



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 06:33 PM EDT

PDB ID : 4J95
Title : Crystal Structure of FGF Receptor 2 (FGFR2) Kinase Domain Harboring the Pathogenic K659N Mutation Responsible for an Unclassified Craniosynostosis Syndrome in Space Group C2.
Authors : Chen, H.; Mohammadi, M.
Deposited on : 2013-02-15
Resolution : 2.38 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

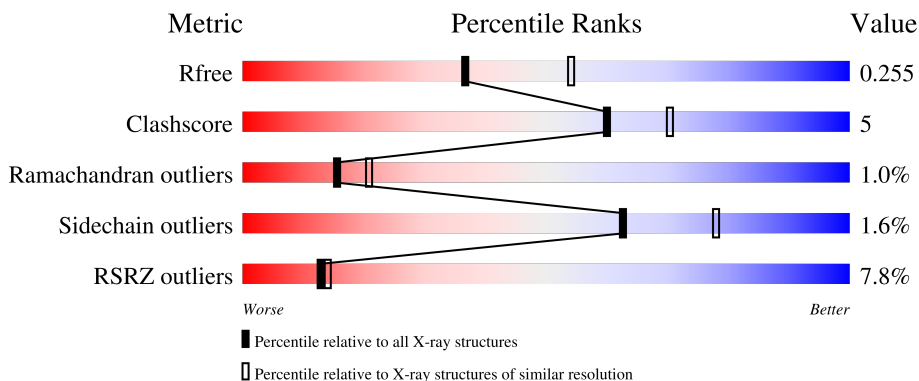
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	324	 4% 75% 11% 14%
1	B	324	 2% 75% 11% 13%
1	C	324	 10% 74% 12% 13%
1	D	324	 10% 73% 10% 16%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9059 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 Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	279	2196	1401	368	405	22	0	2	0
1	B	282	2232	1424	377	408	23	0	3	0
1	C	281	2218	1414	377	407	20	0	0	0
1	D	271	2147	1367	365	394	21	0	1	0

There are 60 discrepancies between the modelled and reference sequences:

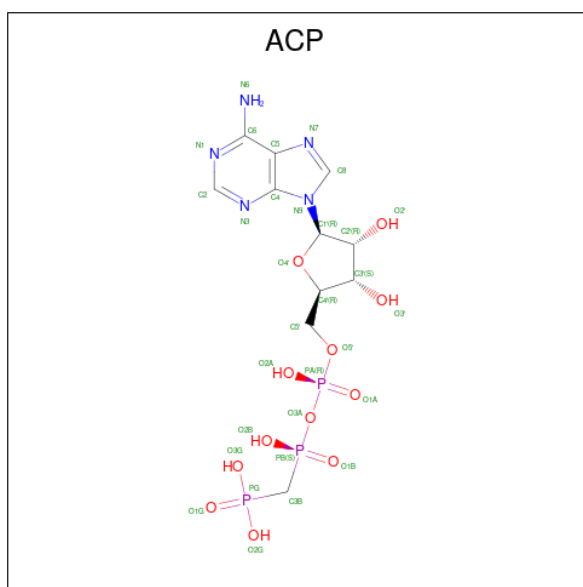
Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	expression tag	UNP P21802
A	446	GLY	-	expression tag	UNP P21802
A	447	SER	-	expression tag	UNP P21802
A	448	SER	-	expression tag	UNP P21802
A	449	HIS	-	expression tag	UNP P21802
A	450	HIS	-	expression tag	UNP P21802
A	451	HIS	-	expression tag	UNP P21802
A	452	HIS	-	expression tag	UNP P21802
A	453	HIS	-	expression tag	UNP P21802
A	454	HIS	-	expression tag	UNP P21802
A	455	SER	-	expression tag	UNP P21802
A	456	GLN	-	expression tag	UNP P21802
A	457	ASP	-	expression tag	UNP P21802
A	491	ALA	CYS	engineered mutation	UNP P21802
A	659	ASN	LYS	engineered mutation	UNP P21802
B	445	MET	-	expression tag	UNP P21802
B	446	GLY	-	expression tag	UNP P21802
B	447	SER	-	expression tag	UNP P21802
B	448	SER	-	expression tag	UNP P21802
B	449	HIS	-	expression tag	UNP P21802
B	450	HIS	-	expression tag	UNP P21802

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	451	HIS	-	expression tag	UNP P21802
B	452	HIS	-	expression tag	UNP P21802
B	453	HIS	-	expression tag	UNP P21802
B	454	HIS	-	expression tag	UNP P21802
B	455	SER	-	expression tag	UNP P21802
B	456	GLN	-	expression tag	UNP P21802
B	457	ASP	-	expression tag	UNP P21802
B	491	ALA	CYS	engineered mutation	UNP P21802
B	659	ASN	LYS	engineered mutation	UNP P21802
C	445	MET	-	expression tag	UNP P21802
C	446	GLY	-	expression tag	UNP P21802
C	447	SER	-	expression tag	UNP P21802
C	448	SER	-	expression tag	UNP P21802
C	449	HIS	-	expression tag	UNP P21802
C	450	HIS	-	expression tag	UNP P21802
C	451	HIS	-	expression tag	UNP P21802
C	452	HIS	-	expression tag	UNP P21802
C	453	HIS	-	expression tag	UNP P21802
C	454	HIS	-	expression tag	UNP P21802
C	455	SER	-	expression tag	UNP P21802
C	456	GLN	-	expression tag	UNP P21802
C	457	ASP	-	expression tag	UNP P21802
C	491	ALA	CYS	engineered mutation	UNP P21802
C	659	ASN	LYS	engineered mutation	UNP P21802
D	445	MET	-	expression tag	UNP P21802
D	446	GLY	-	expression tag	UNP P21802
D	447	SER	-	expression tag	UNP P21802
D	448	SER	-	expression tag	UNP P21802
D	449	HIS	-	expression tag	UNP P21802
D	450	HIS	-	expression tag	UNP P21802
D	451	HIS	-	expression tag	UNP P21802
D	452	HIS	-	expression tag	UNP P21802
D	453	HIS	-	expression tag	UNP P21802
D	454	HIS	-	expression tag	UNP P21802
D	455	SER	-	expression tag	UNP P21802
D	456	GLN	-	expression tag	UNP P21802
D	457	ASP	-	expression tag	UNP P21802
D	491	ALA	CYS	engineered mutation	UNP P21802
D	659	ASN	LYS	engineered mutation	UNP P21802

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

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



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

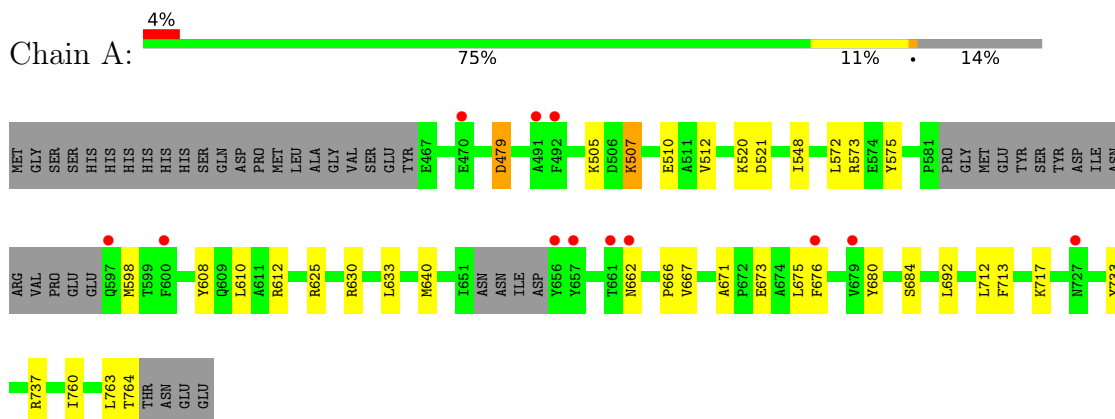
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	37	Total	O	0	0
			37	37		
4	C	19	Total	O	0	0
			19	19		
4	D	13	Total	O	0	0
			13	13		

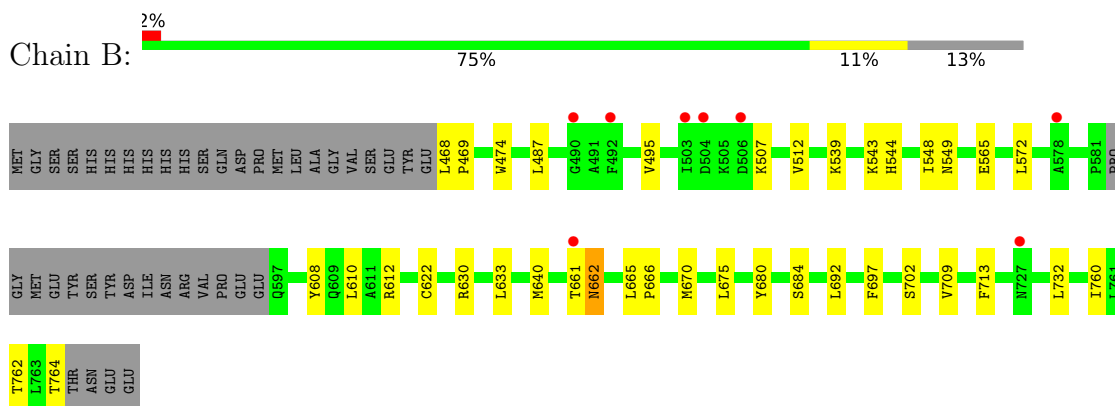
3 Residue-property plots [i](#)

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.

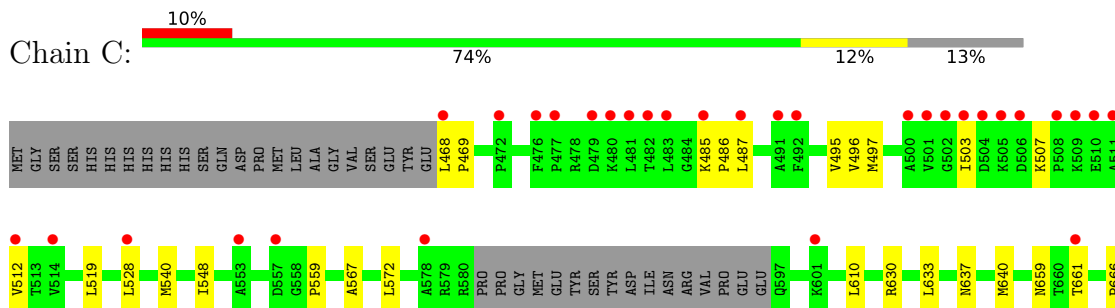
- Molecule 1: Fibroblast growth factor receptor 2



- Molecule 1: Fibroblast growth factor receptor 2

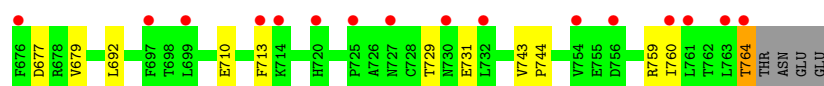
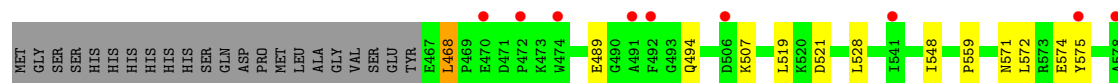
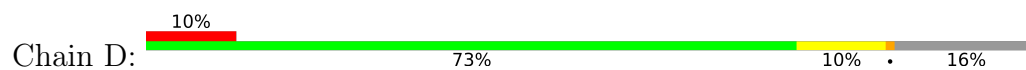


- Molecule 1: Fibroblast growth factor receptor 2





• Molecule 1: Fibroblast growth factor receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	278.63Å 78.12Å 72.79Å 90.00° 101.90° 90.00°	Depositor
Resolution (Å)	37.55 – 2.38 44.84 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.3 (37.55-2.38) 95.4 (44.84-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.08 (at 2.37Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.212 , 0.255 0.212 , 0.255	Depositor DCC
R_{free} test set	2006 reflections (3.30%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9059	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: SO4, ACP

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	0.27	0/2247	0.48	0/3040
1	B	0.28	0/2288	0.49	0/3097
1	C	0.26	0/2264	0.47	0/3063
1	D	0.26	0/2190	0.46	0/2959
All	All	0.27	0/8989	0.48	0/12159

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	2196	0	2177	21	0
1	B	2232	0	2222	19	0
1	C	2218	0	2207	23	0
1	D	2147	0	2138	22	0
2	A	31	0	14	0	0
2	B	31	0	14	1	0
2	C	31	0	14	1	0
2	D	31	0	14	0	0
3	A	10	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	15	0	0	1	0
3	D	5	0	0	1	0
4	A	38	0	0	0	0
4	B	37	0	0	0	0
4	C	19	0	0	0	0
4	D	13	0	0	0	0
All	All	9059	0	8800	81	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 (81) 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:572:LEU:HD13	1:A:640:MET:HE1	1.61	0.83
1:D:572:LEU:HD13	1:D:640:MET:HE1	1.62	0.79
1:B:468:LEU:HD12	1:B:469:PRO:HD2	1.67	0.76
1:B:630:ARG:HH22	1:B:666:PRO:HG2	1.58	0.69
1:C:572:LEU:HD13	1:C:640:MET:HE1	1.75	0.68
1:D:519:LEU:HD11	1:D:528:LEU:HD13	1.76	0.68
1:B:608:TYR:CZ	1:B:612:ARG:HD2	2.29	0.67
1:A:675:LEU:HD21	1:A:713:PHE:HD1	1.60	0.67
1:C:630:ARG:NH2	1:C:666:PRO:HG2	2.10	0.67
1:D:610:LEU:HD13	1:D:692:LEU:HD21	1.80	0.63
1:C:726:ALA:O	1:C:728:CYS:N	2.30	0.63
1:B:572:LEU:HD13	1:B:640:MET:HE1	1.80	0.62
1:C:637:ASN:ND2	3:C:803:SO4:O3	2.32	0.62
1:A:479:ASP:N	1:A:479:ASP:OD1	2.34	0.61
1:D:760:ILE:O	1:D:764:THR:OG1	2.18	0.61
1:D:677:ASP:HB2	1:D:679:VAL:HG22	1.84	0.60
1:A:667:VAL:HG12	1:A:712:LEU:HD23	1.85	0.59
1:A:625:ARG:NH2	3:A:802:SO4:O1	2.31	0.58
1:C:610:LEU:HD13	1:C:692:LEU:HD21	1.85	0.58
1:B:630:ARG:NH2	1:B:666:PRO:HG2	2.18	0.58
1:C:468:LEU:HD12	1:C:469:PRO:HD2	1.85	0.58
1:C:710:GLU:HG3	1:D:559:PRO:HA	1.87	0.57
1:C:485:LYS:HB3	1:C:497:MET:HE3	1.88	0.56
1:D:625:ARG:NH2	3:D:802:SO4:O1	2.31	0.56
1:C:548:ILE:HG13	1:C:633:LEU:HD12	1.88	0.55
1:D:731:GLU:OE2	1:D:759:ARG:NH1	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:PRO:HA	1:D:710:GLU:HG3	1.87	0.55
1:A:610:LEU:HD13	1:A:692:LEU:HD21	1.88	0.54
1:A:675:LEU:HD11	1:A:713:PHE:CE1	2.43	0.54
2:B:801:ACP:H8	2:B:801:ACP:H5'1	1.90	0.53
1:B:680:TYR:CE1	1:B:684:SER:HB2	2.44	0.53
1:C:630:ARG:HH22	1:C:666:PRO:HG2	1.73	0.53
1:A:630:ARG:HH22	1:A:666:PRO:HG2	1.73	0.52
1:D:571:ASN:ND2	1:D:574:GLU:OE1	2.43	0.51
1:B:610:LEU:HD13	1:B:692:LEU:HD21	1.93	0.51
1:A:630:ARG:NH2	1:A:666:PRO:HG2	2.27	0.50
1:B:487:LEU:HD12	1:B:495:VAL:HG12	1.94	0.49
1:C:675:LEU:HD11	1:C:713:PHE:HE1	1.77	0.49
1:A:675:LEU:HD21	1:A:713:PHE:CD1	2.43	0.49
1:B:548:ILE:HG13	1:B:633:LEU:HD12	1.96	0.48
1:A:507:LYS:HD2	1:A:510:GLU:CD	2.33	0.48
1:B:474:TRP:CD1	1:B:539:LYS:HE2	2.48	0.48
1:C:486:PRO:HA	1:C:496:VAL:HG12	1.95	0.48
1:A:676:PHE:CE1	1:A:717:LYS:HE3	2.49	0.48
1:B:675:LEU:HD11	1:B:713:PHE:HE1	1.79	0.48
1:A:675:LEU:HD11	1:A:713:PHE:HE1	1.79	0.47
1:C:659:ASN:O	1:C:678:ARG:NH1	2.45	0.47
1:C:702:SER:HB2	1:D:521:ASP:OD2	2.14	0.47
1:D:575:TYR:HE1	1:D:598:MET:HE1	1.80	0.47
1:D:575:TYR:CE2	1:D:634:VAL:HG11	2.50	0.47
1:D:468:LEU:HD12	1:D:468:LEU:HA	1.83	0.46
1:C:503:ILE:HG22	1:C:512:VAL:HG11	1.97	0.46
1:B:549:ASN:HB2	1:B:565:GLU:OE1	2.15	0.46
1:A:521:ASP:OD2	1:B:702:SER:HB3	2.17	0.45
1:A:671:ALA:HB1	1:A:673:GLU:OE2	2.16	0.45
1:A:548:ILE:HG13	1:A:633:LEU:HD12	1.98	0.45
1:A:575:TYR:HE1	1:A:598:MET:HE1	1.82	0.45
1:C:519:LEU:HD11	1:C:528:LEU:HD13	1.98	0.45
1:A:680:TYR:CE1	1:A:684:SER:HB2	2.51	0.45
1:D:519:LEU:HD21	1:D:528:LEU:HA	1.98	0.44
1:C:666:PRO:O	1:C:670:MET:HG3	2.16	0.44
1:D:671:ALA:HB1	1:D:673:GLU:OE2	2.17	0.44
1:B:662:ASN:HD22	1:B:662:ASN:HA	1.70	0.44
1:D:667:VAL:HG13	1:D:713:PHE:CZ	2.53	0.44
1:C:567:ALA:O	2:C:801:ACP:H2	2.18	0.43
1:B:543:LYS:HD3	1:B:544:HIS:N	2.33	0.43
1:B:697:PHE:CZ	1:B:732:LEU:HD13	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:489:GLU:HA	1:D:494:GLN:HA	2.01	0.42
1:D:675:LEU:HD22	1:D:713:PHE:CZ	2.55	0.42
1:C:724:LYS:HA	1:C:725:PRO:HD3	1.88	0.42
1:B:760:ILE:O	1:B:764:THR:OG1	2.28	0.42
1:C:680:TYR:CE1	1:C:684:SER:HB2	2.53	0.42
1:C:487:LEU:HD12	1:C:495:VAL:HG12	2.01	0.42
1:A:733:TYR:CZ	1:A:737:ARG:HD2	2.55	0.41
1:A:760:ILE:O	1:A:764:THR:OG1	2.31	0.41
1:B:608:TYR:OH	1:B:612:ARG:HD2	2.21	0.41
1:B:665:LEU:HB2	1:B:670[A]:MET:SD	2.61	0.41
1:D:600:PHE:CZ	1:D:729:THR:HG23	2.55	0.41
1:A:608:TYR:CE2	1:A:612:ARG:HD2	2.56	0.41
1:C:710:GLU:CG	1:D:559:PRO:HA	2.51	0.41
1:D:743:VAL:HA	1:D:744:PRO:HD3	1.94	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	275/324 (85%)	267 (97%)	5 (2%)	3 (1%)	14 18
1	B	281/324 (87%)	272 (97%)	7 (2%)	2 (1%)	22 30
1	C	277/324 (86%)	267 (96%)	5 (2%)	5 (2%)	8 9
1	D	266/324 (82%)	259 (97%)	6 (2%)	1 (0%)	34 46
All	All	1099/1296 (85%)	1065 (97%)	23 (2%)	11 (1%)	15 21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	661	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	726	ALA
1	C	727	ASN
1	B	661	THR
1	A	662	ASN
1	C	507	LYS
1	C	763	LEU
1	A	763	LEU
1	A	507	LYS
1	D	507	LYS
1	B	507	LYS

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	236/284 (83%)	231 (98%)	5 (2%)	53	70
1	B	241/284 (85%)	235 (98%)	6 (2%)	47	65
1	C	238/284 (84%)	237 (100%)	1 (0%)	91	96
1	D	231/284 (81%)	227 (98%)	4 (2%)	60	76
All	All	946/1136 (83%)	930 (98%)	16 (2%)	62	76

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	479	ASP
1	A	505	LYS
1	A	512	VAL
1	A	520	LYS
1	A	573	ARG
1	B	512	VAL
1	B	622[A]	CYS
1	B	622[B]	CYS
1	B	662	ASN
1	B	709	VAL
1	B	762	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	540	MET
1	D	468	LEU
1	D	548	ILE
1	D	665	LEU
1	D	764	THR

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](#)

11 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	ACP	C	801	-	27,33,33	2.11	6 (22%)	32,52,52	1.57	4 (12%)
2	ACP	D	801	-	27,33,33	2.07	6 (22%)	32,52,52	1.69	5 (15%)
3	SO4	C	802	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	B	802	-	4,4,4	0.16	0	6,6,6	0.15	0
3	SO4	A	803	-	4,4,4	0.14	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	803	-	4,4,4	0.14	0	6,6,6	0.10	0
2	ACP	A	801	-	27,33,33	2.11	6 (22%)	32,52,52	1.67	4 (12%)
3	SO4	C	804	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	D	802	-	4,4,4	0.14	0	6,6,6	0.09	0
2	ACP	B	801	-	27,33,33	2.14	6 (22%)	32,52,52	1.57	5 (15%)
3	SO4	A	802	-	4,4,4	0.17	0	6,6,6	0.14	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
2	ACP	C	801	-	-	5/15/38/38	0/3/3/3
2	ACP	B	801	-	-	4/15/38/38	0/3/3/3
2	ACP	D	801	-	-	3/15/38/38	0/3/3/3
2	ACP	A	801	-	-	3/15/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ACP	O4'-C1'	6.12	1.49	1.41
2	D	801	ACP	O4'-C1'	5.88	1.49	1.41
2	C	801	ACP	O4'-C1'	5.87	1.49	1.41
2	A	801	ACP	O4'-C1'	5.81	1.49	1.41
2	C	801	ACP	C2'-C1'	-5.68	1.45	1.53
2	B	801	ACP	C2'-C1'	-5.39	1.45	1.53
2	A	801	ACP	C2'-C1'	-5.37	1.45	1.53
2	D	801	ACP	C2'-C1'	-5.32	1.45	1.53
2	C	801	ACP	C2'-C3'	-3.81	1.42	1.53
2	B	801	ACP	C2'-C3'	-3.76	1.43	1.53
2	D	801	ACP	C2'-C3'	-3.71	1.43	1.53
2	A	801	ACP	C2'-C3'	-3.70	1.43	1.53
2	B	801	ACP	C6-N6	3.28	1.46	1.34
2	D	801	ACP	C6-N6	3.27	1.46	1.34
2	C	801	ACP	C6-N6	3.19	1.45	1.34
2	A	801	ACP	C6-N6	3.14	1.45	1.34
2	A	801	ACP	C2-N3	3.13	1.37	1.32
2	B	801	ACP	C2-N3	3.02	1.37	1.32
2	D	801	ACP	C2-N3	2.90	1.36	1.32
2	C	801	ACP	C2-N3	2.80	1.36	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ACP	C3'-C4'	-2.76	1.45	1.53
2	B	801	ACP	C3'-C4'	-2.75	1.46	1.53
2	A	801	ACP	C3'-C4'	-2.66	1.46	1.53
2	D	801	ACP	C3'-C4'	-2.66	1.46	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ACP	N3-C2-N1	-5.54	120.02	128.68
2	B	801	ACP	N3-C2-N1	-5.43	120.20	128.68
2	D	801	ACP	N3-C2-N1	-5.26	120.45	128.68
2	C	801	ACP	N3-C2-N1	-5.03	120.82	128.68
2	D	801	ACP	C3'-C2'-C1'	4.52	107.79	100.98
2	A	801	ACP	C3'-C2'-C1'	4.33	107.49	100.98
2	D	801	ACP	PB-O3A-PA	-3.97	119.98	132.56
2	B	801	ACP	C3'-C2'-C1'	3.96	106.94	100.98
2	C	801	ACP	C3'-C2'-C1'	3.93	106.89	100.98
2	C	801	ACP	PB-O3A-PA	-3.25	122.26	132.56
2	B	801	ACP	PB-O3A-PA	-3.21	122.38	132.56
2	A	801	ACP	PB-O3A-PA	-2.65	124.16	132.56
2	A	801	ACP	C2'-C3'-C4'	2.48	107.47	102.64
2	C	801	ACP	C4-C5-N7	-2.48	106.81	109.40
2	D	801	ACP	C2'-C3'-C4'	2.38	107.27	102.64
2	B	801	ACP	C4-C5-N7	-2.34	106.96	109.40
2	D	801	ACP	C4-C5-N7	-2.11	107.20	109.40
2	B	801	ACP	O3G-PG-O1G	-2.05	106.97	112.39

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ACP	PG-C3B-PB-O1B
2	A	801	ACP	PG-C3B-PB-O3A
2	B	801	ACP	PG-C3B-PB-O1B
2	B	801	ACP	PG-C3B-PB-O2B
2	C	801	ACP	PB-O3A-PA-O5'
2	C	801	ACP	O4'-C4'-C5'-O5'
2	D	801	ACP	PB-O3A-PA-O1A
2	D	801	ACP	O4'-C4'-C5'-O5'
2	D	801	ACP	C3'-C4'-C5'-O5'
2	B	801	ACP	O4'-C4'-C5'-O5'
2	B	801	ACP	PB-O3A-PA-O5'

Continued on next page...

Continued from previous page...

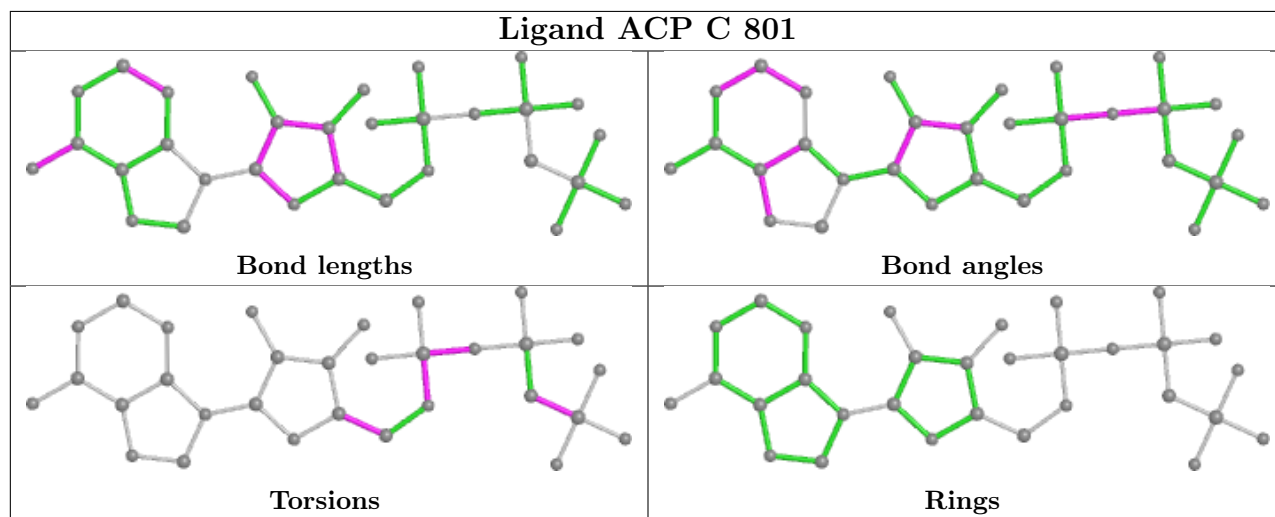
Mol	Chain	Res	Type	Atoms
2	A	801	ACP	O4'-C4'-C5'-O5'
2	C	801	ACP	C3'-C4'-C5'-O5'
2	C	801	ACP	PB-C3B-PG-O2G
2	C	801	ACP	C5'-O5'-PA-O1A

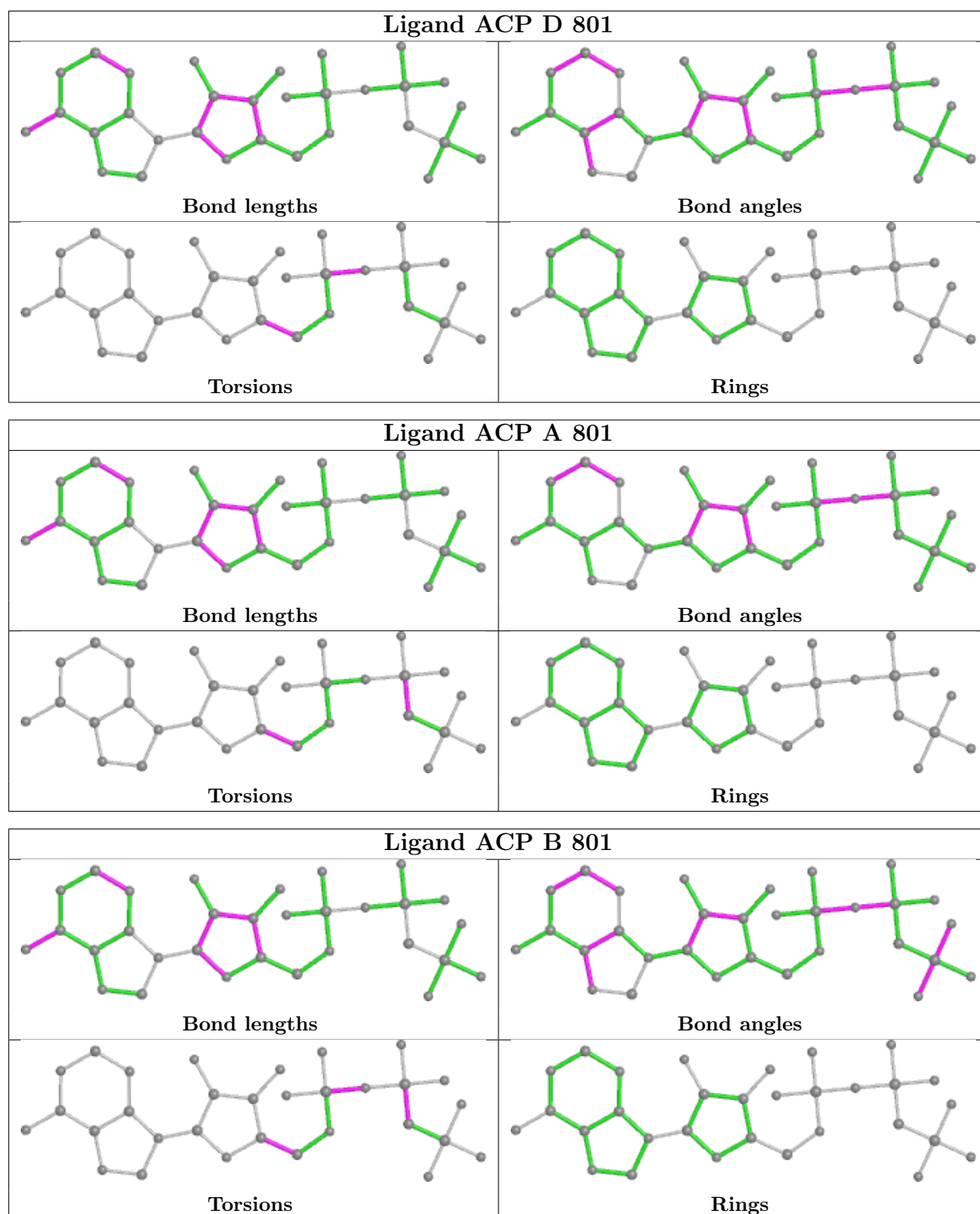
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	ACP	1	0
3	C	803	SO4	1	0
3	D	802	SO4	1	0
2	B	801	ACP	1	0
3	A	802	SO4	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

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	279/324 (86%)	0.48	12 (4%) 35 38	31, 48, 80, 116	1 (0%)
1	B	282/324 (87%)	0.48	8 (2%) 53 55	26, 43, 76, 110	0
1	C	281/324 (86%)	0.75	33 (11%) 4 5	30, 56, 101, 134	0
1	D	271/324 (83%)	0.79	34 (12%) 3 4	39, 68, 97, 122	0
All	All	1113/1296 (85%)	0.63	87 (7%) 13 14	26, 53, 93, 134	1 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	492	PHE	6.9
1	C	501	VAL	6.3
1	A	656	TYR	6.0
1	C	511	ALA	5.6
1	C	508	PRO	5.5
1	D	761	LEU	5.2
1	C	481	LEU	4.7
1	A	657	TYR	4.6
1	D	727	ASN	4.5
1	D	713	PHE	4.4
1	C	510	GLU	4.4
1	C	502	GLY	4.3
1	D	600	PHE	4.2
1	D	491	ALA	4.0
1	C	504	ASP	3.9
1	C	503	ILE	3.9
1	B	661	THR	3.8
1	C	727	ASN	3.8
1	C	512	VAL	3.8
1	C	482	THR	3.7
1	D	763	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	477	PRO	3.6
1	A	679	VAL	3.5
1	C	479	ASP	3.4
1	C	483	LEU	3.4
1	D	697	PHE	3.4
1	C	472	PRO	3.4
1	D	604	VAL	3.3
1	D	578	ALA	3.2
1	D	720	HIS	3.2
1	A	597	GLN	3.2
1	A	662	ASN	3.2
1	D	730	ASN	3.2
1	D	732	LEU	3.1
1	A	492	PHE	3.1
1	C	487	LEU	2.9
1	D	601	LYS	2.9
1	C	578	ALA	2.9
1	D	575	TYR	2.9
1	B	492	PHE	2.9
1	B	727	ASN	2.9
1	A	491	ALA	2.8
1	B	504	ASP	2.8
1	C	485	LYS	2.8
1	C	480	LYS	2.7
1	D	725	PRO	2.7
1	D	638	ASN	2.7
1	C	491	ALA	2.6
1	D	676	PHE	2.6
1	C	509	LYS	2.6
1	C	661	THR	2.6
1	D	474	TRP	2.5
1	C	500	ALA	2.5
1	C	601	LYS	2.5
1	D	764	THR	2.5
1	B	503	ILE	2.5
1	B	578	ALA	2.5
1	C	468	LEU	2.5
1	C	505	LYS	2.4
1	A	600	PHE	2.4
1	A	727	ASN	2.4
1	C	506	ASP	2.4
1	C	553	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	661	THR	2.4
1	C	514	VAL	2.4
1	D	472	PRO	2.3
1	C	476	PHE	2.3
1	D	579	ARG	2.3
1	D	760	ILE	2.3
1	C	557	ASP	2.3
1	D	470	GLU	2.3
1	D	637	ASN	2.3
1	D	597	GLN	2.3
1	C	528	LEU	2.2
1	D	598	MET	2.2
1	B	490	GLY	2.2
1	C	492	PHE	2.2
1	B	506	ASP	2.2
1	D	756	ASP	2.2
1	D	754	VAL	2.2
1	A	676	PHE	2.1
1	D	675	LEU	2.1
1	D	699	LEU	2.1
1	D	714	LYS	2.1
1	D	506	ASP	2.1
1	D	541	ILE	2.0
1	A	470	GLU	2.0

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](#)

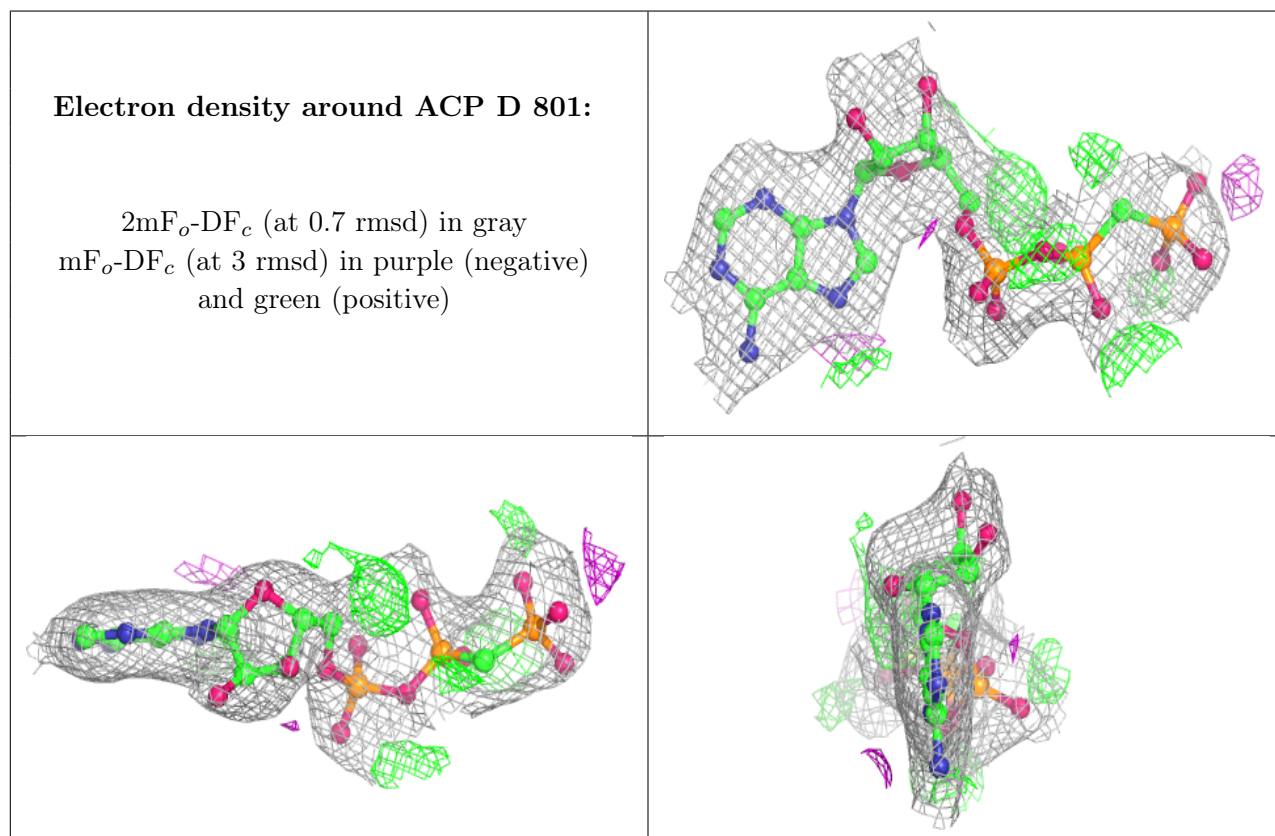
There are no monosaccharides in this entry.

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.

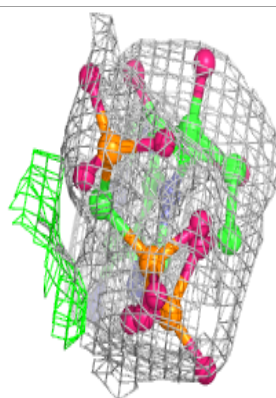
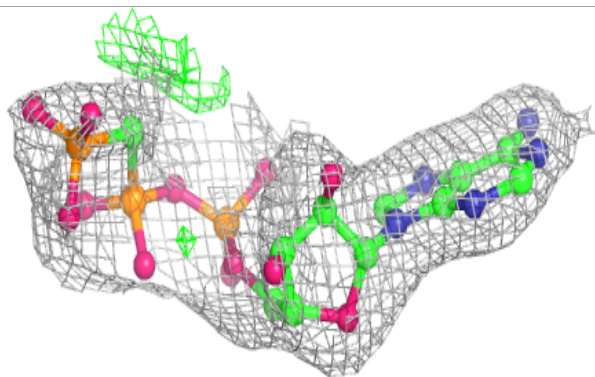
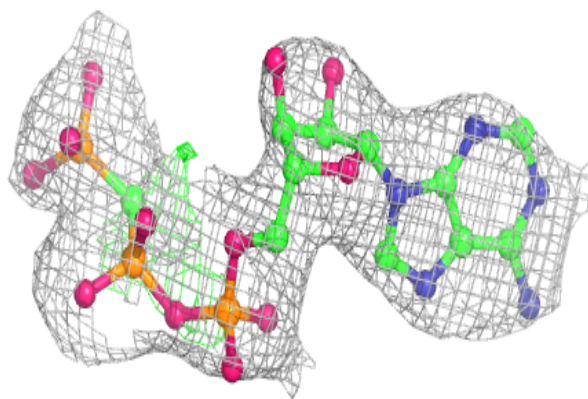
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	C	804	5/5	0.79	0.33	108,112,113,113	0
3	SO4	C	803	5/5	0.81	0.23	129,131,131,132	0
3	SO4	A	802	5/5	0.82	0.19	115,117,119,120	0
3	SO4	A	803	5/5	0.84	0.19	101,103,111,112	0
2	ACP	D	801	31/31	0.88	0.21	53,82,140,190	0
2	ACP	C	801	31/31	0.89	0.16	68,82,146,189	0
2	ACP	B	801	31/31	0.89	0.17	30,67,170,206	0
3	SO4	D	802	5/5	0.89	0.18	96,99,103,109	0
2	ACP	A	801	31/31	0.92	0.19	34,59,103,203	0
3	SO4	C	802	5/5	0.97	0.16	60,62,67,74	0
3	SO4	B	802	5/5	0.97	0.18	54,61,68,71	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.

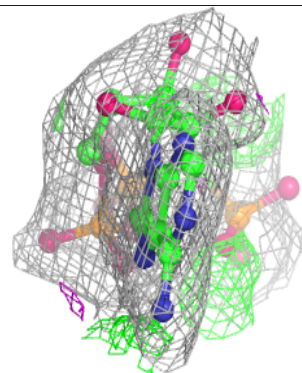
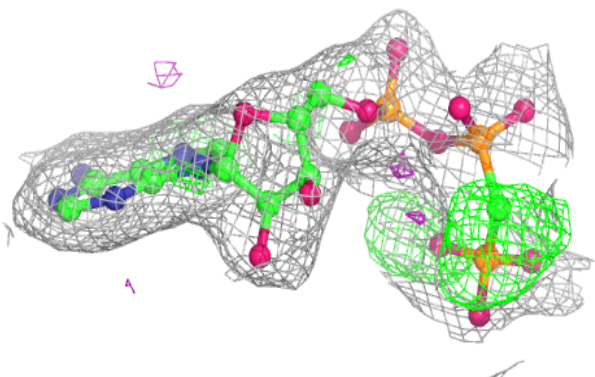
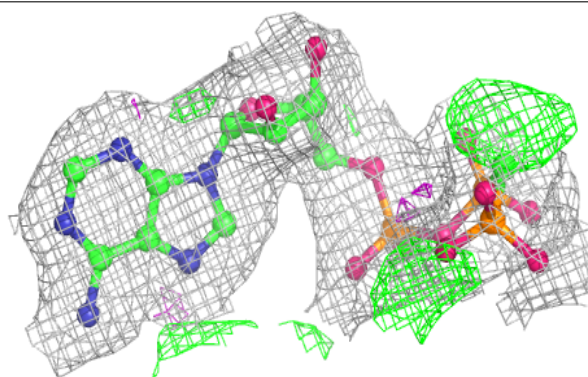


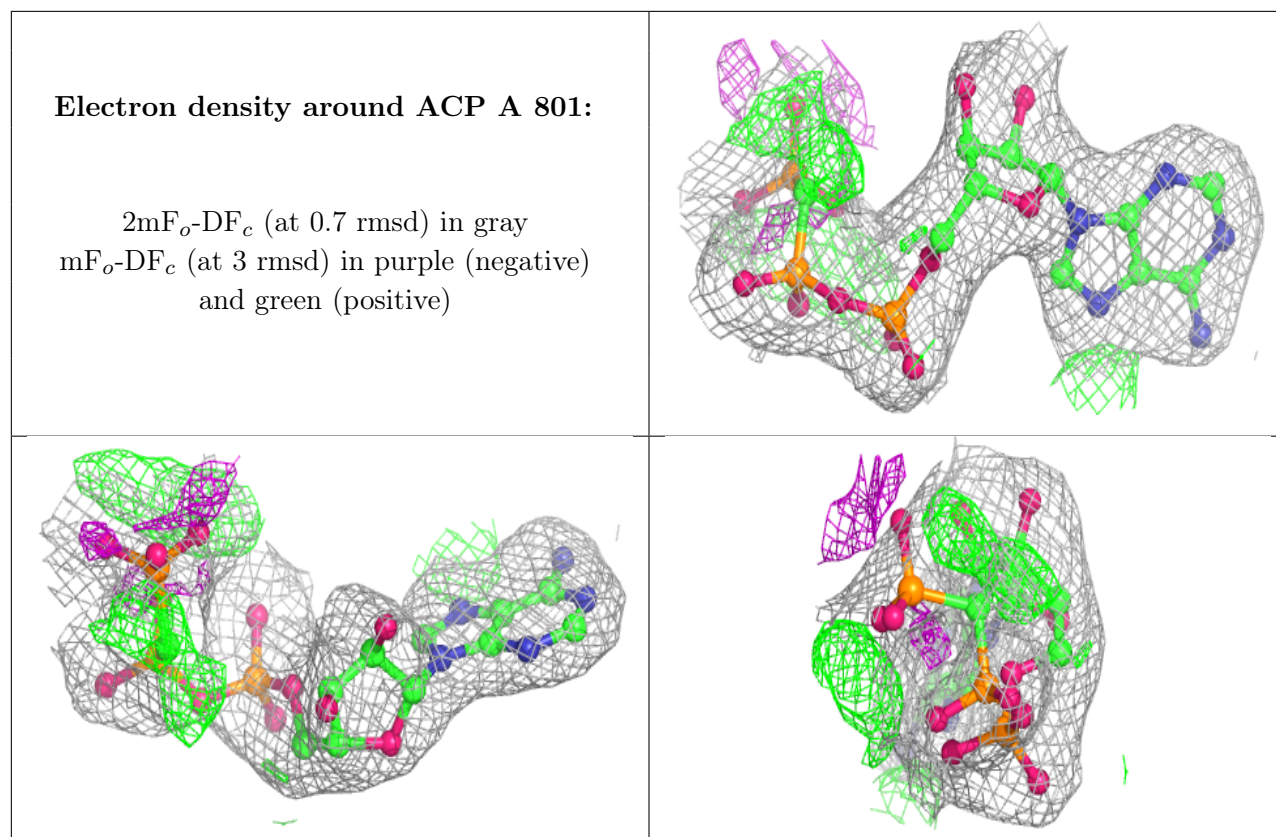
Electron density around ACP C 801:

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

**Electron density around ACP B 801:**

$2mF_o-DF_c$ (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.