



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 09:42 PM EDT

PDB ID : 6D26
Title : Crystal structure of the prostaglandin D2 receptor CRTH2 with fevipiprant
Authors : Wang, L.; Yao, D.; Deepak, K.; Liu, H.; Gong, W.; Fan, H.; Wei, Z.; Zhang, C.
Deposited on : 2018-04-13
Resolution : 2.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

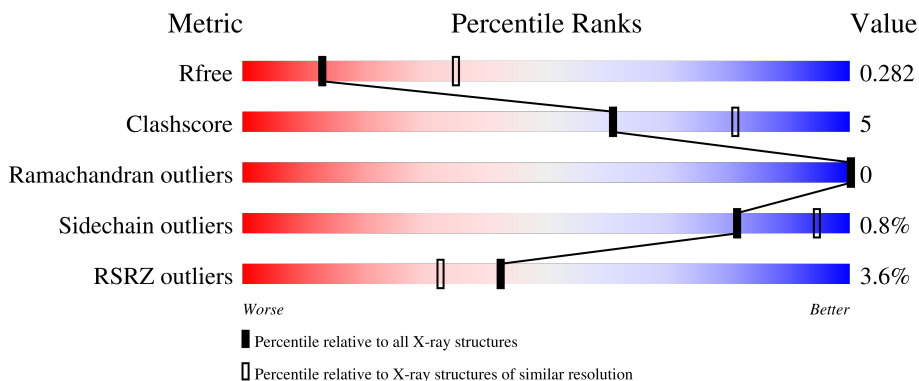
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	470	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SIN	A	2414	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3650 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.

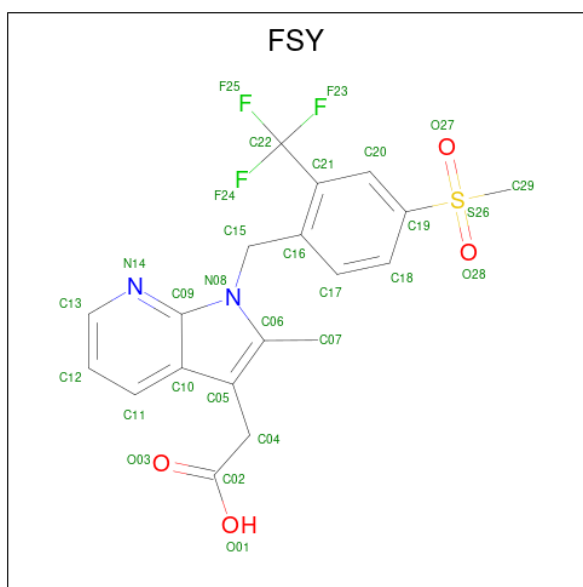
- Molecule 1 is a protein called Prostaglandin D2 receptor 2, Endolysin chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3498	2254	634	592	18	0	1	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q9Y5Y4
A	25	ALA	ASN	engineered mutation	UNP Q9Y5Y4
A	204	ALA	VAL	variant	UNP Q9Y5Y4
A	1238	ALA	-	insertion	UNP Q9Y5Y4
A	1239	ASP	-	insertion	UNP Q9Y5Y4
A	1240	LEU	-	insertion	UNP Q9Y5Y4
A	1241	GLY	-	insertion	UNP Q9Y5Y4
A	1242	LEU	-	insertion	UNP Q9Y5Y4
A	1243	GLN	-	insertion	UNP Q9Y5Y4
A	1244	HIS	-	insertion	UNP Q9Y5Y4
A	1245	ARG	-	insertion	UNP Q9Y5Y4
A	1257	GLY	-	insertion	UNP D9IEF7
A	1258	GLY	-	insertion	UNP D9IEF7
A	1259	SER	-	insertion	UNP D9IEF7
A	1260	GLY	-	insertion	UNP D9IEF7
A	1261	GLY	-	insertion	UNP D9IEF7
A	1298	ALA	CYS	engineered mutation	UNP D9IEF7
A	2340	LEU	-	expression tag	UNP Q9Y5Y4
A	2341	GLU	-	expression tag	UNP Q9Y5Y4
A	2342	VAL	-	expression tag	UNP Q9Y5Y4
A	2343	LEU	-	expression tag	UNP Q9Y5Y4
A	2344	PHE	-	expression tag	UNP Q9Y5Y4
A	2345	GLN	-	expression tag	UNP Q9Y5Y4

- Molecule 2 is fevipiprant (three-letter code: FSY) (formula: $C_{19}H_{17}F_3N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
2	A	1	29	19	3	2	4	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



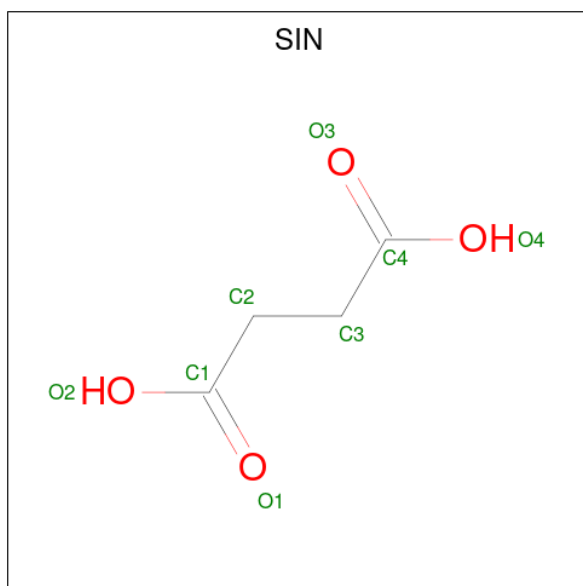
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O S		
3	A	1	5	4 1	0	0
3	A	1	5	4 1	0	0
3	A	1	5	4 1	0	0

Continued on next page...

Continued from previous page...

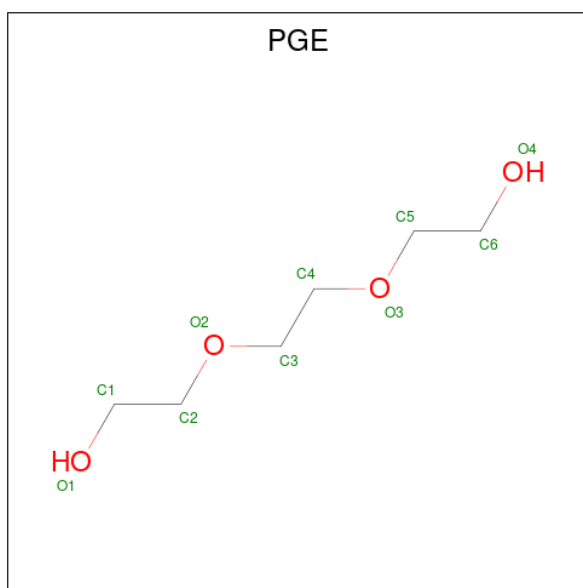
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is SUCCINIC ACID (three-letter code: SIN) (formula: C₄H₆O₄).



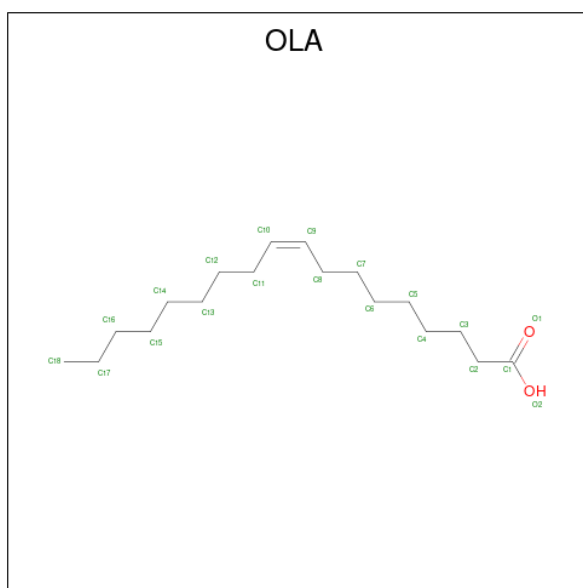
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 4 4	0	0
4	A	1	Total C O 8 4 4	0	0
4	A	1	Total C O 8 4 4	0	0
4	A	1	Total C O 8 4 4	0	0
4	A	1	Total C O 8 4 4	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



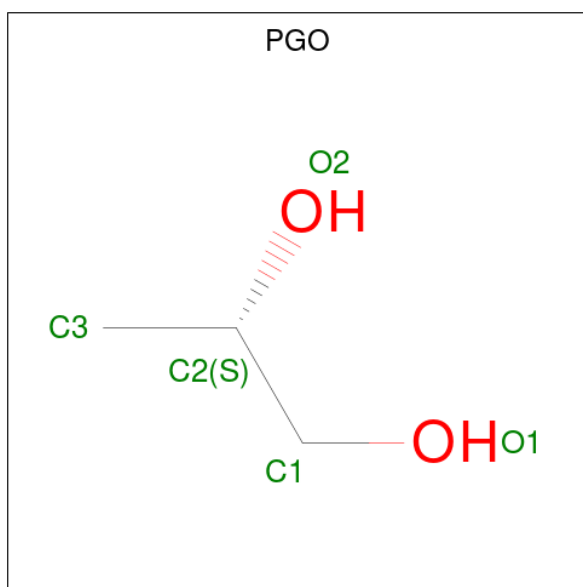
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			20	18	2		

- Molecule 7 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			5	3	2		

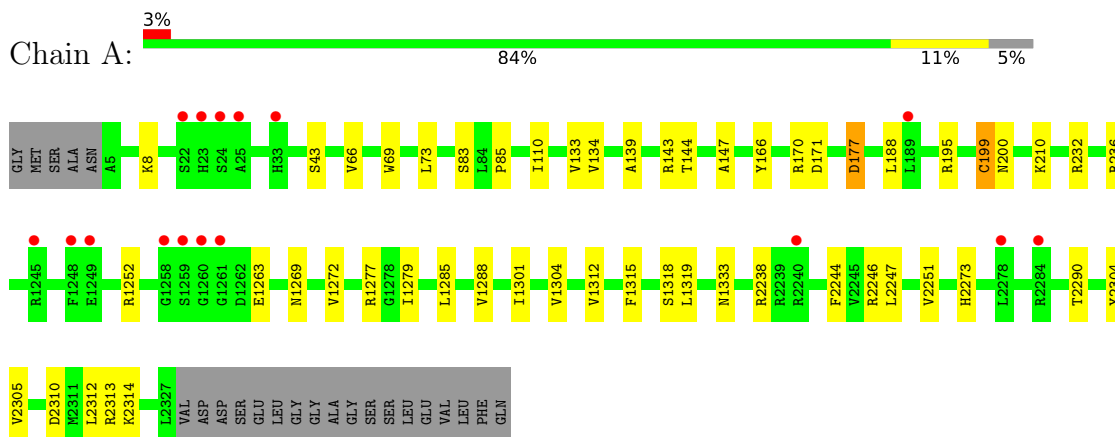
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	O	0	0
			3	3		

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: Prostaglandin D2 receptor 2, Endolysin chimera



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.46Å 61.71Å 266.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.33 – 2.80 29.33 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (29.33-2.80) 84.6 (29.33-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.80Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.250 , 0.280 0.254 , 0.282	Depositor DCC
R_{free} test set	979 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtrriage
Anisotropy	0.763	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3650	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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: PGE, PGO, SO4, YCM, SIN, FSY, OLA

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	0.21	0/3570	0.36	0/4853

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	3498	0	3565	33	0
2	A	29	0	0	2	0
3	A	45	0	0	3	0
4	A	40	0	20	1	0
5	A	10	0	14	0	0
6	A	20	0	33	0	0
7	A	5	0	8	0	0
8	A	3	0	0	0	0
All	All	3650	0	3640	33	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 (33) 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:2246:ARG:HH22	4:A:2412:SIN:H31	1.61	0.65
1:A:170:ARG:NH2	2:A:2401:FSY:O03	2.29	0.64
1:A:1318:SER:OG	1:A:1333:ASN:ND2	2.32	0.62
1:A:2305:VAL:HG13	1:A:2312:LEU:HB2	1.83	0.60
1:A:1315:PHE:HB3	1:A:1318:SER:HB2	1.87	0.55
1:A:2247:LEU:HD11	1:A:2304:TYR:HD1	1.70	0.55
1:A:1252:ARG:HB2	1:A:2238:ARG:NH1	2.25	0.52
1:A:133:VAL:O	1:A:236:ARG:NH2	2.43	0.52
1:A:1263:GLU:O	1:A:1269:ASN:ND2	2.43	0.50
1:A:2247:LEU:HD11	1:A:2304:TYR:CD1	2.45	0.50
1:A:43:SER:HB3	1:A:85:PRO:HG3	1.94	0.49
1:A:1279:ILE:HG23	1:A:1285:LEU:HB3	1.95	0.48
1:A:139:ALA:O	1:A:143:ARG:HB2	2.13	0.48
1:A:66:VAL:HA	1:A:69:TRP:HD1	1.79	0.48
1:A:1288:VAL:HG21	1:A:1319:LEU:HB3	1.95	0.47
1:A:1333:ASN:ND2	3:A:2403:SO4:O4	2.47	0.47
1:A:1272:VAL:HG13	1:A:1301:ILE:HG21	1.97	0.46
1:A:73:LEU:HD21	1:A:2251:VAL:HG11	1.98	0.46
1:A:195:ARG:O	1:A:199:CYS:HB2	2.16	0.46
1:A:134:VAL:O	1:A:232:ARG:NH1	2.49	0.45
1:A:177:ASP:N	1:A:177:ASP:OD1	2.48	0.45
1:A:1304:VAL:HG12	1:A:1312:VAL:HG21	1.97	0.45
1:A:171:ASP:HB2	1:A:188:LEU:HD22	1.99	0.45
1:A:2244:PHE:N	3:A:2404:SO4:O2	2.41	0.45
1:A:8:LYS:NZ	1:A:171:ASP:OD2	2.40	0.44
1:A:83:SER:HB3	1:A:110:ILE:HD12	2.00	0.44
1:A:2290:THR:HG21	2:A:2401:FSY:C06	2.48	0.43
1:A:144:THR:HG23	1:A:147:ALA:H	1.82	0.43
1:A:1277:ARG:NH1	3:A:2409:SO4:O1	2.52	0.42
1:A:2310:ASP:OD1	1:A:2313:ARG:NH2	2.45	0.41
1:A:200:ASN:HB2	1:A:2273:HIS:CD2	2.56	0.41
1:A:143:ARG:HE	1:A:143:ARG:HB3	1.73	0.40
1:A:166:TYR:OH	1:A:210:LYS:HB2	2.22	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	445/470 (95%)	429 (96%)	16 (4%)	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	366/389 (94%)	363 (99%)	3 (1%)	81 94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ASP
1	A	199	CYS
1	A	2314	LYS

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](#)

1 non-standard protein/DNA/RNA residue is 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
1	YCM	A	2308	1	7,9,10	1.07	0	4,10,12	0.46	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
1	YCM	A	2308	1	-	0/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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	SO4	A	2409	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	2404	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	A	2403	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	A	2405	-	4,4,4	0.14	0	6,6,6	0.05	0
7	PGO	A	2418	-	3,4,4	0.25	0	1,4,4	0.19	0
2	FSY	A	2401	-	29,31,31	2.15	11 (37%)	40,48,48	1.67	8 (20%)
3	SO4	A	2407	-	4,4,4	0.14	0	6,6,6	0.11	0
4	SIN	A	2412	-	7,7,7	1.01	0	8,8,8	1.71	3 (37%)
4	SIN	A	2411	-	7,7,7	1.02	0	8,8,8	1.71	2 (25%)
4	SIN	A	2415	-	7,7,7	1.02	0	8,8,8	1.70	2 (25%)
4	SIN	A	2413	-	7,7,7	1.03	0	8,8,8	1.69	1 (12%)
6	OLA	A	2417	-	19,19,19	0.78	1 (5%)	19,19,19	0.95	1 (5%)
4	SIN	A	2414	-	7,7,7	1.01	0	8,8,8	1.69	3 (37%)
5	PGE	A	2416	-	9,9,9	0.31	0	8,8,8	0.31	0
3	SO4	A	2406	-	4,4,4	0.13	0	6,6,6	0.06	0
3	SO4	A	2410	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	A	2408	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	A	2402	-	4,4,4	0.14	0	6,6,6	0.08	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
7	PGO	A	2418	-	-	0/2/2/2	-
2	FSY	A	2401	-	-	5/20/20/20	0/3/3/3
4	SIN	A	2411	-	-	2/5/5/5	-
4	SIN	A	2415	-	-	0/5/5/5	-
4	SIN	A	2413	-	-	4/5/5/5	-
4	SIN	A	2414	-	-	4/5/5/5	-
5	PGE	A	2416	-	-	4/7/7/7	-
6	OLA	A	2417	-	-	13/17/17/17	-
4	SIN	A	2412	-	-	3/5/5/5	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2401	FSY	C19-S26	4.45	1.81	1.77
2	A	2401	FSY	C06-N08	-4.43	1.30	1.39
2	A	2401	FSY	O27-S26	4.37	1.56	1.44
2	A	2401	FSY	C15-C16	3.60	1.58	1.51
2	A	2401	FSY	C15-N08	-3.48	1.42	1.48
2	A	2401	FSY	F25-C22	2.90	1.43	1.32
6	A	2417	OLA	C10-C9	2.69	1.47	1.31
2	A	2401	FSY	O28-S26	2.49	1.51	1.44
2	A	2401	FSY	C07-C06	2.44	1.54	1.49
2	A	2401	FSY	C04-C05	2.17	1.58	1.51
2	A	2401	FSY	C10-C09	-2.08	1.38	1.43
2	A	2401	FSY	C12-C11	2.05	1.41	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2401	FSY	O28-S26-O27	-4.62	109.97	117.92
2	A	2401	FSY	C29-S26-C19	3.93	109.22	104.58
2	A	2401	FSY	C13-N14-C09	3.62	121.26	116.77
2	A	2401	FSY	C22-C21-C16	2.76	124.31	121.22
2	A	2401	FSY	C05-C06-N08	2.66	109.27	106.86
2	A	2401	FSY	F24-C22-C21	-2.40	108.51	112.70
4	A	2412	SIN	C3-C2-C1	-2.25	108.77	113.60
2	A	2401	FSY	F23-C22-C21	-2.23	108.82	112.70
4	A	2412	SIN	O4-C4-C3	2.14	120.91	114.03
4	A	2411	SIN	O4-C4-C3	2.14	120.89	114.03
2	A	2401	FSY	C12-C13-N14	-2.09	120.73	123.94
4	A	2413	SIN	C2-C3-C4	-2.09	109.11	113.60
6	A	2417	OLA	O2-C1-C2	2.04	120.60	114.03
4	A	2411	SIN	C2-C3-C4	-2.04	109.22	113.60
4	A	2415	SIN	C3-C2-C1	-2.03	109.23	113.60
4	A	2415	SIN	O4-C4-C3	2.02	120.52	114.03
4	A	2414	SIN	O2-C1-C2	2.02	120.50	114.03
4	A	2414	SIN	O4-C4-C3	2.01	120.49	114.03
4	A	2414	SIN	C3-C2-C1	-2.01	109.28	113.60
4	A	2412	SIN	O2-C1-C2	2.00	120.47	114.03

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2417	OLA	C1-C2-C3-C4
4	A	2412	SIN	C1-C2-C3-C4
6	A	2417	OLA	C3-C4-C5-C6
5	A	2416	PGE	O2-C3-C4-O3
2	A	2401	FSY	C16-C21-C22-F23
6	A	2417	OLA	C12-C13-C14-C15
6	A	2417	OLA	C11-C12-C13-C14
2	A	2401	FSY	C16-C21-C22-F24
2	A	2401	FSY	C16-C21-C22-F25
6	A	2417	OLA	C11-C10-C9-C8
6	A	2417	OLA	C4-C5-C6-C7
5	A	2416	PGE	C4-C3-O2-C2
6	A	2417	OLA	C14-C15-C16-C17
5	A	2416	PGE	O1-C1-C2-O2
6	A	2417	OLA	C10-C11-C12-C13
4	A	2414	SIN	O2-C1-C2-C3
4	A	2414	SIN	C2-C3-C4-O3
4	A	2413	SIN	O2-C1-C2-C3
4	A	2414	SIN	C2-C3-C4-O4
4	A	2413	SIN	O1-C1-C2-C3
6	A	2417	OLA	C5-C6-C7-C8
4	A	2414	SIN	O1-C1-C2-C3
6	A	2417	OLA	C7-C8-C9-C10
4	A	2412	SIN	C2-C3-C4-O4
6	A	2417	OLA	O2-C1-C2-C3
5	A	2416	PGE	C3-C4-O3-C5
4	A	2413	SIN	C2-C3-C4-O4
2	A	2401	FSY	N08-C15-C16-C17
4	A	2412	SIN	C2-C3-C4-O3
6	A	2417	OLA	C9-C10-C11-C12
6	A	2417	OLA	O1-C1-C2-C3
2	A	2401	FSY	C20-C21-C22-F23
4	A	2411	SIN	O2-C1-C2-C3
4	A	2413	SIN	C2-C3-C4-O3
4	A	2411	SIN	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 6 short contacts:

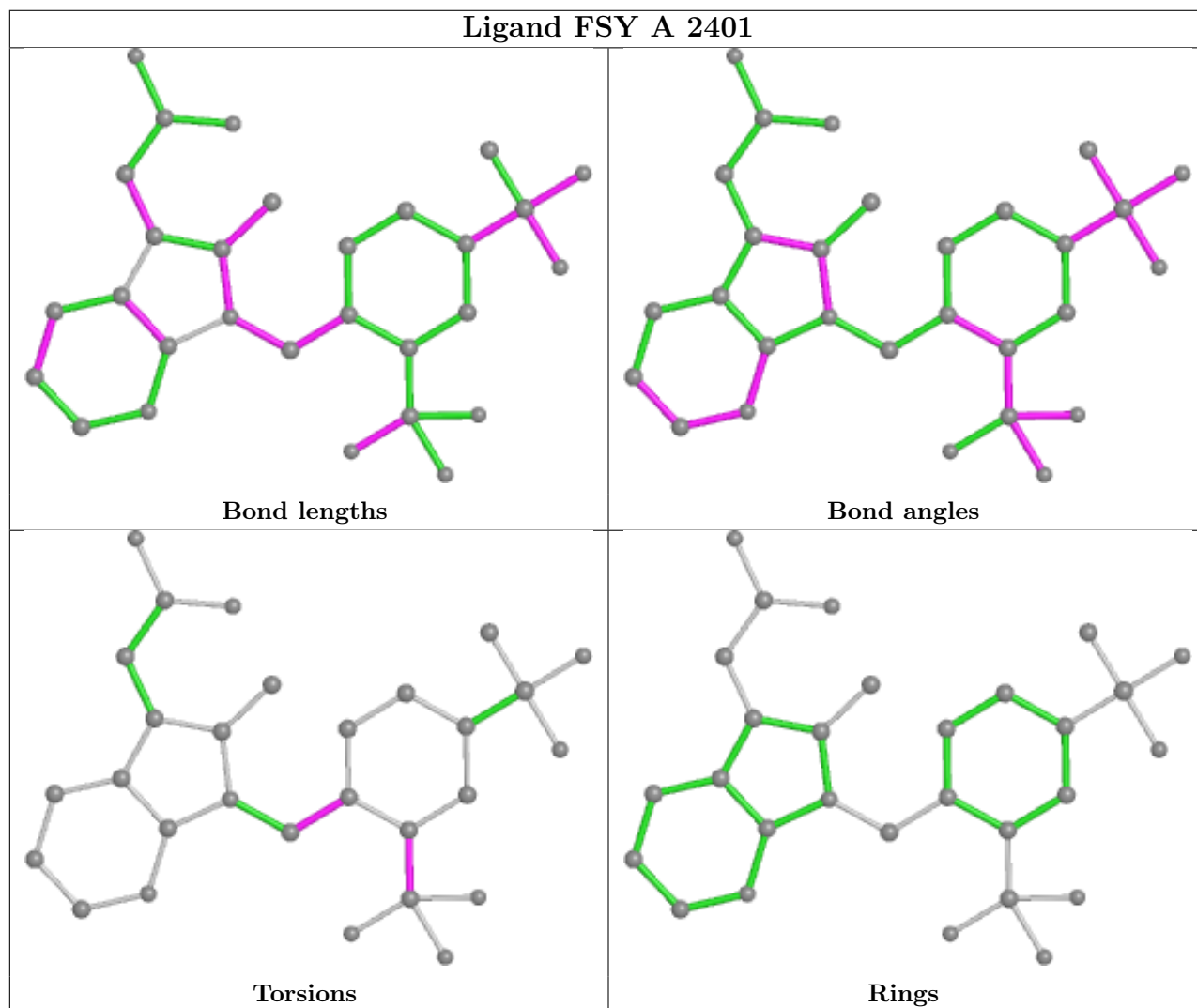
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2409	SO4	1	0
3	A	2404	SO4	1	0
3	A	2403	SO4	1	0

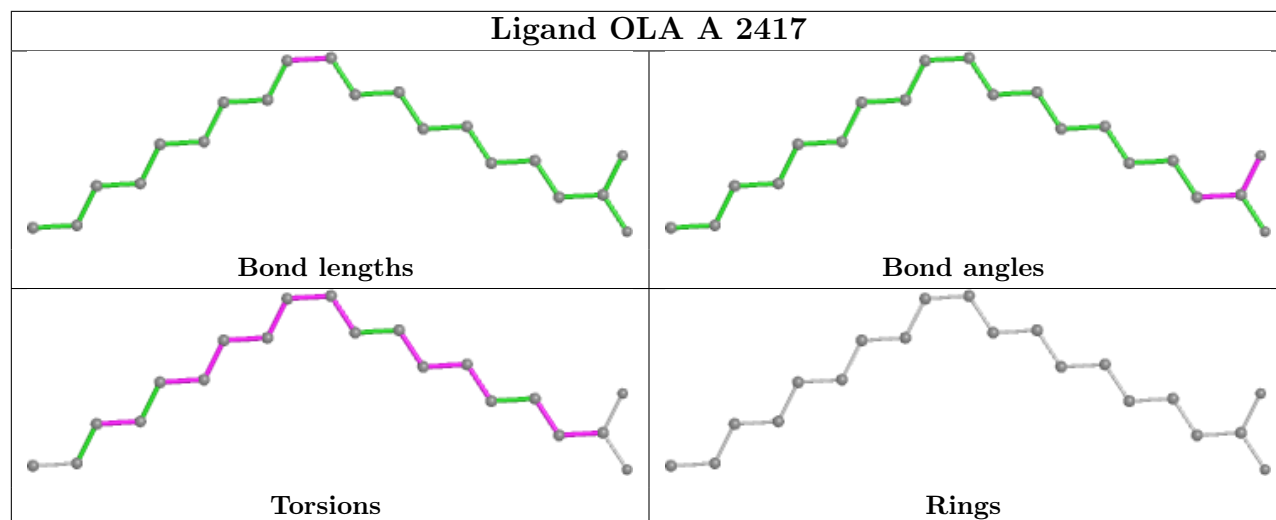
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2401	FSY	2	0
4	A	2412	SIN	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.





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	446/470 (94%)	0.28	16 (3%) 42 32	50, 78, 135, 175	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1261	GLY	5.2
1	A	1260	GLY	5.1
1	A	25	ALA	5.1
1	A	2284	ARG	4.6
1	A	24	SER	4.1
1	A	1245	ARG	4.0
1	A	2278	LEU	3.7
1	A	22	SER	3.6
1	A	1259	SER	3.2
1	A	189	LEU	3.1
1	A	1249	GLU	2.6
1	A	23	HIS	2.4
1	A	1258	GLY	2.2
1	A	1248	PHE	2.1
1	A	33	HIS	2.0
1	A	2240	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	YCM	A	2308	10/11	0.96	0.14	61,66,94,98	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

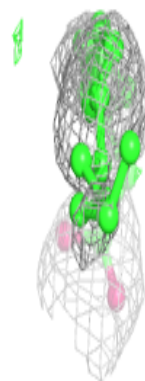
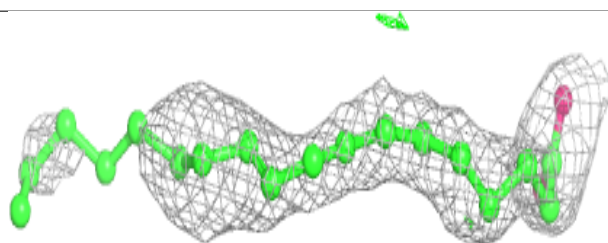
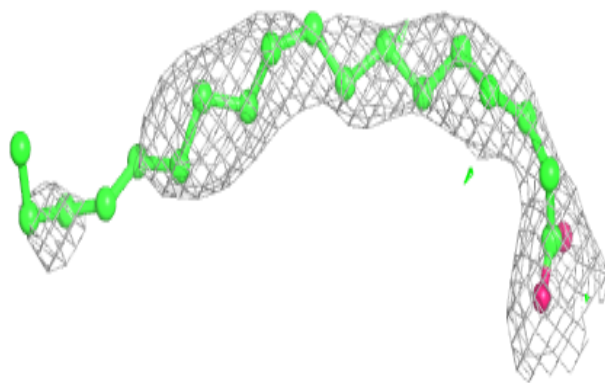
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SIN	A	2414	8/8	0.59	0.50	100,105,106,106	0
4	SIN	A	2413	8/8	0.62	0.29	112,115,120,123	0
3	SO4	A	2408	5/5	0.68	0.33	164,166,167,168	0
6	OLA	A	2417	20/20	0.75	0.39	80,86,102,102	0
5	PGE	A	2416	10/10	0.79	0.37	107,108,113,113	0
4	SIN	A	2415	8/8	0.84	0.34	103,109,111,112	0
7	PGO	A	2418	5/5	0.87	0.29	83,84,84,86	0
3	SO4	A	2409	5/5	0.88	0.28	160,160,160,161	0
3	SO4	A	2405	5/5	0.89	0.32	69,71,72,72	5
4	SIN	A	2411	8/8	0.90	0.28	91,93,101,104	0
3	SO4	A	2410	5/5	0.92	0.22	66,68,74,74	5
3	SO4	A	2403	5/5	0.92	0.13	90,91,93,100	0
4	SIN	A	2412	8/8	0.93	0.11	71,78,81,82	0
3	SO4	A	2407	5/5	0.94	0.15	84,90,92,94	0
2	FSY	A	2401	29/29	0.95	0.21	43,64,95,96	0
3	SO4	A	2404	5/5	0.98	0.10	63,65,72,72	0
3	SO4	A	2402	5/5	0.98	0.12	67,67,69,70	0
3	SO4	A	2406	5/5	0.98	0.13	87,88,92,97	0

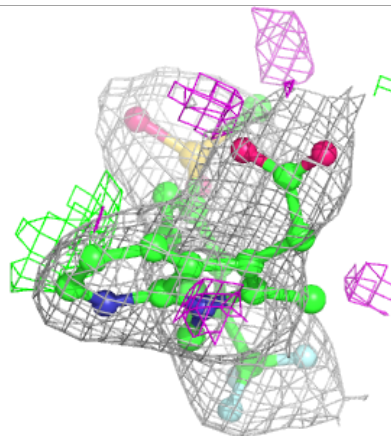
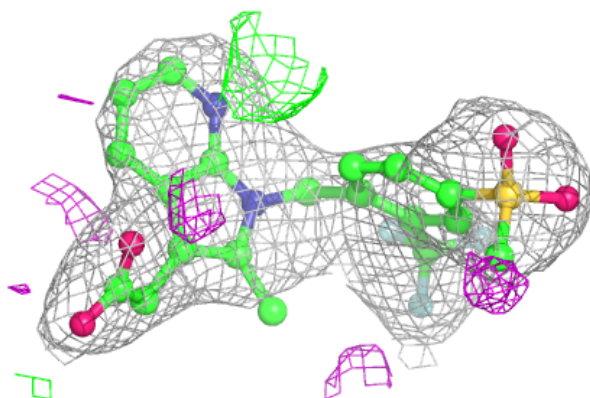
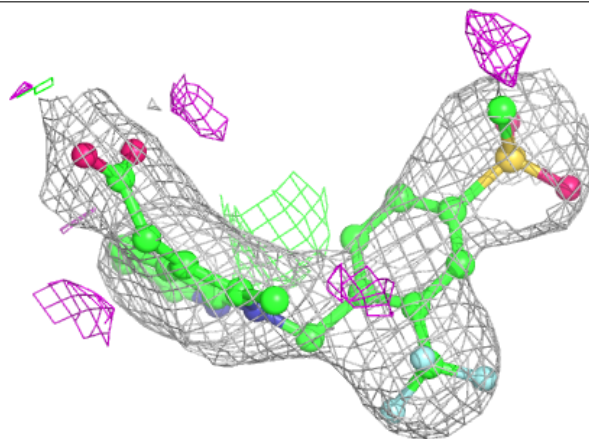
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 2417:

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

**Electron density around FSY A 2401:**

$2mF_o-DF_c$ (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.