	B	130	SER
1	B	131	ARG
1	B	172	GLU
1	B	179	MET
1	B	185	ASP
1	B	186	ASP
1	B	197	ASP
1	B	254	LEU
1	B	266	MET
1	B	269	VAL
1	B	272	LYS
1	B	283	SER
1	B	288	VAL
1	B	305	LYS
1	B	314	LYS
1	B	318	LYS
1	B	324	LEU
1	B	326	LYS
1	C	10	ASP
1	C	18	GLN
1	C	19	THR

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Mol	Chain	Res	Type
1	C	29	THR
1	C	104	ARG
1	C	107	LYS
1	C	139	ARG
1	C	165	GLN
1	C	179	MET
1	C	181	ILE
1	C	219	GLU
1	C	254	LEU
1	D	0	LYS
1	D	18	GLN
1	D	19	THR
1	D	37	ARG
1	D	104	ARG
1	D	115	GLN
1	D	127	THR
1	D	130	SER
1	D	139	ARG
1	D	186	ASP
1	D	197	ASP
1	D	252	ARG
1	D	258	LEU
1	D	277	GLU
1	D	279	GLU
1	D	282	ILE
1	D	284	LYS
1	D	285	ILE
1	D	288	VAL
1	D	324	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	40	HIS
1	A	97	HIS
1	A	165	GLN
1	B	18	GLN
1	B	124	GLN
1	B	243	HIS
1	C	18	GLN
1	C	124	GLN

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Mol	Chain	Res	Type
1	D	8	ASN
1	D	18	GLN
1	D	165	GLN
1	D	193	ASN
1	D	202	HIS
1	D	243	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	C0X	D	401	-	27,27,27	1.86	7 (25%)	30,34,34	2.24	11 (36%)
2	C0X	D	402	-	17,17,27	2.26	7 (41%)	18,22,34	1.19	1 (5%)

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
2	C0X	D	401	-	-	16/34/34/34	-
2	C0X	D	402	-	-	7/22/22/34	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	C0X	P20-O21	4.22	1.69	1.56
2	D	402	C0X	P20-O19	3.99	1.68	1.56
2	D	401	C0X	P20-O23	3.86	1.68	1.56
2	D	401	C0X	P20-O19	3.66	1.67	1.56
2	D	402	C0X	C18-C17	3.60	1.56	1.51
2	D	402	C0X	C15-C14	3.57	1.59	1.49
2	D	402	C0X	P20-O21	3.37	1.67	1.56
2	D	401	C0X	C17-C26	2.93	1.55	1.52
2	D	402	C0X	C3-C2	2.82	1.57	1.50
2	D	402	C0X	P20-O23	2.73	1.65	1.56
2	D	402	C0X	O28-C26	2.59	1.29	1.22
2	D	401	C0X	C3-C2	2.53	1.56	1.51
2	D	401	C0X	C15-C14	2.52	1.56	1.49
2	D	401	C0X	C9-C10	2.13	1.56	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	C0X	O16-C17-C26	4.79	119.50	112.17
2	D	401	C0X	C7-C6-C8	4.66	123.31	115.23
2	D	401	C0X	C15-O16-C17	4.49	121.23	113.15
2	D	401	C0X	C8-C6-C5	-4.47	111.13	121.17
2	D	401	C0X	O27-C26-C17	3.10	120.77	112.71
2	D	402	C0X	C15-O16-C17	3.01	118.56	113.15
2	D	401	C0X	C1-C2-C3	2.92	120.30	115.23
2	D	401	C0X	C15-C14-C2	-2.89	121.46	126.20
2	D	401	C0X	O27-C26-O28	-2.84	117.64	124.08
2	D	401	C0X	C9-C10-C11	-2.51	119.26	127.64
2	D	401	C0X	O19-P20-O25	-2.44	105.06	114.20
2	D	401	C0X	C12-C11-C13	2.02	119.24	114.59

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	C0X	C26-C17-O16-C15

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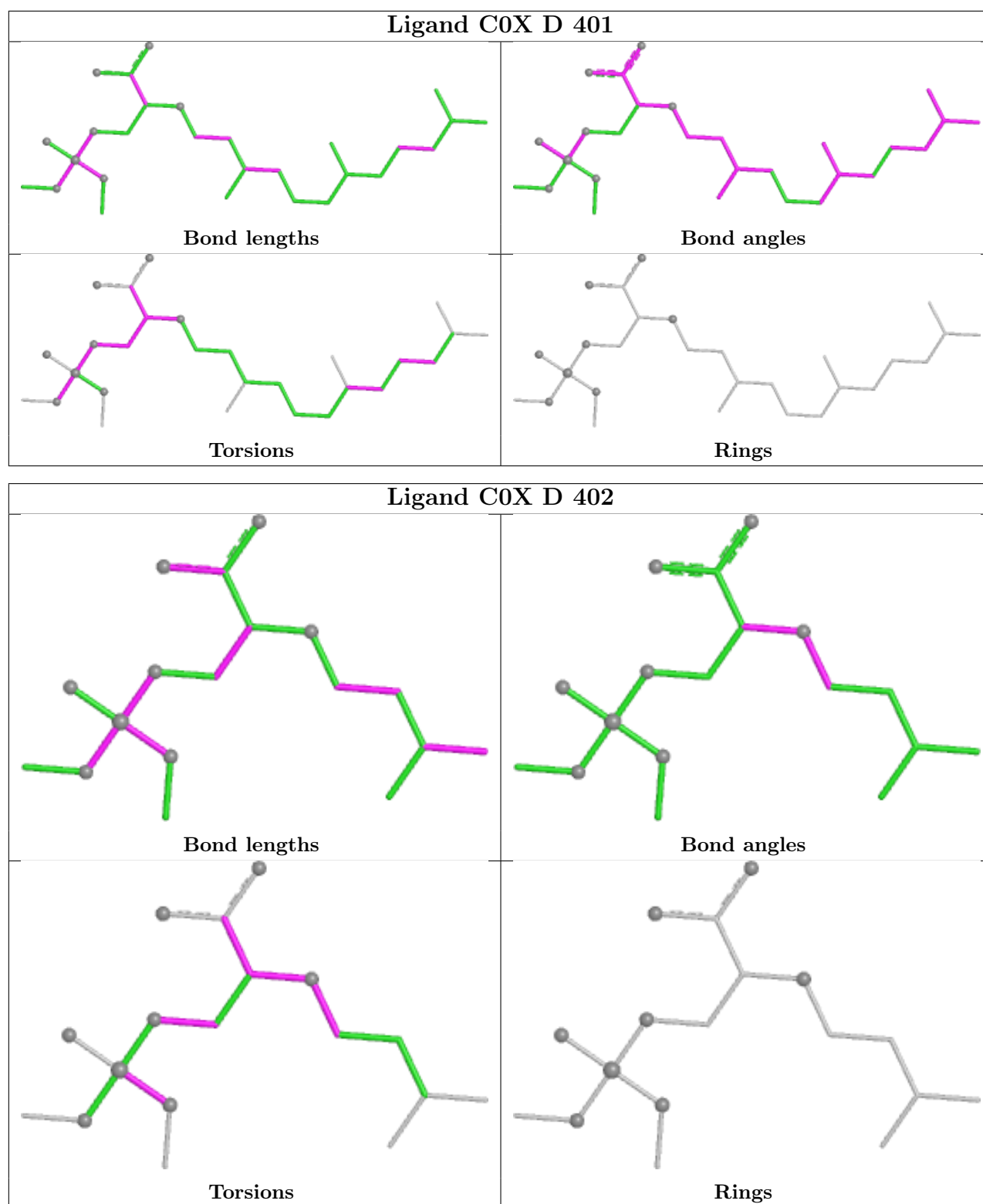
Mol	Chain	Res	Type	Atoms
2	D	401	C0X	O16-C17-C18-O19
2	D	401	C0X	C26-C17-C18-O19
2	D	401	C0X	O16-C17-C26-O28
2	D	401	C0X	O16-C17-C26-O27
2	D	401	C0X	C22-O21-P20-O19
2	D	401	C0X	C22-O21-P20-O25
2	D	402	C0X	C14-C15-O16-C17
2	D	402	C0X	C18-C17-O16-C15
2	D	402	C0X	C26-C17-O16-C15
2	D	402	C0X	O16-C17-C26-O27
2	D	402	C0X	C24-O23-P20-O21
2	D	402	C0X	C24-O23-P20-O25
2	D	401	C0X	C7-C6-C8-C9
2	D	401	C0X	C5-C6-C8-C9
2	D	401	C0X	C18-O19-P20-O25
2	D	401	C0X	C18-O19-P20-O23
2	D	401	C0X	C18-C17-C26-O28
2	D	401	C0X	C18-C17-C26-O27
2	D	401	C0X	C18-C17-O16-C15
2	D	401	C0X	C17-C18-O19-P20
2	D	402	C0X	C17-C18-O19-P20
2	D	401	C0X	C11-C10-C9-C8

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	402	C0X	8	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 ⓘ

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	260/343 (75%)	-0.22	7 (2%) 56 63	25, 45, 81, 133	1 (0%)
1	B	333/343 (97%)	-0.05	7 (2%) 63 68	33, 49, 104, 138	0
1	C	262/343 (76%)	-0.20	3 (1%) 78 82	31, 48, 73, 113	0
1	D	304/343 (88%)	-0.09	6 (1%) 65 70	32, 46, 124, 160	0
All	All	1159/1372 (84%)	-0.13	23 (1%) 65 70	25, 48, 98, 160	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-5	VAL	4.9
1	D	258	LEU	4.8
1	B	263	ALA	4.5
1	A	-5	VAL	4.3
1	B	261	ALA	4.0
1	C	145	TYR	3.7
1	B	304	GLY	3.3
1	A	190	TYR	2.9
1	A	162	GLY	2.8
1	D	252	ARG	2.8
1	A	192	ARG	2.7
1	C	219	GLU	2.6
1	B	262	GLY	2.6
1	D	322	GLN	2.5
1	D	320	LEU	2.5
1	A	197	ASP	2.5
1	A	189	ASP	2.5
1	A	163	GLU	2.4
1	D	282	ILE	2.3
1	C	259	GLY	2.2
1	B	303	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	300	ASP	2.1
1	B	264	GLY	2.1

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](#)

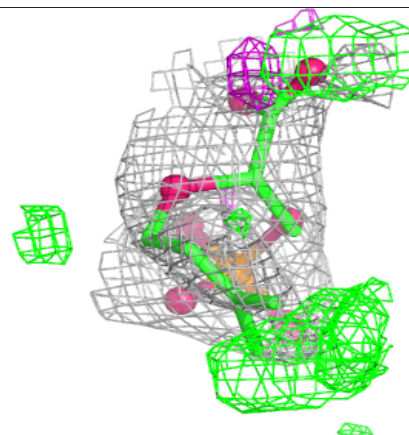
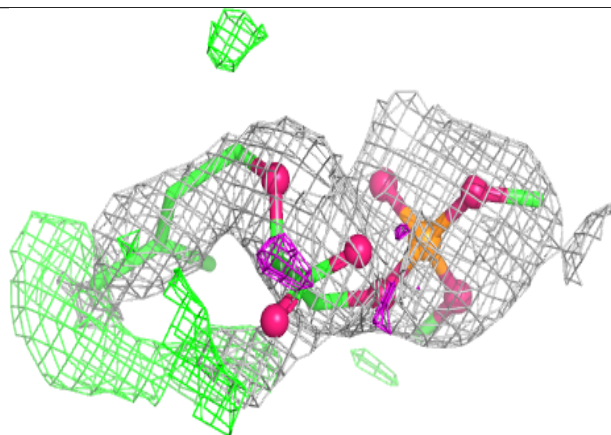
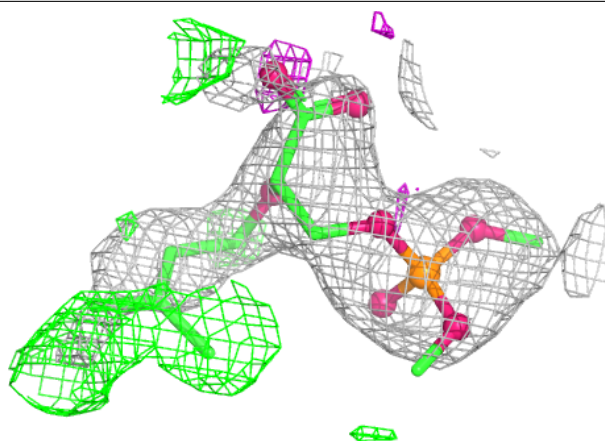
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	C0X	D	402	18/28	0.63	0.20	92,108,115,115	0
2	C0X	D	401	28/28	0.85	0.17	56,83,124,139	0

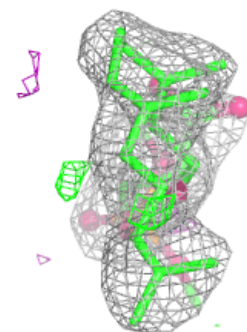
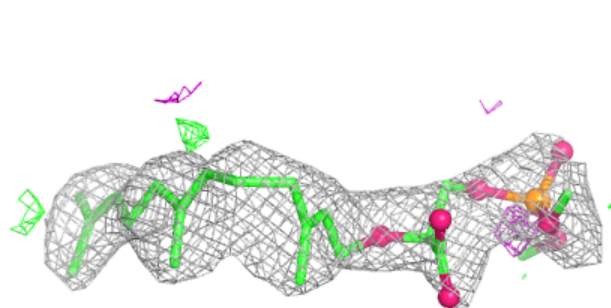
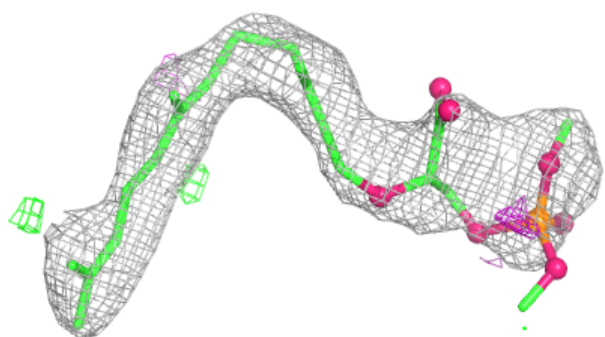
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C0X D 402:

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

**Electron density around C0X D 401:**

$2mF_o-DF_c$ (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.