Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:53 AM EDT

PDB ID	:	7M8W
Title	:	XFEL crystal structure of the prostaglandin D2 receptor CRTH2 in complex with 15R-methyl-PGD2
Authors	:	Shiriaeva, A.; Han, G.W.; Cherezov, V.
Deposited on	:	2021-03-30
Resolution	:	2.61 Å(reported)

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 2.61 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.
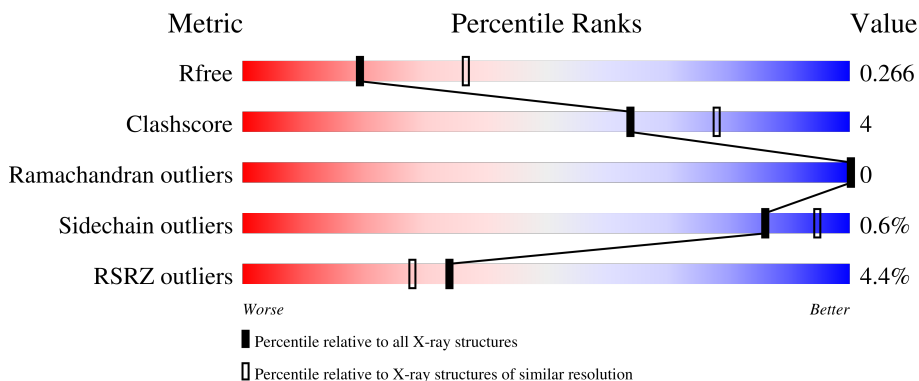
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	470	

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 3501 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	437	3424	2210	624	573	17	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	900	ALA	-	linker	UNP Q9Y5Y4
A	901	ASP	-	linker	UNP Q9Y5Y4
A	902	LEU	-	linker	UNP Q9Y5Y4
A	903	GLY	-	linker	UNP Q9Y5Y4
A	904	LEU	-	linker	UNP Q9Y5Y4
A	905	GLN	-	linker	UNP Q9Y5Y4
A	906	HIS	-	linker	UNP Q9Y5Y4
A	907	ARG	-	linker	UNP Q9Y5Y4
A	1056	GLY	-	linker	UNP D9IEF7
A	1057	GLY	-	linker	UNP D9IEF7
A	1058	SER	-	linker	UNP D9IEF7
A	1059	GLY	-	linker	UNP D9IEF7
A	1060	GLY	-	linker	UNP D9IEF7
A	1097	ALA	CYS	engineered mutation	UNP D9IEF7
A	340	LEU	-	expression tag	UNP Q9Y5Y4
A	341	GLU	-	expression tag	UNP Q9Y5Y4
A	342	VAL	-	expression tag	UNP Q9Y5Y4
A	343	LEU	-	expression tag	UNP Q9Y5Y4
A	344	PHE	-	expression tag	UNP Q9Y5Y4
A	345	GLN	-	expression tag	UNP Q9Y5Y4

- Molecule 2 is 15R-methyl-prostaglandin D2 (three-letter code: YSS) (formula: $C_{21}H_{34}O_5$) (labeled as "Ligand of Interest" by depositor).
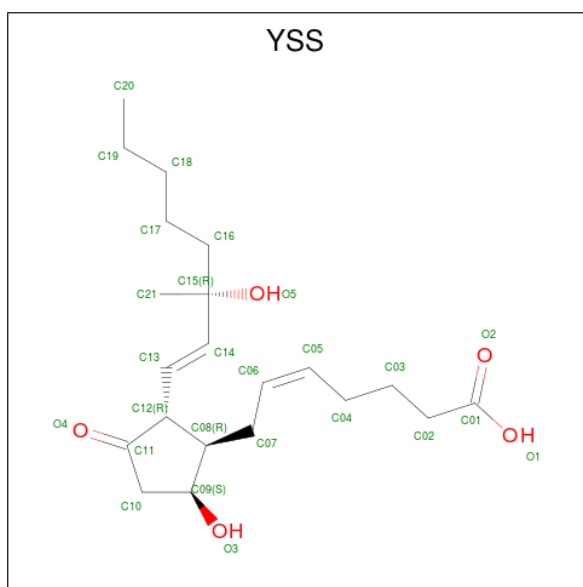
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 26	C 21	O 5	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).
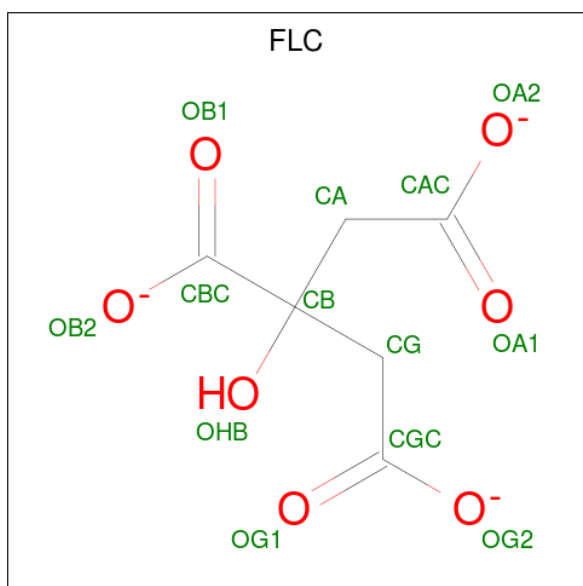
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 13	C 6	O 7	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
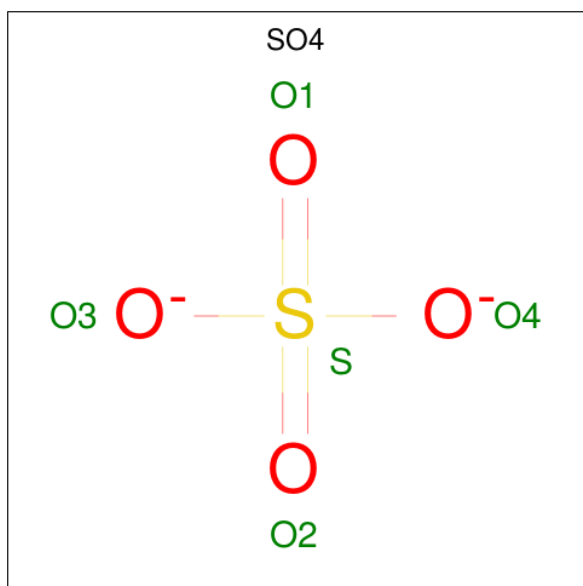
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total 12	O 12	0	0

3 Residue-property plots ⓘ

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
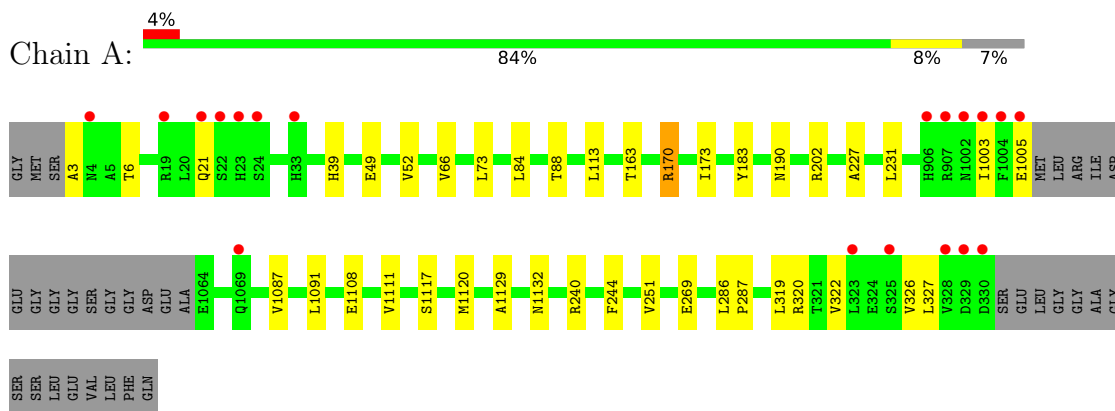
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.40Å 67.80Å 265.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.43 – 2.61 32.43 – 2.61	Depositor EDS
% Data completeness (in resolution range)	53.4 (32.43-2.61) 53.4 (32.43-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.229 , 0.267 0.232 , 0.266	Depositor DCC
R_{free} test set	781 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 71.5	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3501	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: YCM, YSS, FLC, SO4, NA

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	0.24	0/3495	0.41	0/4757

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3424	0	3495	29	0
2	A	26	0	0	1	0
3	A	1	0	0	0	0
4	A	13	0	5	1	0
5	A	25	0	0	0	0
6	A	12	0	0	0	0
All	All	3501	0	3500	29	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASN:OD1	1:A:202:ARG:NH2	2.30	0.65
1:A:1120:MET:HB2	1:A:1129:ALA:HB2	1.83	0.60
1:A:39:HIS:HB3	1:A:88:THR:HG22	1.83	0.60
1:A:3:ALA:N	1:A:6:THR:HG1	2.00	0.58
1:A:1003:ILE:HG13	1:A:1005:GLU:HG2	1.86	0.58
1:A:326:VAL:HG23	1:A:327:LEU:HD12	1.87	0.57
1:A:3:ALA:N	1:A:6:THR:OG1	2.37	0.57
1:A:1003:ILE:CG1	1:A:1005:GLU:HG2	2.38	0.54
1:A:66:VAL:HG23	4:A:2403:FLC:OB1	2.08	0.53
1:A:1003:ILE:CG1	1:A:1005:GLU:CG	2.91	0.49
1:A:73:LEU:HD21	1:A:251:VAL:HG11	1.95	0.48
1:A:1003:ILE:HD11	1:A:1005:GLU:HG3	1.96	0.47
1:A:170:ARG:NH2	2:A:2401:YSS:O2	2.48	0.46
1:A:1117:SER:OG	1:A:1132:ASN:OD1	2.34	0.46
1:A:1003:ILE:HG13	1:A:1003:ILE:O	2.16	0.46
1:A:21:GLN:O	1:A:21:GLN:HG3	2.15	0.45
1:A:1087:VAL:O	1:A:1091:LEU:HD13	2.16	0.45
1:A:183:TYR:OH	1:A:269:GLU:OE2	2.28	0.45
1:A:319:LEU:HD23	1:A:320:ARG:HH21	1.82	0.44
1:A:66:VAL:HG11	1:A:244:PHE:CD2	2.53	0.44
1:A:319:LEU:O	1:A:322:VAL:HG12	2.17	0.44
1:A:39:HIS:CB	1:A:88:THR:HG22	2.45	0.43
1:A:227:ALA:O	1:A:231:LEU:HD13	2.18	0.43
1:A:1108:GLU:HA	1:A:1111:VAL:HG22	2.00	0.43
1:A:49:GLU:O	1:A:52:VAL:HG22	2.19	0.42
1:A:84:LEU:O	1:A:88:THR:HG23	2.20	0.42
1:A:173:ILE:HD12	1:A:173:ILE:N	2.35	0.41
1:A:286:LEU:N	1:A:287:PRO:CD	2.83	0.41
1:A:113:LEU:HA	1:A:163:THR:HG21	2.03	0.41

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	433/470 (92%)	412 (95%)	21 (5%)	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	359/389 (92%)	357 (99%)	2 (1%)	86	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	ARG
1	A	240	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	308	1	7,9,10	1.08	0	4,10,12	0.37	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	308	1	-	2/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	308	YCM	CE-CD-SG-CB
1	A	308	YCM	SG-CD-CE-NZ2

There are no ring outliers.

No monomer is involved in short contacts.

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	SO4	A	2404	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	A	2405	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	A	2408	-	4,4,4	0.14	0	6,6,6	0.07	0
2	YSS	A	2401	-	26,26,26	2.11	10 (38%)	25,34,34	1.94	3 (12%)
4	FLC	A	2403	-	12,12,12	1.36	1 (8%)	17,17,17	0.53	0
5	SO4	A	2406	-	4,4,4	0.13	0	6,6,6	0.05	0
5	SO4	A	2407	-	4,4,4	0.15	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
4	FLC	A	2403	-	-	9/16/16/16	-
2	YSS	A	2401	-	-	7/21/37/37	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2401	YSS	C12-C11	-4.44	1.47	1.53
4	A	2403	FLC	CB-CBC	3.89	1.57	1.53
2	A	2401	YSS	C08-C09	3.66	1.58	1.53
2	A	2401	YSS	C10-C11	-3.66	1.45	1.51
2	A	2401	YSS	O4-C11	3.42	1.27	1.21
2	A	2401	YSS	C10-C09	3.33	1.56	1.52
2	A	2401	YSS	C15-C14	3.03	1.55	1.51
2	A	2401	YSS	C02-C01	2.45	1.56	1.50
2	A	2401	YSS	C13-C14	2.39	1.37	1.31
2	A	2401	YSS	C08-C12	-2.34	1.52	1.55
2	A	2401	YSS	C16-C15	2.21	1.56	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2401	YSS	C15-C14-C13	-7.46	115.85	127.11
2	A	2401	YSS	C21-C15-C14	-3.32	103.47	110.83
2	A	2401	YSS	C07-C06-C05	-2.49	117.16	126.40

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2401	YSS	C21-C15-C16-C17
4	A	2403	FLC	CAC-CA-CB-CBC
4	A	2403	FLC	CAC-CA-CB-CG
4	A	2403	FLC	CAC-CA-CB-OHB
4	A	2403	FLC	CG-CB-CBC-OB1
4	A	2403	FLC	CG-CB-CBC-OB2
4	A	2403	FLC	OHB-CB-CBC-OB1
4	A	2403	FLC	OHB-CB-CBC-OB2
2	A	2401	YSS	C16-C17-C18-C19
2	A	2401	YSS	C05-C06-C07-C08
2	A	2401	YSS	C11-C12-C13-C14
2	A	2401	YSS	C14-C15-C16-C17
4	A	2403	FLC	CB-CG-CGC-OG1
2	A	2401	YSS	C13-C14-C15-C21
2	A	2401	YSS	C13-C14-C15-O5
4	A	2403	FLC	CB-CG-CGC-OG2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2401	YSS	1	0
4	A	2403	FLC	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 YSS A 2401

Bond lengths

Bond angles

Torsions

Rings
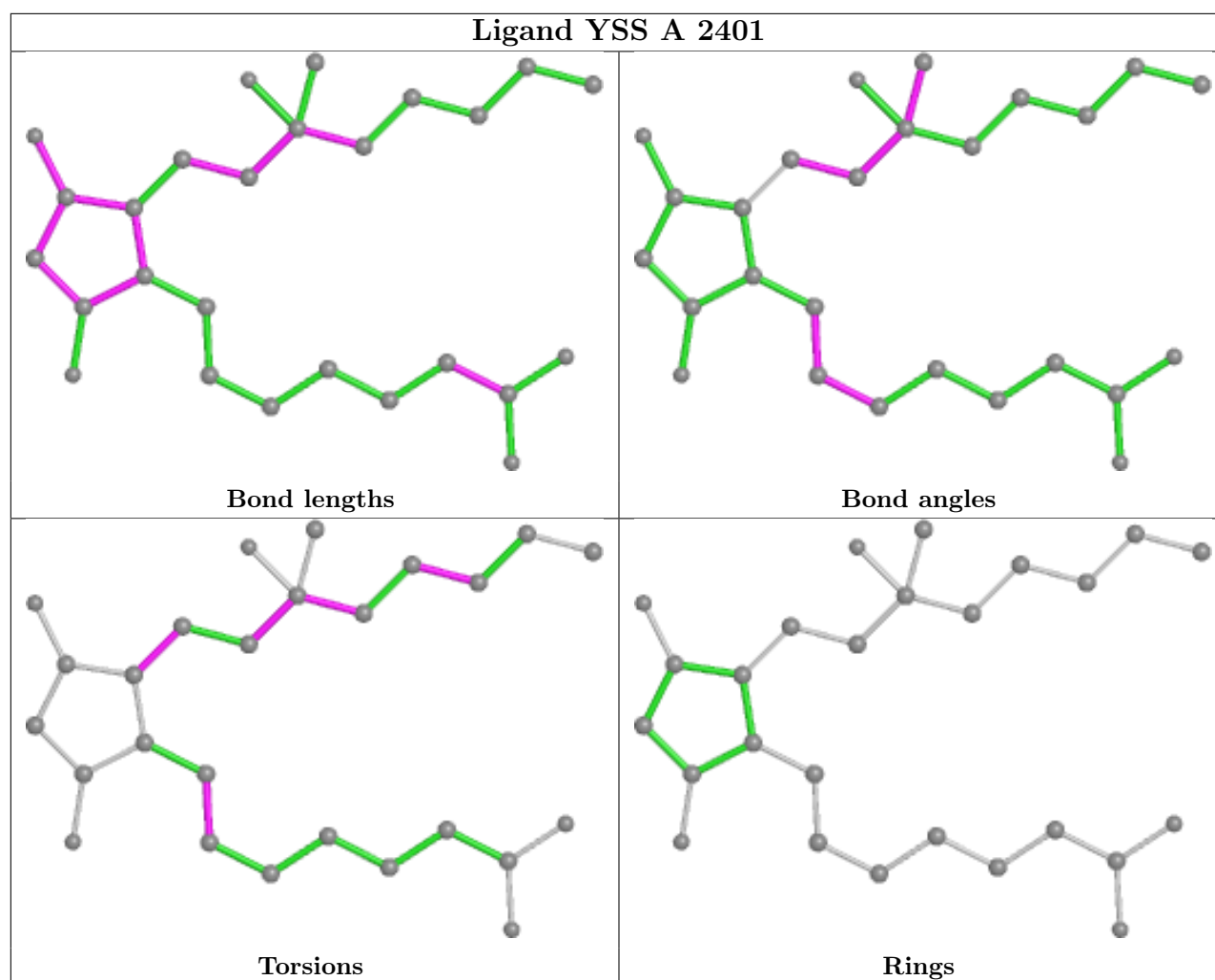
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	436/470 (92%)	-0.27	19 (4%)	34	28	18, 47, 101, 145	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1003	ILE	8.9
1	A	1005	GLU	8.0
1	A	328	VAL	7.1
1	A	21	GLN	6.4
1	A	1004	PHE	5.5
1	A	24	SER	5.1
1	A	329	ASP	5.0
1	A	23	HIS	4.1
1	A	22	SER	4.1
1	A	330	ASP	4.0
1	A	906	HIS	3.7
1	A	1069	GLN	3.3
1	A	907	ARG	3.2
1	A	4	ASN	2.9
1	A	19	ARG	2.8
1	A	325	SER	2.6
1	A	323	LEU	2.5
1	A	1002	ASN	2.1
1	A	33	HIS	2.0

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

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.

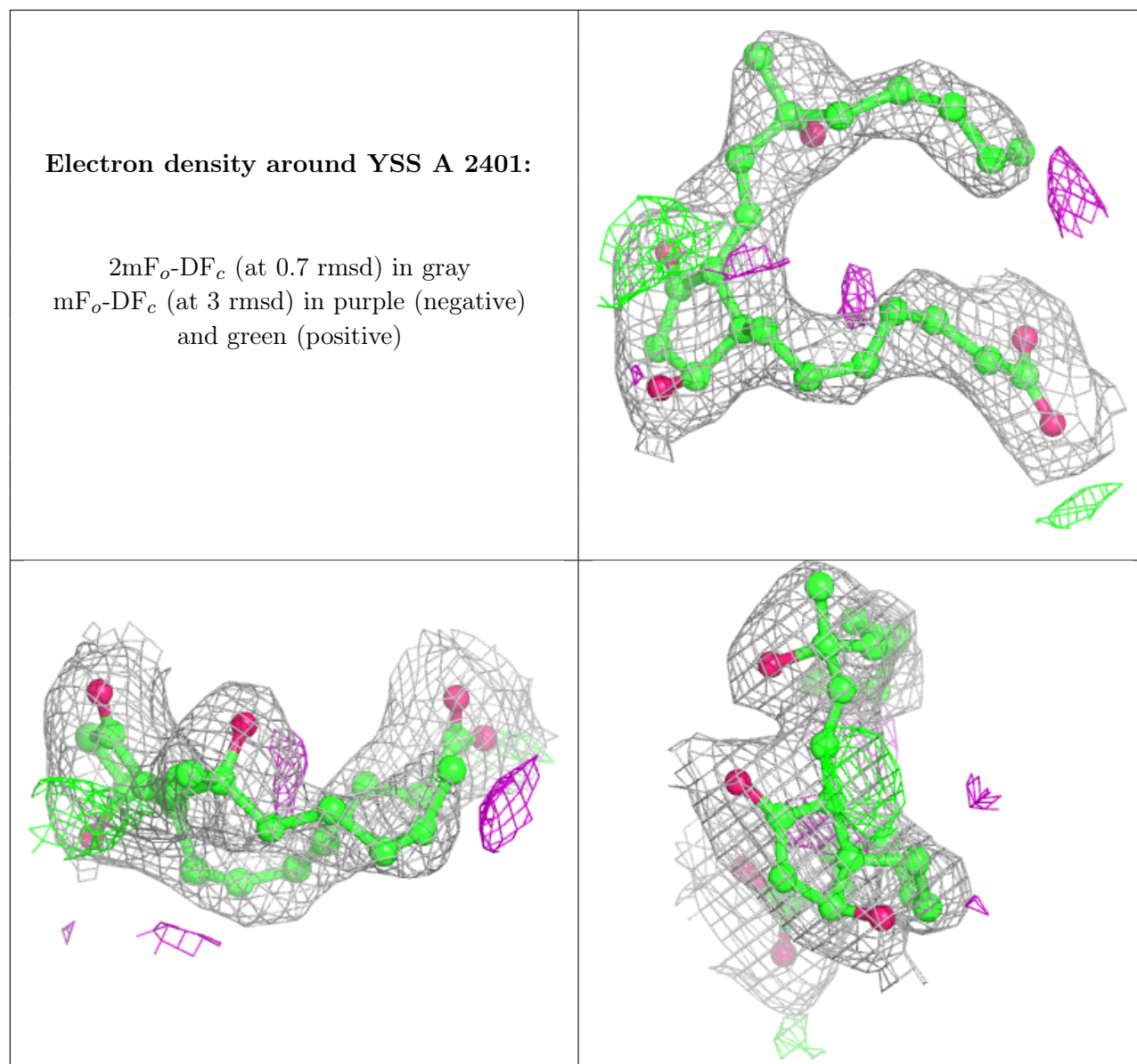| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
1	YCM	A	308	10/11	0.97	0.12	28,44,58,65	0

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($\mathring{A}^2$)	Q<0.9
4	FLC	A	2403	13/13	0.79	0.26	69,95,114,114	0
5	SO4	A	2406	5/5	0.86	0.31	100,103,114,137	0
5	SO4	A	2408	5/5	0.87	0.43	107,116,131,139	0
5	SO4	A	2407	5/5	0.93	0.10	76,79,86,99	0
2	YSS	A	2401	26/26	0.96	0.22	25,35,47,55	0
3	NA	A	2402	1/1	0.98	0.24	31,31,31,31	0
5	SO4	A	2405	5/5	0.99	0.09	52,61,64,67	0
5	SO4	A	2404	5/5	0.99	0.11	46,48,59,62	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 YSS 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 ⓘ

There are no such residues in this entry.