Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 08:16 AM EST

PDB ID	:	6BR9
Title	:	Structure of A6 reveals a novel lipid transporter
Authors	:	Deng, J.; Peng, S.; Pathak, P.
Deposited on	:	2017-11-30
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

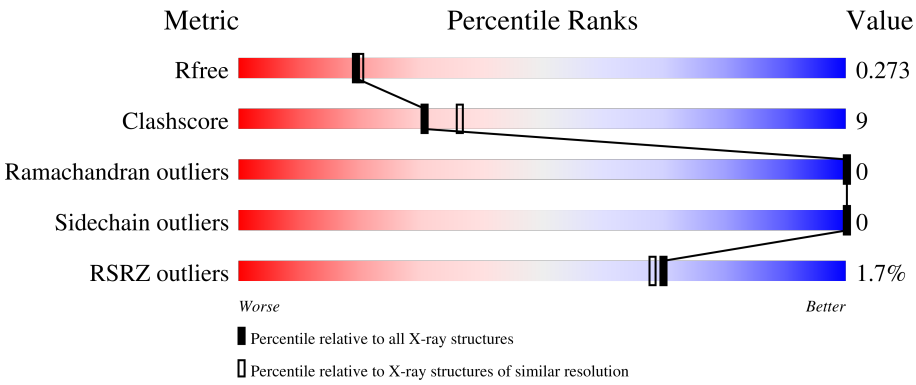
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

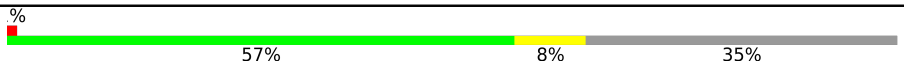
The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	359	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2215 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 Protein A6 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	233	1917	1250	303	357	7	167	0	0

There are 107 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	expression tag	UNP Q9J563
A	17	GLY	-	expression tag	UNP Q9J563
A	18	HIS	-	expression tag	UNP Q9J563
A	19	HIS	-	expression tag	UNP Q9J563
A	20	HIS	-	expression tag	UNP Q9J563
A	21	HIS	-	expression tag	UNP Q9J563
A	22	HIS	-	expression tag	UNP Q9J563
A	23	HIS	-	expression tag	UNP Q9J563
A	24	GLY	-	expression tag	UNP Q9J563
A	25	SER	-	expression tag	UNP Q9J563
A	26	ASP	-	expression tag	UNP Q9J563
A	27	SER	-	expression tag	UNP Q9J563
A	28	GLU	-	expression tag	UNP Q9J563
A	29	VAL	-	expression tag	UNP Q9J563
A	30	ASN	-	expression tag	UNP Q9J563
A	31	GLN	-	expression tag	UNP Q9J563
A	32	GLU	-	expression tag	UNP Q9J563
A	33	ALA	-	expression tag	UNP Q9J563
A	34	LYS	-	expression tag	UNP Q9J563
A	35	PRO	-	expression tag	UNP Q9J563
A	36	GLU	-	expression tag	UNP Q9J563
A	37	VAL	-	expression tag	UNP Q9J563
A	38	LYS	-	expression tag	UNP Q9J563
A	39	PRO	-	expression tag	UNP Q9J563
A	40	GLU	-	expression tag	UNP Q9J563
A	41	VAL	-	expression tag	UNP Q9J563
A	42	LYS	-	expression tag	UNP Q9J563

Continued on next page...

Continued from previous page...

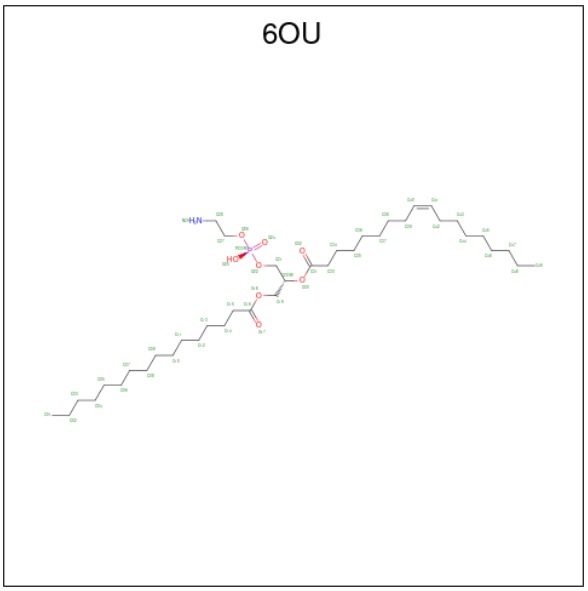
Chain	Residue	Modelled	Actual	Comment	Reference
A	43	PRO	-	expression tag	UNP Q9J563
A	44	GLU	-	expression tag	UNP Q9J563
A	45	THR	-	expression tag	UNP Q9J563
A	46	HIS	-	expression tag	UNP Q9J563
A	47	ILE	-	expression tag	UNP Q9J563
A	48	ASN	-	expression tag	UNP Q9J563
A	49	LEU	-	expression tag	UNP Q9J563
A	50	LYS	-	expression tag	UNP Q9J563
A	51	VAL	-	expression tag	UNP Q9J563
A	52	SER	-	expression tag	UNP Q9J563
A	53	ASP	-	expression tag	UNP Q9J563
A	54	GLY	-	expression tag	UNP Q9J563
A	55	SER	-	expression tag	UNP Q9J563
A	56	SER	-	expression tag	UNP Q9J563
A	57	GLU	-	expression tag	UNP Q9J563
A	58	ILE	-	expression tag	UNP Q9J563
A	59	PHE	-	expression tag	UNP Q9J563
A	60	PHE	-	expression tag	UNP Q9J563
A	61	LYS	-	expression tag	UNP Q9J563
A	62	ILE	-	expression tag	UNP Q9J563
A	63	LYS	-	expression tag	UNP Q9J563
A	64	LYS	-	expression tag	UNP Q9J563
A	65	THR	-	expression tag	UNP Q9J563
A	66	THR	-	expression tag	UNP Q9J563
A	67	PRO	-	expression tag	UNP Q9J563
A	68	LEU	-	expression tag	UNP Q9J563
A	69	ARG	-	expression tag	UNP Q9J563
A	70	ARG	-	expression tag	UNP Q9J563
A	71	LEU	-	expression tag	UNP Q9J563
A	72	MET	-	expression tag	UNP Q9J563
A	73	GLU	-	expression tag	UNP Q9J563
A	74	ALA	-	expression tag	UNP Q9J563
A	75	PHE	-	expression tag	UNP Q9J563
A	76	ALA	-	expression tag	UNP Q9J563
A	77	LYS	-	expression tag	UNP Q9J563
A	78	ARG	-	expression tag	UNP Q9J563
A	79	GLN	-	expression tag	UNP Q9J563
A	80	GLY	-	expression tag	UNP Q9J563
A	81	LYS	-	expression tag	UNP Q9J563
A	82	GLU	-	expression tag	UNP Q9J563
A	83	MET	-	expression tag	UNP Q9J563
A	84	ASP	-	expression tag	UNP Q9J563

Continued on next page...

Continued from previous page...

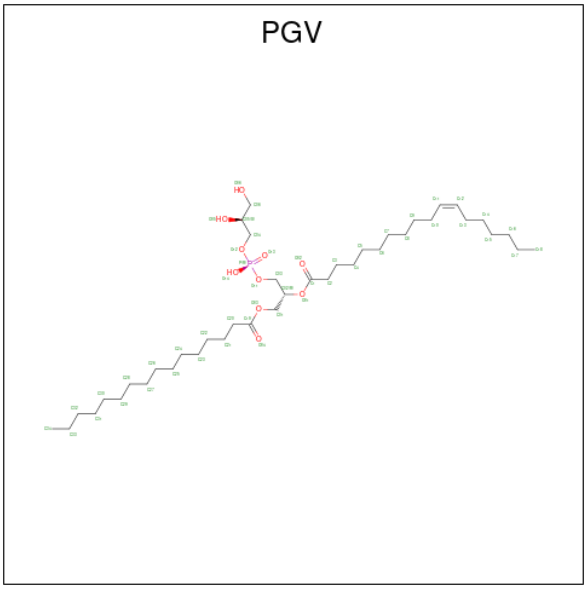
Chain	Residue	Modelled	Actual	Comment	Reference
A	85	SER	-	expression tag	UNP Q9J563
A	86	LEU	-	expression tag	UNP Q9J563
A	87	ARG	-	expression tag	UNP Q9J563
A	88	PHE	-	expression tag	UNP Q9J563
A	89	LEU	-	expression tag	UNP Q9J563
A	90	TYR	-	expression tag	UNP Q9J563
A	91	ASP	-	expression tag	UNP Q9J563
A	92	GLY	-	expression tag	UNP Q9J563
A	93	ILE	-	expression tag	UNP Q9J563
A	94	ARG	-	expression tag	UNP Q9J563
A	95	ILE	-	expression tag	UNP Q9J563
A	96	GLN	-	expression tag	UNP Q9J563
A	97	ALA	-	expression tag	UNP Q9J563
A	98	ASP	-	expression tag	UNP Q9J563
A	99	GLN	-	expression tag	UNP Q9J563
A	100	THR	-	expression tag	UNP Q9J563
A	101	PRO	-	expression tag	UNP Q9J563
A	102	GLU	-	expression tag	UNP Q9J563
A	103	ASP	-	expression tag	UNP Q9J563
A	104	LEU	-	expression tag	UNP Q9J563
A	105	ASP	-	expression tag	UNP Q9J563
A	106	MET	-	expression tag	UNP Q9J563
A	107	GLU	-	expression tag	UNP Q9J563
A	108	ASP	-	expression tag	UNP Q9J563
A	109	ASN	-	expression tag	UNP Q9J563
A	110	ASP	-	expression tag	UNP Q9J563
A	111	ILE	-	expression tag	UNP Q9J563
A	112	ILE	-	expression tag	UNP Q9J563
A	113	GLU	-	expression tag	UNP Q9J563
A	114	ALA	-	expression tag	UNP Q9J563
A	115	HIS	-	expression tag	UNP Q9J563
A	116	ARG	-	expression tag	UNP Q9J563
A	117	GLU	-	expression tag	UNP Q9J563
A	118	GLN	-	expression tag	UNP Q9J563
A	120	GLY	ASN	conflict	UNP Q9J563
A	121	GLY	ASN	conflict	UNP Q9J563
A	122	HIS	MET	conflict	UNP Q9J563
A	123	MET	TYR	conflict	UNP Q9J563

- Molecule 2 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propan-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: $C_{39}H_{76}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	49	39	1	8	1	1	0
			Total	C	N	O	P		
2	A	1	49	39	1	8	1	11	0
			Total	C	N	O	P		
2	A	1	49	39	1	8	1	10	0
			Total	C	N	O	P		
2	A	1	49	39	1	8	1	12	0

- Molecule 3 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	51	40	10	1	6	0

- Molecule 4 is water.

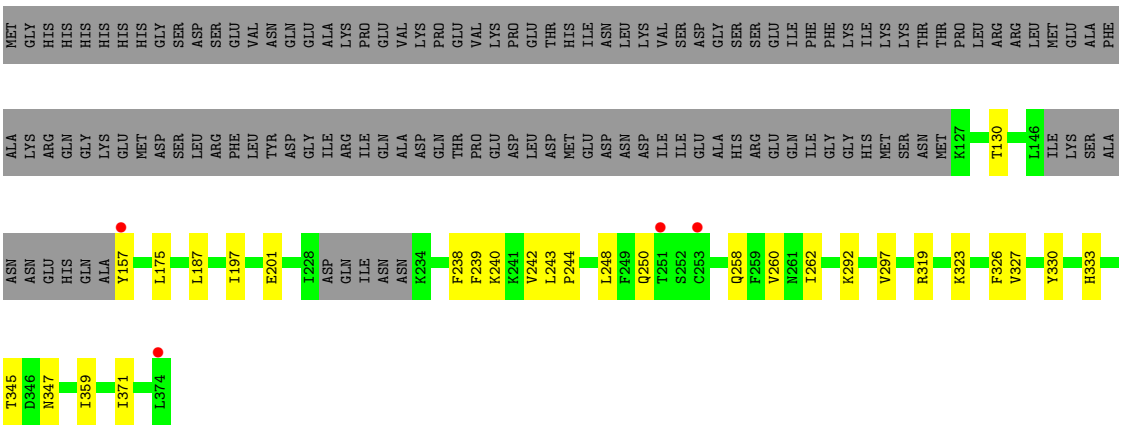
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	51	51	51	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein A6 homolog

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	54.70Å 74.15Å 143.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.53 – 2.20 37.53 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.9 (37.53-2.20) 94.1 (37.53-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.216 , 0.270 0.221 , 0.273	Depositor DCC
R_{free} test set	1518 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2215	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 6OU, PGV

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	0.44	0/1945	0.51	0/2614

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	1917	0	1984	24	0
2	A	196	0	0	5	0
3	A	51	0	76	14	0
4	A	51	0	0	2	0
All	All	2215	0	2060	34	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 9.

All (34) 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:A:323:LYS:HG3	3:A:404:PGV:H42	1.59	0.85
1:A:319:ARG:HG3	2:A:405:6OU:C19	2.13	0.78
1:A:371:ILE:HG21	3:A:404:PGV:H221	1.73	0.71
1:A:244:PRO:O	1:A:250:GLN:NE2	2.23	0.70
3:A:404:PGV:H031	3:A:404:PGV:H22	1.78	0.65
3:A:404:PGV:H05	3:A:404:PGV:H032	1.78	0.65
1:A:248:LEU:HD12	1:A:248:LEU:N	2.13	0.64
1:A:175:LEU:HB3	1:A:248:LEU:HD22	1.80	0.64
1:A:197:ILE:O	1:A:201:GLU:HG2	1.99	0.62
1:A:327:VAL:HG22	3:A:404:PGV:H202	1.83	0.59
1:A:319:ARG:CG	2:A:405:6OU:C19	2.82	0.57
1:A:248:LEU:N	1:A:248:LEU:CD1	2.68	0.56
3:A:404:PGV:H22	3:A:404:PGV:H202	1.89	0.54
1:A:330:TYR:CZ	3:A:404:PGV:H242	2.43	0.54
1:A:345:THR:HG21	1:A:359:ILE:HD11	1.92	0.51
1:A:323:LYS:HG3	3:A:404:PGV:C4	2.36	0.50
3:A:404:PGV:H151	3:A:404:PGV:H291	1.93	0.50
1:A:326:PHE:HE2	3:A:404:PGV:H222	1.78	0.49
1:A:371:ILE:HG13	3:A:404:PGV:H251	1.95	0.49
1:A:347:ASN:HB3	4:A:535:HOH:O	2.11	0.49
3:A:404:PGV:C19	3:A:404:PGV:C03	2.91	0.49
1:A:130:THR:HB	1:A:187:LEU:HG	1.95	0.48
1:A:333:HIS:NE2	4:A:502:HOH:O	2.36	0.47
1:A:240:LYS:HG3	1:A:260:VAL:HG21	1.95	0.47
1:A:292:LYS:HE3	1:A:297:VAL:HG21	1.97	0.46
3:A:404:PGV:H032	3:A:404:PGV:C05	2.47	0.44
2:A:402:6OU:O32	2:A:403:6OU:C19	2.65	0.44
3:A:404:PGV:H031	3:A:404:PGV:H202	2.00	0.43
1:A:239:PHE:HA	1:A:242:VAL:HG22	2.00	0.43
1:A:258:GLN:O	1:A:262:ILE:HG22	2.19	0.42
1:A:157:TYR:HE2	1:A:238:PHE:HB2	1.86	0.41
2:A:401:6OU:O17	2:A:401:6OU:C20	2.69	0.41
2:A:403:6OU:O32	2:A:403:6OU:C21	2.70	0.40
1:A:242:VAL:HG23	1:A:243:LEU:N	2.37	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	227/359 (63%)	220 (97%)	7 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	225/337 (67%)	225 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
3	PGV	A	404	-	50,50,50	1.35	6 (12%)	53,56,56	1.08	4 (7%)
2	6OU	A	403	-	48,48,48	0.87	4 (8%)	51,53,53	0.94	2 (3%)
2	6OU	A	401	-	48,48,48	0.94	4 (8%)	51,53,53	1.08	3 (5%)
2	6OU	A	405	-	48,48,48	0.93	3 (6%)	51,53,53	1.01	4 (7%)
2	6OU	A	402	-	48,48,48	0.90	3 (6%)	51,53,53	0.95	2 (3%)

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
3	PGV	A	404	-	-	23/55/55/55	-
2	6OU	A	403	-	-	27/52/52/52	-
2	6OU	A	401	-	-	26/52/52/52	-
2	6OU	A	405	-	-	31/52/52/52	-
2	6OU	A	402	-	-	24/52/52/52	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	PGV	C01-C02	4.12	1.63	1.50
2	A	401	6OU	O30-C20	-3.14	1.38	1.46
2	A	405	6OU	O30-C20	-2.95	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	PGV	P-O11	2.88	1.71	1.59
2	A	401	6OU	O18-C19	-2.87	1.38	1.45
2	A	402	6OU	O18-C16	2.67	1.41	1.33
2	A	405	6OU	O18-C19	-2.65	1.39	1.45
3	A	404	PGV	P-O12	2.61	1.69	1.59
3	A	404	PGV	C04-C05	2.47	1.59	1.51
2	A	401	6OU	O17-C16	-2.45	1.15	1.22
2	A	403	6OU	O30-C20	-2.40	1.40	1.46
3	A	404	PGV	C03-C02	2.35	1.57	1.50
2	A	403	6OU	O18-C16	2.29	1.40	1.33
2	A	402	6OU	O30-C31	2.26	1.40	1.34
2	A	405	6OU	O17-C16	-2.25	1.15	1.22
3	A	404	PGV	O03-C19	2.22	1.39	1.33
2	A	401	6OU	O32-C31	-2.15	1.16	1.22
2	A	402	6OU	O30-C20	-2.08	1.41	1.46
2	A	403	6OU	O32-C31	-2.05	1.16	1.22
2	A	403	6OU	O18-C19	-2.02	1.40	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	404	PGV	O01-C1-C2	4.93	122.13	111.50
2	A	402	6OU	O30-C31-C33	4.53	121.27	111.50
2	A	401	6OU	O30-C31-C33	4.29	120.75	111.50
2	A	403	6OU	O30-C31-C33	4.00	120.13	111.50
3	A	404	PGV	O03-C19-C20	3.63	123.31	111.91
2	A	401	6OU	O18-C16-C15	3.38	122.53	111.91
2	A	405	6OU	O30-C31-C33	3.18	118.35	111.50
2	A	402	6OU	O18-C16-C15	2.99	121.29	111.91
3	A	404	PGV	O03-C19-O04	-2.73	116.70	123.59
2	A	405	6OU	O18-C16-C15	2.61	120.10	111.91
3	A	404	PGV	O01-C1-O02	-2.54	117.56	123.70
2	A	405	6OU	C20-O30-C31	2.48	123.89	117.79
2	A	405	6OU	O30-C20-C19	2.20	116.36	108.40
2	A	403	6OU	O18-C16-C15	2.11	118.52	111.91
2	A	401	6OU	O30-C31-O32	-2.05	118.75	123.70

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	6OU	C28-C27-O26-P23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	401	6OU	O26-C27-C28-N29
2	A	402	6OU	C15-C16-O18-C19
2	A	402	6OU	O17-C16-O18-C19
2	A	402	6OU	C33-C31-O30-C20
2	A	403	6OU	O26-C27-C28-N29
2	A	405	6OU	C21-O22-P23-O25
2	A	405	6OU	C27-O26-P23-O24
2	A	405	6OU	C27-O26-P23-O25
2	A	405	6OU	C33-C31-O30-C20
3	A	404	PGV	C03-O11-P-O12
3	A	404	PGV	C03-O11-P-O13
3	A	404	PGV	C03-O11-P-O14
3	A	404	PGV	O02-C1-O01-C02
3	A	404	PGV	O04-C19-O03-C01
3	A	404	PGV	C20-C19-O03-C01
2	A	402	6OU	O32-C31-O30-C20
3	A	404	PGV	C2-C1-O01-C02
2	A	403	6OU	C15-C16-O18-C19
2	A	405	6OU	O32-C31-O30-C20
2	A	403	6OU	O17-C16-O18-C19
3	A	404	PGV	O12-C04-C05-O05
2	A	405	6OU	C05-C06-C07-C08
3	A	404	PGV	C13-C14-C15-C16
3	A	404	PGV	O12-C04-C05-C06
2	A	401	6OU	C15-C16-O18-C19
2	A	401	6OU	C13-C14-C15-C16
2	A	401	6OU	O17-C16-O18-C19
2	A	403	6OU	C39-C40-C41-C42
2	A	401	6OU	C31-C33-C34-C35
3	A	404	PGV	C19-C20-C21-C22
2	A	405	6OU	C07-C08-C09-C10
2	A	403	6OU	C21-O22-P23-O26
2	A	405	6OU	C21-O22-P23-O26
2	A	401	6OU	O32-C31-O30-C20
2	A	403	6OU	O32-C31-O30-C20
2	A	401	6OU	C41-C42-C43-C44
2	A	401	6OU	C07-C08-C09-C10
2	A	401	6OU	C33-C31-O30-C20
2	A	403	6OU	C33-C31-O30-C20
2	A	405	6OU	C11-C12-C13-C14
2	A	405	6OU	C19-C20-O30-C31
2	A	405	6OU	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	403	6OU	C36-C37-C38-C39
3	A	404	PGV	C20-C21-C22-C23
2	A	401	6OU	C08-C09-C10-C11
2	A	403	6OU	C02-C03-C04-C05
2	A	403	6OU	C03-C04-C05-C06
2	A	405	6OU	C42-C43-C44-C45
2	A	405	6OU	C43-C44-C45-C46
2	A	403	6OU	C07-C08-C09-C10
2	A	402	6OU	C43-C44-C45-C46
2	A	402	6OU	C42-C43-C44-C45
2	A	401	6OU	C05-C06-C07-C08
3	A	404	PGV	C23-C24-C25-C26
2	A	401	6OU	C36-C37-C38-C39
2	A	402	6OU	C35-C36-C37-C38
2	A	403	6OU	C08-C09-C10-C11
2	A	405	6OU	C44-C45-C46-C47
2	A	405	6OU	C39-C40-C41-C42
3	A	404	PGV	C24-C25-C26-C27
2	A	405	6OU	C04-C05-C06-C07
2	A	403	6OU	C43-C44-C45-C46
2	A	402	6OU	C33-C34-C35-C36
3	A	404	PGV	C21-C22-C23-C24
2	A	401	6OU	C09-C10-C11-C12
2	A	405	6OU	C06-C07-C08-C09
2	A	402	6OU	C04-C05-C06-C07
3	A	404	PGV	C30-C31-C32-C33
2	A	402	6OU	C09-C10-C11-C12
2	A	403	6OU	C12-C13-C14-C15
2	A	405	6OU	C27-O26-P23-O22
2	A	402	6OU	C45-C46-C47-C48
3	A	404	PGV	C12-C13-C14-C15
2	A	401	6OU	O18-C19-C20-C21
2	A	403	6OU	C05-C06-C07-C08
2	A	401	6OU	C46-C47-C48-C49
2	A	403	6OU	C01-C02-C03-C04
2	A	402	6OU	C40-C41-C42-C43
2	A	402	6OU	C05-C06-C07-C08
2	A	402	6OU	C12-C13-C14-C15
3	A	404	PGV	C22-C23-C24-C25
2	A	403	6OU	C41-C42-C43-C44
2	A	405	6OU	C35-C36-C37-C38
2	A	401	6OU	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	402	6OU	C19-C20-C21-O22
2	A	403	6OU	O18-C19-C20-C21
2	A	402	6OU	O30-C20-C21-O22
2	A	405	6OU	O30-C20-C21-O22
2	A	401	6OU	C42-C43-C44-C45
3	A	404	PGV	C6-C7-C8-C9
2	A	403	6OU	C13-C14-C15-C16
3	A	404	PGV	C5-C6-C7-C8
2	A	402	6OU	O18-C19-C20-O30
2	A	402	6OU	C10-C11-C12-C13
2	A	405	6OU	C45-C46-C47-C48
2	A	401	6OU	C27-O26-P23-O24
2	A	403	6OU	C21-O22-P23-O24
2	A	403	6OU	C21-O22-P23-O25
2	A	405	6OU	C21-O22-P23-O24
2	A	405	6OU	C19-C20-C21-O22
2	A	401	6OU	C45-C46-C47-C48
2	A	402	6OU	O18-C19-C20-C21
2	A	401	6OU	O18-C19-C20-O30
2	A	403	6OU	O18-C19-C20-O30
2	A	403	6OU	C21-C20-O30-C31
3	A	404	PGV	C01-C02-O01-C1
2	A	402	6OU	C44-C45-C46-C47
2	A	402	6OU	C20-C21-O22-P23
2	A	403	6OU	C45-C46-C47-C48
2	A	405	6OU	C34-C35-C36-C37
2	A	405	6OU	O26-C27-C28-N29
2	A	405	6OU	C37-C38-C39-C40
3	A	404	PGV	C31-C32-C33-C34
2	A	405	6OU	C02-C03-C04-C05
2	A	401	6OU	C19-C20-O30-C31
2	A	401	6OU	C03-C04-C05-C06
2	A	401	6OU	C27-O26-P23-O22
2	A	402	6OU	C01-C02-C03-C04
3	A	404	PGV	C9-C10-C11-C12
2	A	405	6OU	C40-C41-C42-C43
2	A	402	6OU	O30-C31-C33-C34
2	A	403	6OU	C14-C15-C16-O18
2	A	401	6OU	C43-C44-C45-C46
2	A	405	6OU	C46-C47-C48-C49
2	A	405	6OU	O18-C19-C20-O30
2	A	403	6OU	C38-C39-C40-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	403	6OU	C46-C47-C48-C49
2	A	401	6OU	C21-C20-O30-C31
2	A	402	6OU	C28-C27-O26-P23
2	A	405	6OU	C38-C39-C40-C41

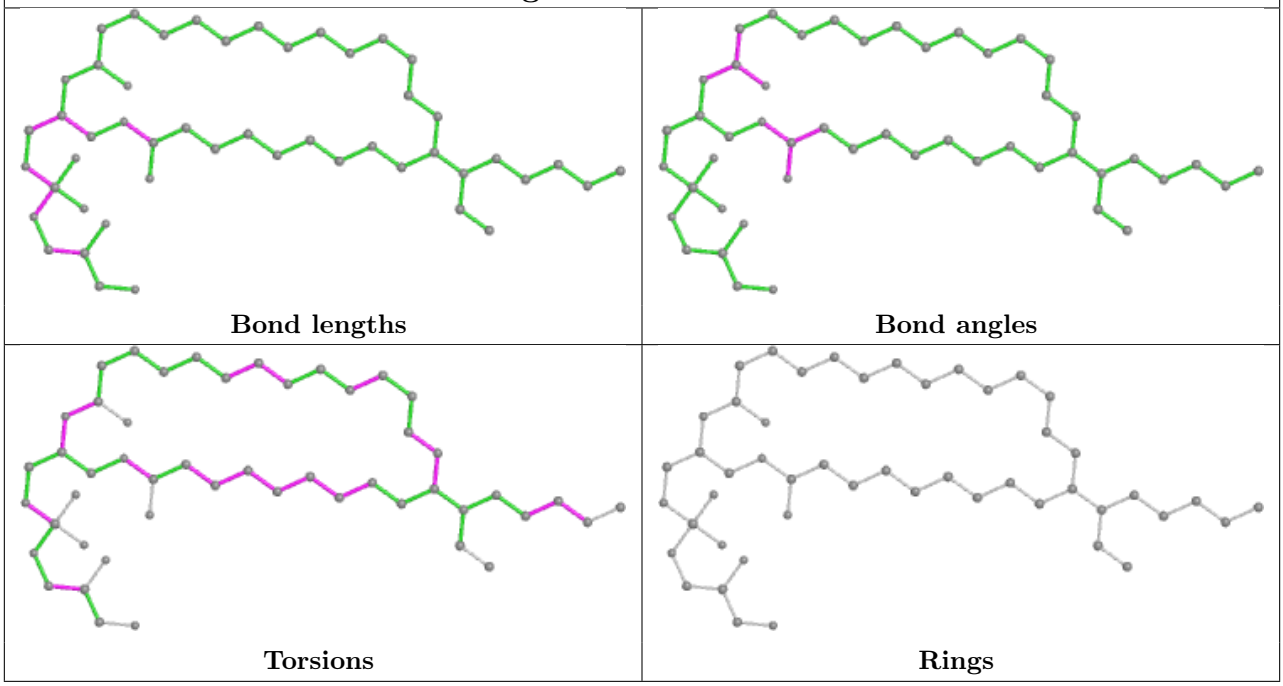
There are no ring outliers.

5 monomers are involved in 19 short contacts:

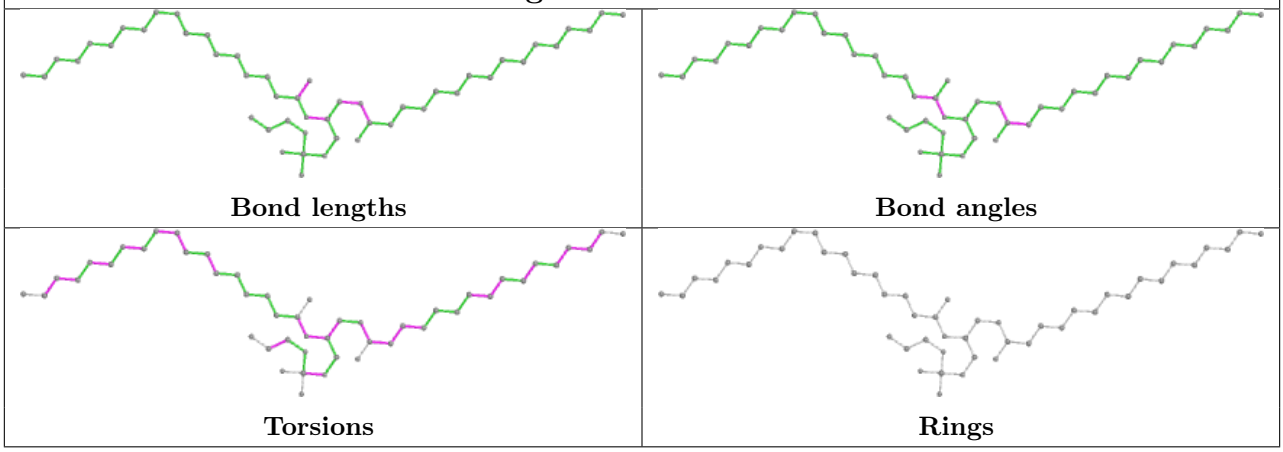
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	PGV	14	0
2	A	403	6OU	2	0
2	A	401	6OU	1	0
2	A	405	6OU	2	0
2	A	402	6OU	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

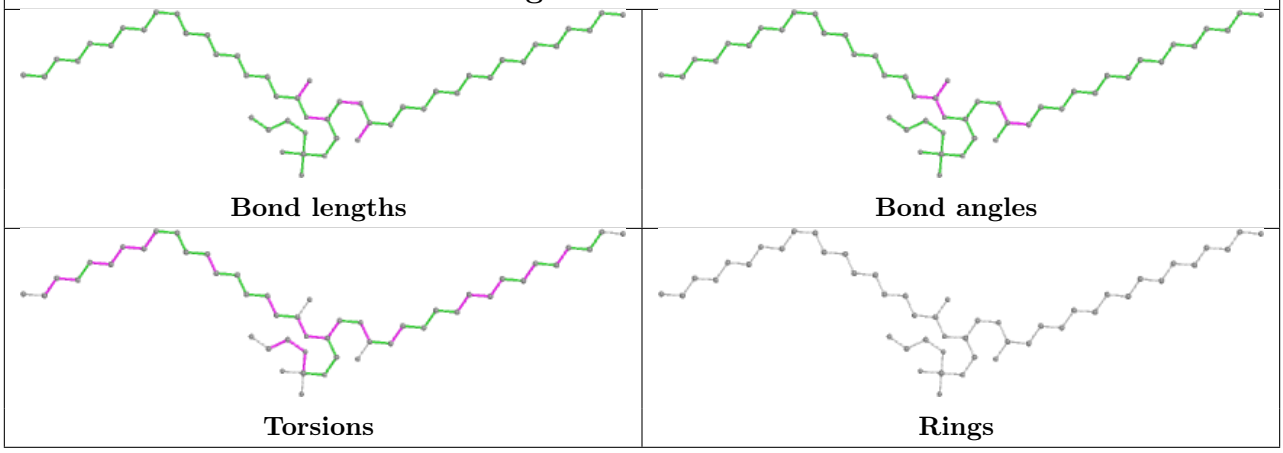
Ligand PGV A 404

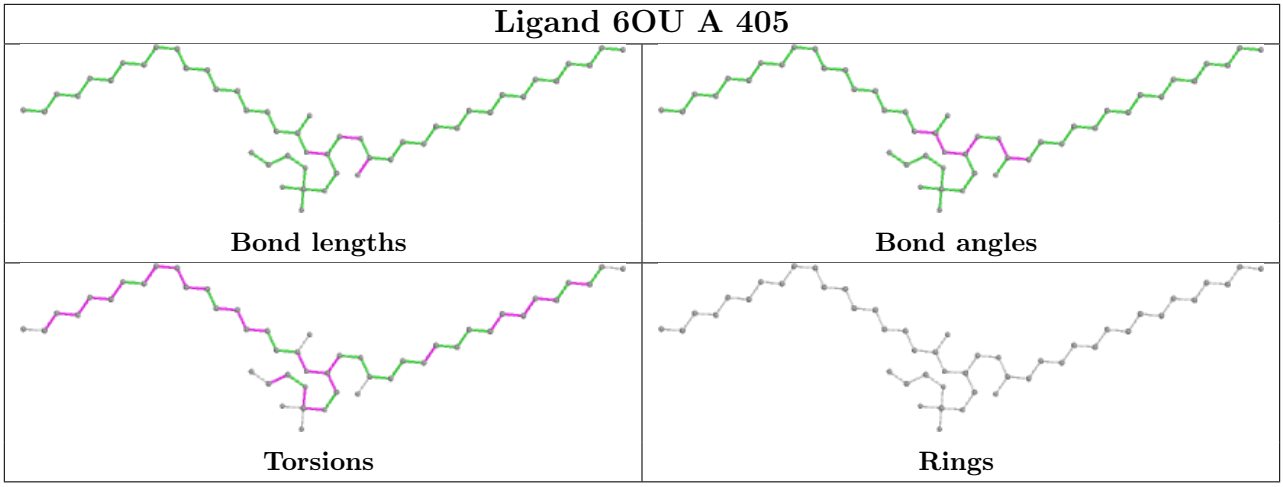


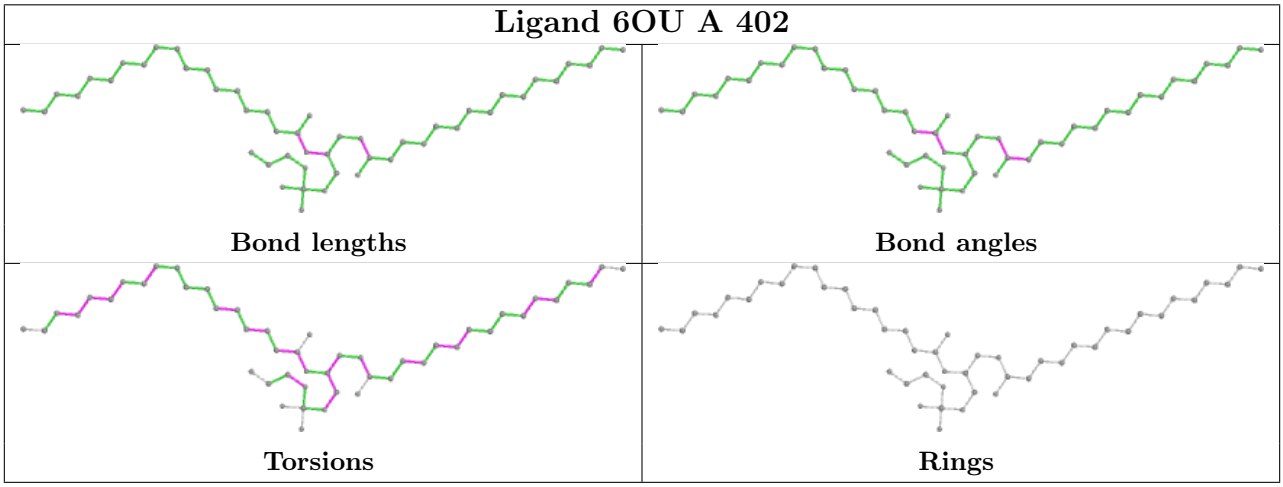
Ligand 6OU A 403



Ligand 6OU A 401







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 (i)

6.1 Protein, DNA and RNA chains (i)

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	233/359 (64%)	-0.20	4 (1%) 70 68	31, 59, 99, 122	61 (26%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	CYS	3.8
1	A	374	LEU	2.9
1	A	157	TYR	2.7
1	A	251	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	6OU	A	402	49/49	0.74	0.21	65,77,86,87	11
3	PGV	A	404	51/51	0.74	0.28	45,70,89,90	6
2	6OU	A	403	49/49	0.80	0.17	65,72,99,105	10

Continued on next page...

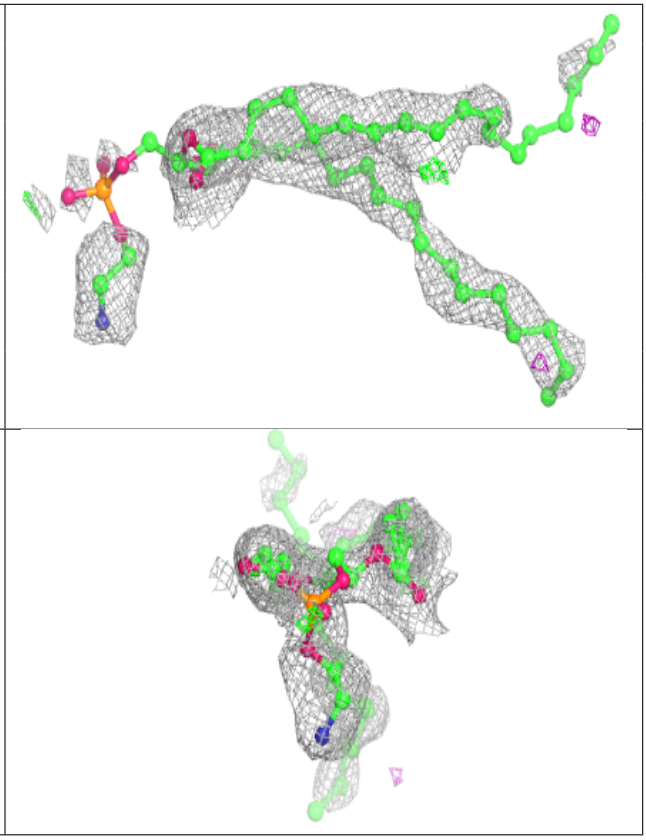
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	6OU	A	401	49/49	0.85	0.16	61,74,84,85	1
2	6OU	A	405	49/49	0.89	0.18	57,67,88,96	12

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.

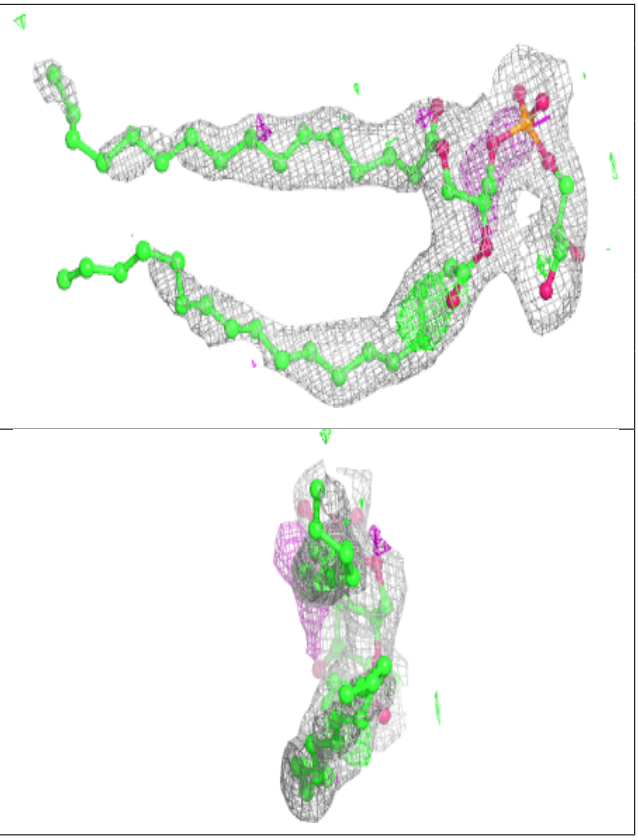
Electron density around 6OU A 402:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



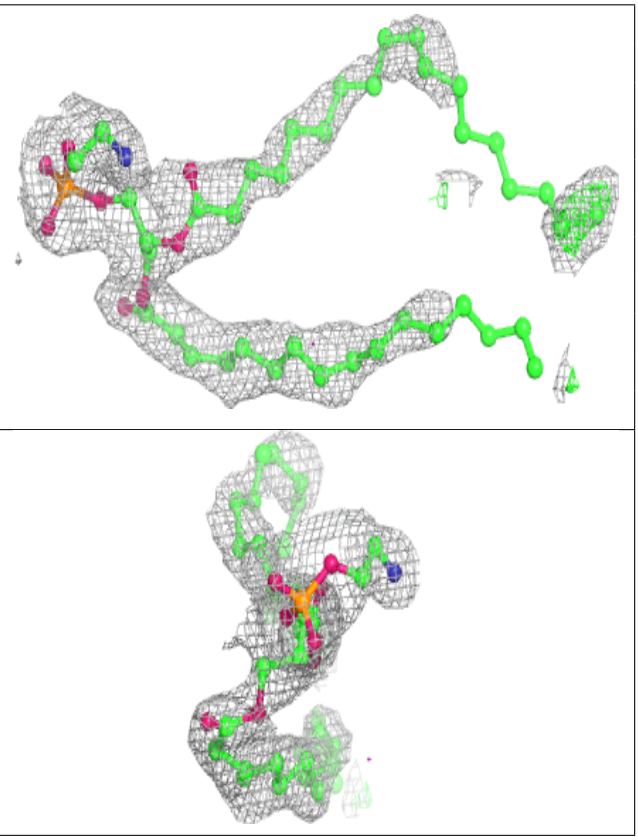
Electron density around PGV A 404:

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



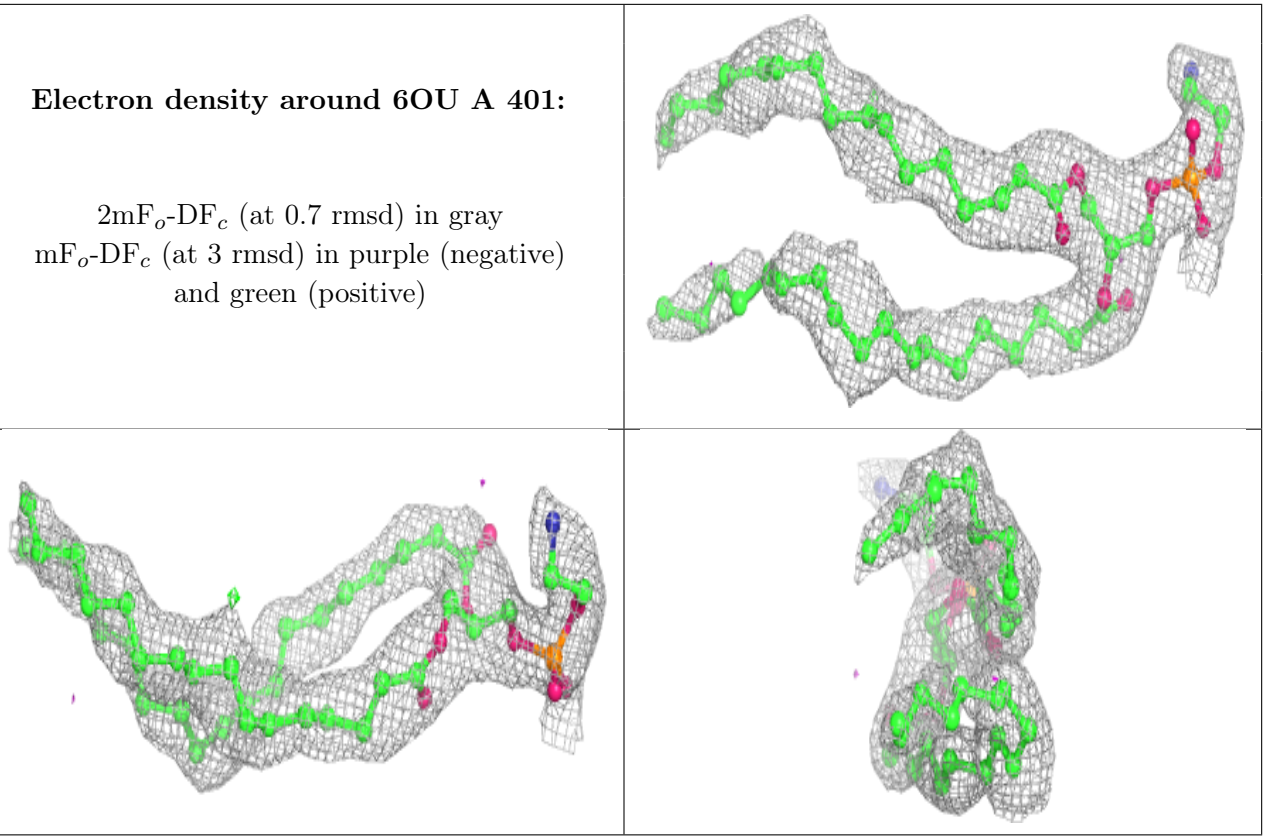
Electron density around 6OU A 403:

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



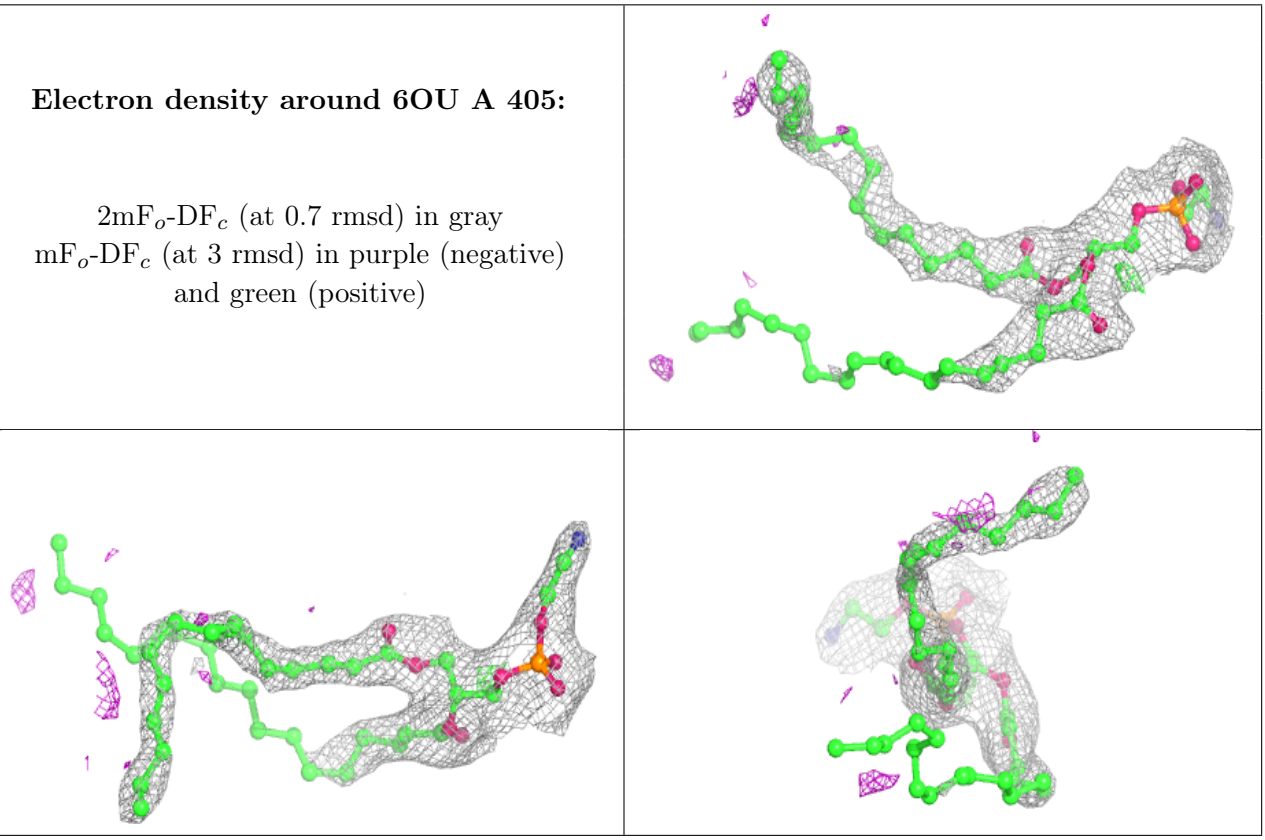
Electron density around 6OU A 401:

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



Electron density around 6OU A 405:

$2mF_o$-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.