



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:14 AM UTC

PDB ID : 4J95 / pdb_00004j95
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

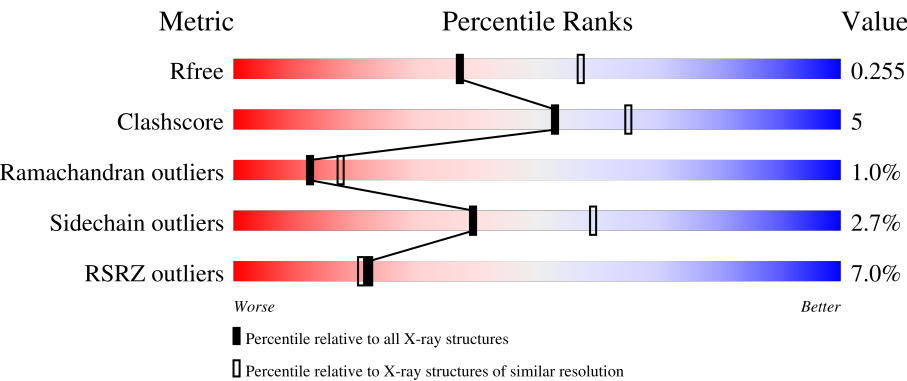
1 Overall quality at a glance i

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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (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	5% 74%11%•14%
1	B	324	5% 74%13%13%
1	C	324	7% 73%13%•13%
1	D	324	8% 70%12%•16%

2 Entry composition

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

There are 60 discrepancies between the modelled and reference sequences:

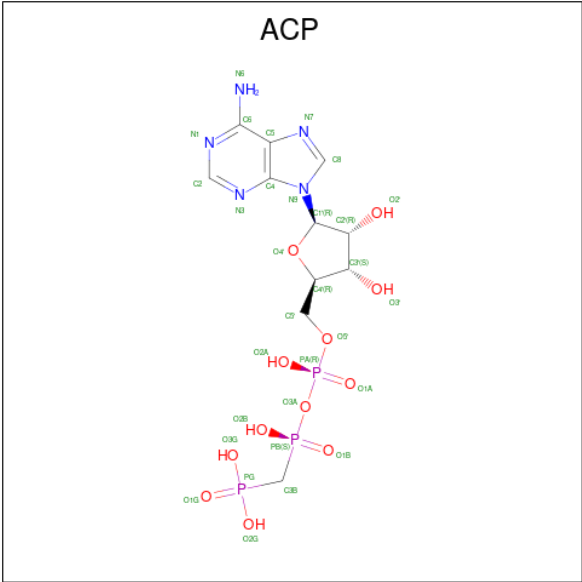
Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	expression tag	UNP P21802
A	446	GLY	-	expression tag	UNP P21802
A	447	SER	-	expression tag	UNP P21802
A	448	SER	-	expression tag	UNP P21802
A	449	HIS	-	expression tag	UNP P21802
A	450	HIS	-	expression tag	UNP P21802
A	451	HIS	-	expression tag	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

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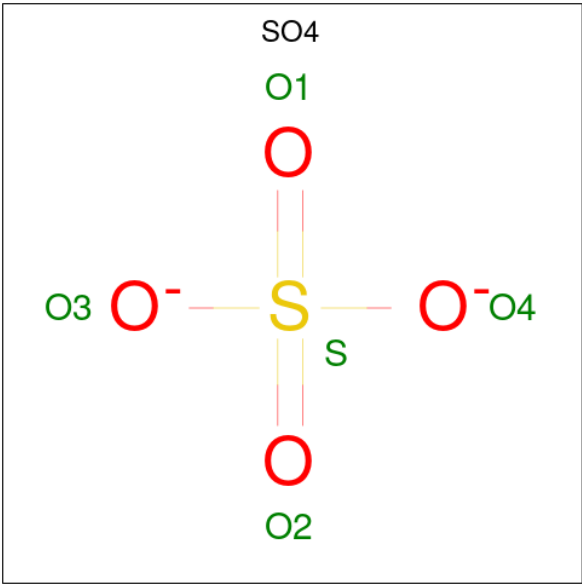
Chain	Residue	Modelled	Actual	Comment	Reference
B	451	HIS	-	expression tag	UNP P21802
B	452	HIS	-	expression tag	UNP P21802
B	453	HIS	-	expression tag	UNP P21802
B	454	HIS	-	expression tag	UNP P21802
B	455	SER	-	expression tag	UNP P21802
B	456	GLN	-	expression tag	UNP P21802
B	457	ASP	-	expression tag	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 (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (CCD ID: SO4) (formula: O₄S).



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	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

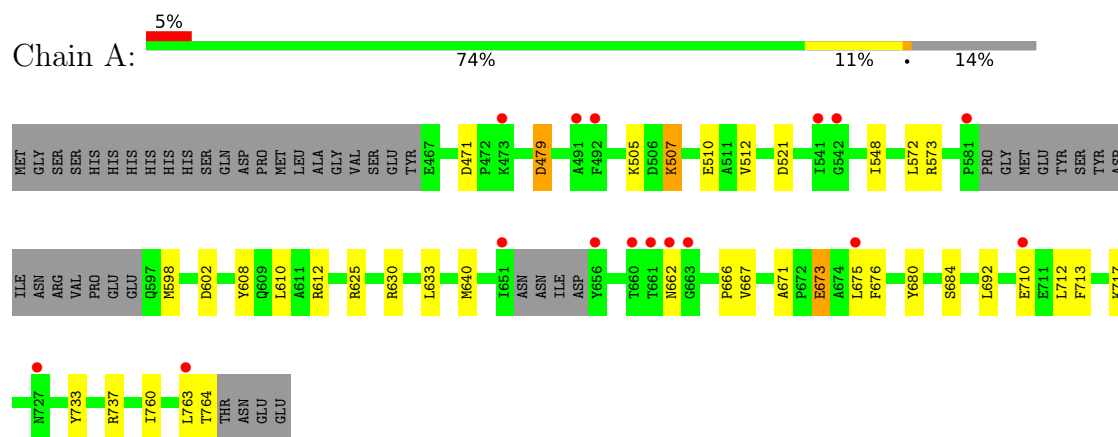
- Molecule 4 is water.

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

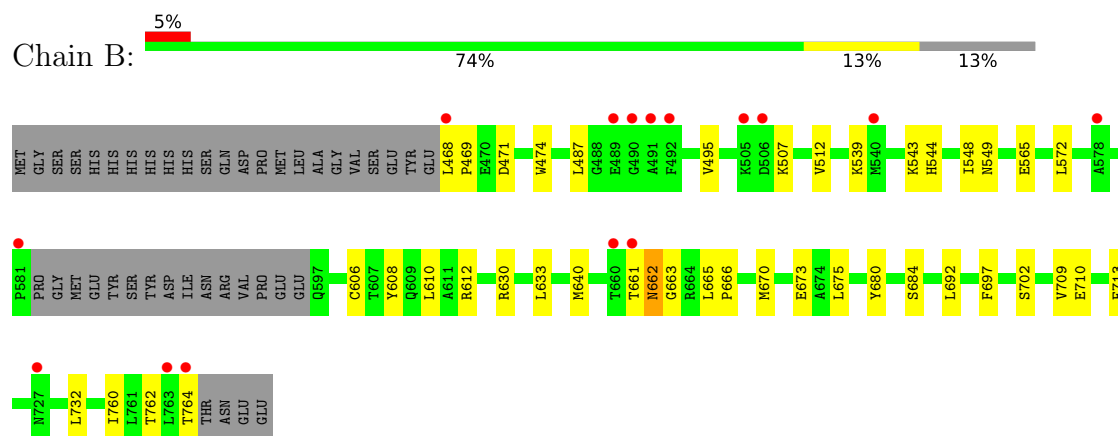
3 Residue-property plots [i](#)

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.

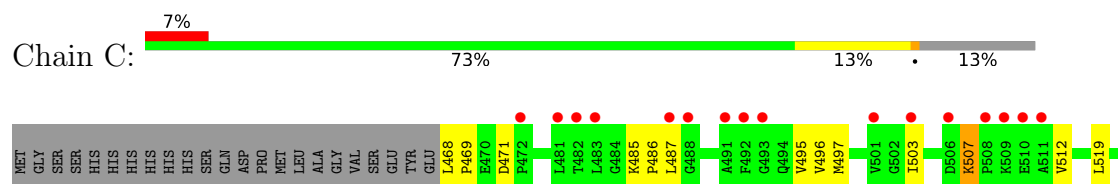
• Molecule 1: Fibroblast growth factor receptor 2

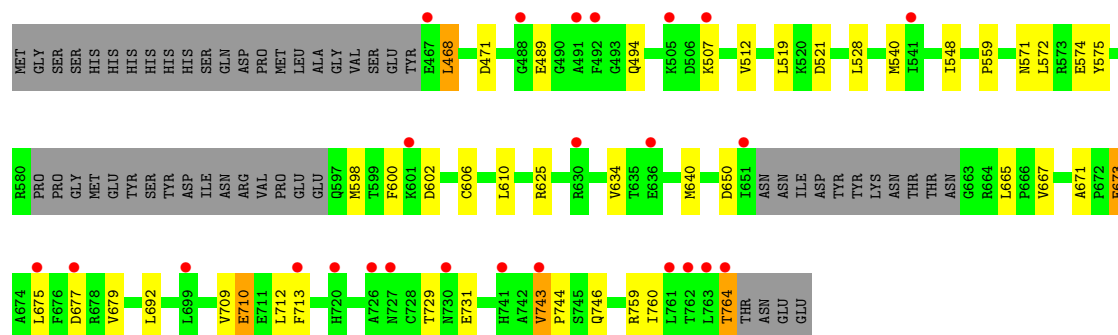


• Molecule 1: Fibroblast growth factor receptor 2



• 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 37.55 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.3 (37.55-2.38) 95.4 (37.55-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.08 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.212 , 0.255 0.213 , 0.255	Depositor DCC
R_{free} test set	2006 reflections (2.10%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, SO4

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	0.31	0/2247	0.81	2/3040 (0.1%)
1	B	0.34	0/2288	0.79	3/3097 (0.1%)
1	C	0.31	0/2264	0.80	4/3063 (0.1%)
1	D	0.31	0/2190	0.79	5/2959 (0.2%)
All	All	0.32	0/8989	0.80	14/12159 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	ASP	CA-C-N	6.84	126.65	119.05
1	B	471	ASP	C-N-CA	6.84	126.65	119.05
1	B	663	GLY	N-CA-C	6.79	119.31	111.36
1	D	712	LEU	N-CA-C	6.77	118.45	111.14
1	C	507	LYS	CA-C-N	5.77	125.48	119.82
1	C	507	LYS	C-N-CA	5.77	125.48	119.82
1	A	471	ASP	CA-C-N	5.59	125.43	119.28
1	A	471	ASP	C-N-CA	5.59	125.43	119.28
1	D	471	ASP	CA-C-N	5.44	125.09	119.05
1	D	471	ASP	C-N-CA	5.44	125.09	119.05
1	C	471	ASP	CA-C-N	5.29	125.10	119.28
1	C	471	ASP	C-N-CA	5.29	125.10	119.28
1	D	743	VAL	CA-C-N	5.07	124.51	119.24
1	D	743	VAL	C-N-CA	5.07	124.51	119.24

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	2196	0	2177	21	0
1	B	2232	0	2222	21	0
1	C	2218	0	2207	23	0
1	D	2147	0	2138	27	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
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	88	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 (88) 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: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:A:572:LEU:HD13	1:A: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	1.81	0.63
1:C:637:ASN:ND2	3:C:803:SO4:O3	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ASP:OD1	1:A:479:ASP:N	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:D:572:LEU:HD13	1:D:640:MET:HE1	1.85	0.59
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:572:LEU:HD13	1:C:640:MET:HE1	1.84	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:598:MET:HE3	1:D:602:ASP:HB3	1.87	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
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:507:LYS:HD2	1:A:510:GLU:CD	2.33	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:A:598:MET:HE3	1:A:602:ASP:HB3	1.93	0.49
1:B:487:LEU:HD12	1:B:495:VAL:HG12	1.94	0.49
1:B:665:LEU:HB3	1:B:670[B]:MET:HE3	1.95	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: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:D:606:CYS:SG	1:D:640:MET:HE2	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:606[B]:CYS:SG	1:B:640:MET:HE2	2.56	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: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:B:760:ILE:O	1:B:764:THR:OG1	2.28	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
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:D:540:MET:HE1	1:D:650:ASP:CG	2.44	0.42
1:D:572:LEU:HD13	1:D:640:MET:CE	2.49	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:D:571:ASN:HD21	1:D:574:GLU:CD	2.28	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:D:673:GLU:H	1:D:673:GLU:CD	2.29	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

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	275/324 (85%)	267 (97%)	5 (2%)	3 (1%)	11	16
1	B	281/324 (87%)	272 (97%)	7 (2%)	2 (1%)	18	26
1	C	277/324 (86%)	267 (96%)	5 (2%)	5 (2%)	6	8
1	D	266/324 (82%)	259 (97%)	6 (2%)	1 (0%)	30	40
All	All	1099/1296 (85%)	1065 (97%)	23 (2%)	11 (1%)	12	17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	661	THR
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

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%)	230 (98%)	6 (2%)	42	61
1	B	241/284 (85%)	235 (98%)	6 (2%)	42	61
1	C	238/284 (84%)	234 (98%)	4 (2%)	53	72
1	D	231/284 (81%)	222 (96%)	9 (4%)	28	45
All	All	946/1136 (83%)	921 (97%)	25 (3%)	39	60

All (25) 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	573	ARG
1	A	673	GLU
1	A	710	GLU
1	B	512	VAL
1	B	662	ASN
1	B	673	GLU
1	B	709	VAL
1	B	710	GLU
1	B	762	THR
1	C	540	MET
1	C	673	GLU
1	C	709	VAL
1	C	710	GLU
1	D	468	LEU
1	D	512	VAL
1	D	548	ILE
1	D	665	LEU
1	D	673	GLU
1	D	709	VAL
1	D	710	GLU
1	D	746	GLN
1	D	764	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	720	HIS
1	B	571	ASN
1	D	571	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
3	SO4	B	802	-	4,4,4	0.23	0	6,6,6	0.12	0
2	ACP	C	801	-	31,33,33	1.73	7 (22%)	47,52,52	1.95	10 (21%)
2	ACP	D	801	-	31,33,33	1.72	7 (22%)	47,52,52	1.98	11 (23%)
3	SO4	C	803	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	A	802	-	4,4,4	0.25	0	6,6,6	0.16	0
2	ACP	A	801	-	31,33,33	1.74	7 (22%)	47,52,52	1.98	10 (21%)
3	SO4	A	803	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	C	804	-	4,4,4	0.24	0	6,6,6	0.10	0
2	ACP	B	801	-	31,33,33	1.75	7 (22%)	47,52,52	1.97	11 (23%)
3	SO4	D	802	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	C	802	-	4,4,4	0.24	0	6,6,6	0.06	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	-	-	5/19/38/38	0/3/3/3
2	ACP	D	801	-	-	3/19/38/38	0/3/3/3
2	ACP	B	801	-	-	4/19/38/38	0/3/3/3
2	ACP	A	801	-	-	5/19/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ACP	C6-N6	4.62	1.46	1.34
2	D	801	ACP	C6-N6	4.60	1.46	1.34
2	C	801	ACP	C6-N6	4.50	1.45	1.34
2	A	801	ACP	C6-N6	4.43	1.45	1.34
2	C	801	ACP	C2'-C3'	-3.85	1.42	1.53
2	B	801	ACP	C2'-C3'	-3.81	1.43	1.53
2	D	801	ACP	C2'-C3'	-3.76	1.43	1.53
2	A	801	ACP	C2'-C3'	-3.74	1.43	1.53
2	B	801	ACP	O4'-C1'	3.30	1.49	1.42
2	D	801	ACP	O4'-C1'	3.15	1.49	1.42
2	C	801	ACP	O4'-C1'	3.14	1.49	1.42
2	A	801	ACP	C5-N7	-3.11	1.33	1.39
2	A	801	ACP	O4'-C1'	3.11	1.49	1.42
2	D	801	ACP	C5-N7	-3.10	1.33	1.39
2	C	801	ACP	C5-N7	-3.05	1.33	1.39
2	B	801	ACP	C5-N7	-2.99	1.33	1.39
2	C	801	ACP	C3'-C4'	-2.78	1.45	1.53
2	B	801	ACP	C3'-C4'	-2.77	1.46	1.53
2	A	801	ACP	C3'-C4'	-2.68	1.46	1.53
2	D	801	ACP	C3'-C4'	-2.68	1.46	1.53
2	C	801	ACP	C2'-C1'	-2.65	1.45	1.53
2	B	801	ACP	C2'-C1'	-2.52	1.45	1.53
2	A	801	ACP	C2'-C1'	-2.51	1.45	1.53
2	D	801	ACP	C2'-C1'	-2.48	1.45	1.53
2	C	801	ACP	C1'-N9	-2.22	1.40	1.46
2	D	801	ACP	C1'-N9	-2.09	1.40	1.46
2	A	801	ACP	C1'-N9	-2.09	1.40	1.46
2	B	801	ACP	C1'-N9	-2.08	1.40	1.46

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ACP	N3-C2-N1	-5.65	120.02	128.58
2	B	801	ACP	C5-C4-N3	-5.63	118.96	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ACP	C5-C4-N3	-5.61	118.99	126.72
2	B	801	ACP	N3-C2-N1	-5.54	120.20	128.58
2	D	801	ACP	C5-C4-N3	-5.46	119.19	126.72
2	C	801	ACP	C5-C4-N3	-5.46	119.20	126.72
2	D	801	ACP	N3-C2-N1	-5.37	120.45	128.58
2	C	801	ACP	N3-C2-N1	-5.13	120.82	128.58
2	A	801	ACP	N3-C4-N9	4.63	135.05	127.17
2	B	801	ACP	N3-C4-N9	4.41	134.67	127.17
2	D	801	ACP	N3-C4-N9	4.31	134.49	127.17
2	C	801	ACP	N3-C4-N9	4.12	134.18	127.17
2	B	801	ACP	C5-N7-C8	3.94	109.64	103.45
2	C	801	ACP	C5-N7-C8	3.89	109.56	103.45
2	A	801	ACP	C2-N3-C4	3.81	121.15	111.83
2	B	801	ACP	C2-N3-C4	3.81	121.14	111.83
2	D	801	ACP	PB-O3A-PA	-3.80	119.98	132.37
2	D	801	ACP	C5-N7-C8	3.71	109.28	103.45
2	D	801	ACP	C2-N3-C4	3.64	120.72	111.83
2	C	801	ACP	C2-N3-C4	3.59	120.61	111.83
2	A	801	ACP	C5-N7-C8	3.58	109.08	103.45
2	D	801	ACP	C3'-C2'-C1'	3.34	107.79	101.46
2	C	801	ACP	C4-C5-N7	-3.30	106.81	110.58
2	A	801	ACP	C3'-C2'-C1'	3.19	107.49	101.46
2	B	801	ACP	C4-C5-N7	-3.17	106.96	110.58
2	C	801	ACP	PB-O3A-PA	-3.10	122.26	132.37
2	B	801	ACP	PB-O3A-PA	-3.06	122.38	132.37
2	D	801	ACP	C4-C5-N7	-2.96	107.20	110.58
2	B	801	ACP	C3'-C2'-C1'	2.90	106.94	101.46
2	C	801	ACP	C3'-C2'-C1'	2.87	106.89	101.46
2	C	801	ACP	N9-C8-N7	-2.80	109.97	113.94
2	B	801	ACP	N9-C8-N7	-2.70	110.10	113.94
2	A	801	ACP	C4-C5-N7	-2.68	107.52	110.58
2	D	801	ACP	N9-C8-N7	-2.64	110.19	113.94
2	A	801	ACP	PB-O3A-PA	-2.52	124.16	132.37
2	A	801	ACP	C2'-C3'-C4'	2.52	107.47	102.61
2	A	801	ACP	N9-C8-N7	-2.48	110.41	113.94
2	D	801	ACP	C2'-C3'-C4'	2.41	107.27	102.61
2	C	801	ACP	C4'-O4'-C1'	-2.40	104.16	109.47
2	B	801	ACP	C4'-O4'-C1'	-2.16	104.69	109.47
2	D	801	ACP	C4'-O4'-C1'	-2.13	104.77	109.47
2	B	801	ACP	O3G-PG-O1G	-2.09	106.97	112.39

There are no chirality outliers.

All (17) 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	O4'-C4'-C5'-O5'
2	D	801	ACP	C3'-C4'-C5'-O5'
2	D	801	ACP	PB-O3A-PA-O1A
2	B	801	ACP	PB-O3A-PA-O5'
2	A	801	ACP	O4'-C4'-C5'-O5'
2	C	801	ACP	C3'-C4'-C5'-O5'
2	A	801	ACP	PG-C3B-PB-O2B
2	C	801	ACP	PB-C3B-PG-O2G
2	C	801	ACP	C5'-O5'-PA-O1A
2	B	801	ACP	O4'-C4'-C5'-O5'
2	A	801	ACP	C3'-C4'-C5'-O5'

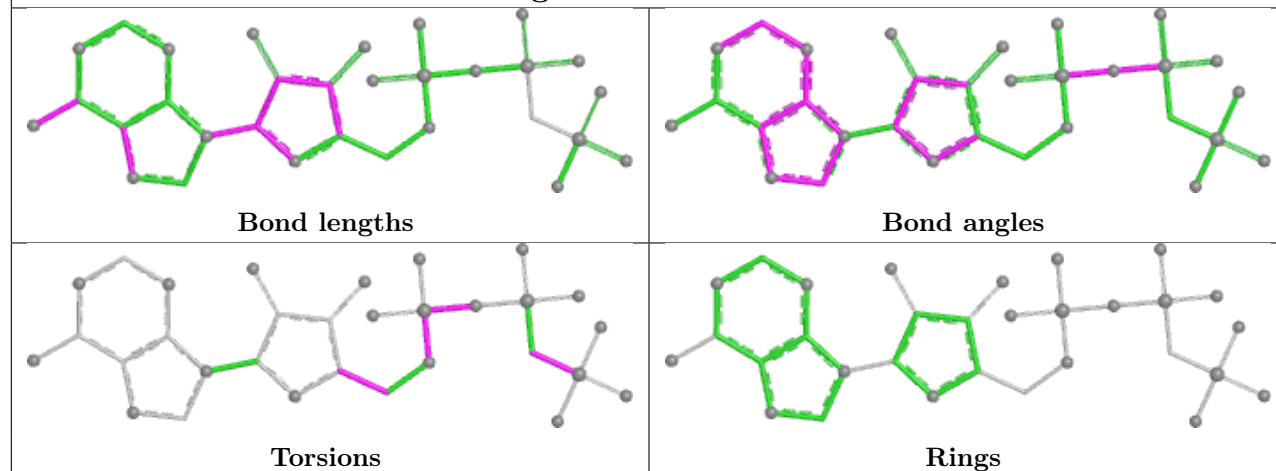
There are no ring outliers.

5 monomers are involved in 5 short contacts:

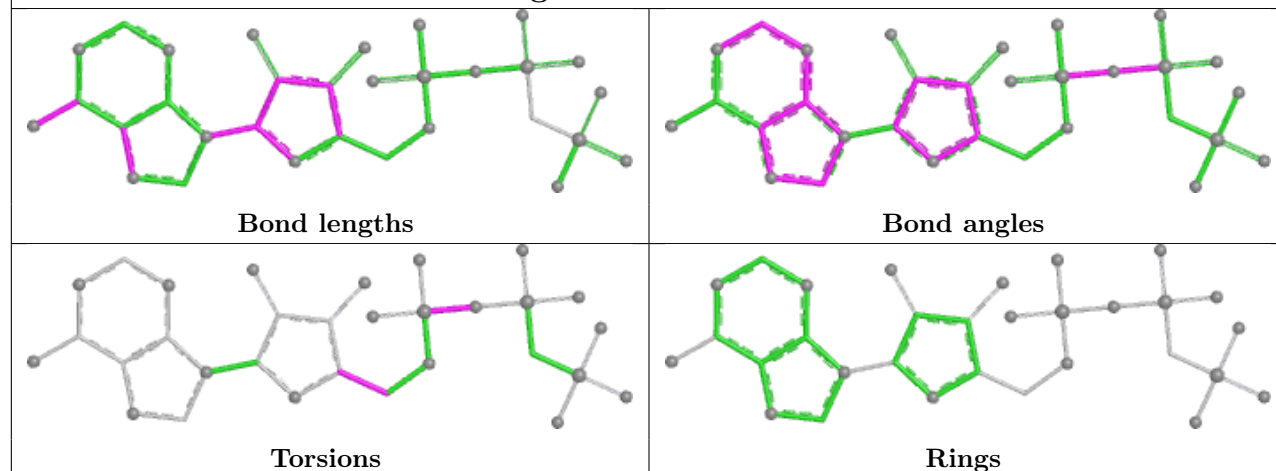
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	ACP	1	0
3	C	803	SO4	1	0
3	A	802	SO4	1	0
2	B	801	ACP	1	0
3	D	802	SO4	1	0

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.

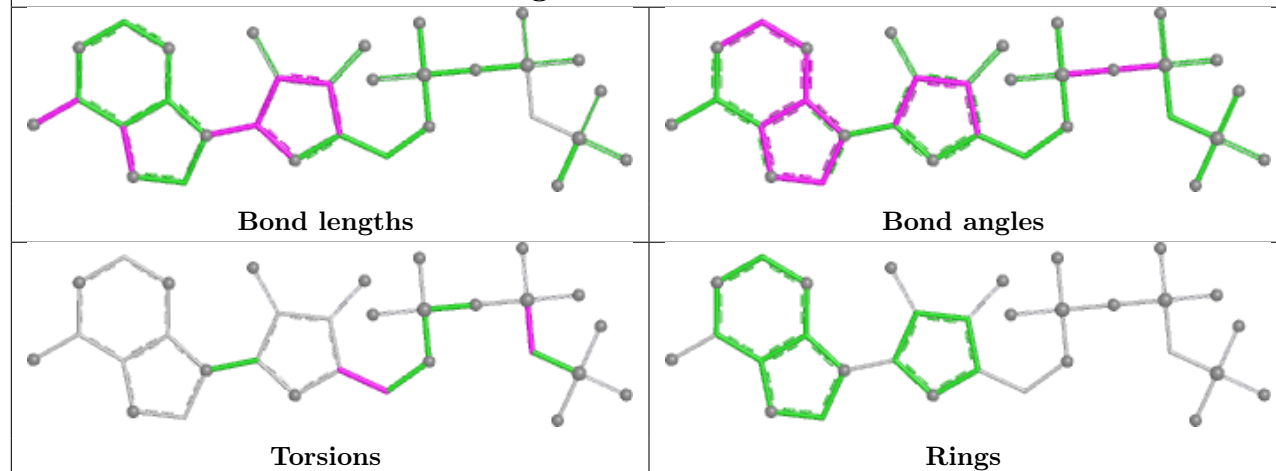
Ligand ACP C 801

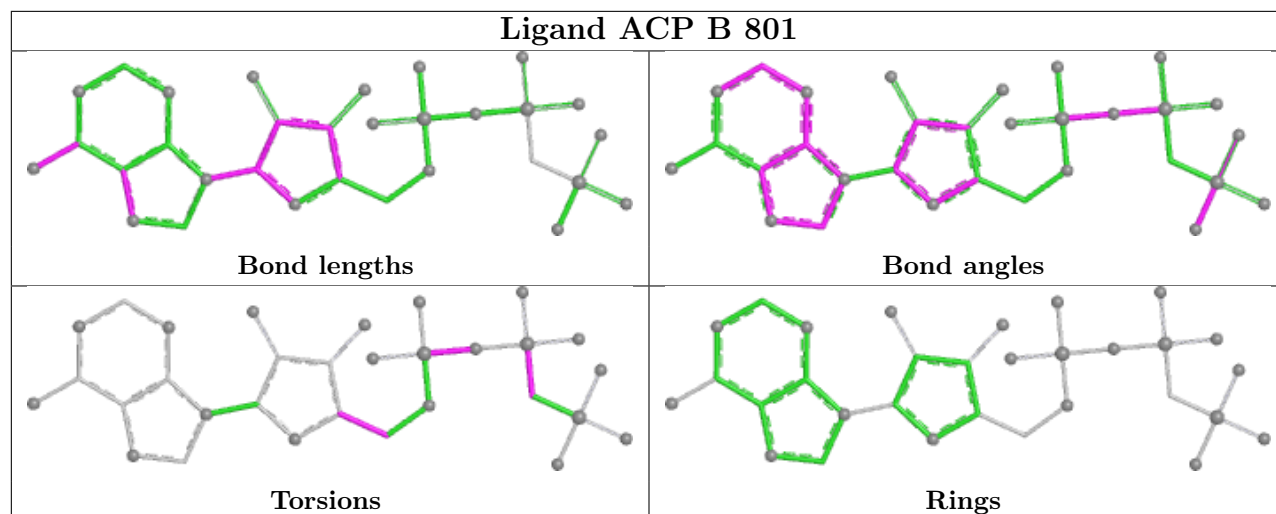


Ligand ACP D 801



Ligand ACP A 801





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 ⓘ

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%)	0.31	16 (5%)	29 28	24, 48, 80, 116	2 (0%)
1	B	282/324 (87%)	0.21	15 (5%)	32 31	19, 43, 76, 110	3 (1%)
1	C	281/324 (86%)	0.54	22 (7%)	19 17	30, 56, 101, 134	0
1	D	271/324 (83%)	0.76	25 (9%)	14 13	32, 68, 97, 122	1 (0%)
All	All	1113/1296 (85%)	0.45	78 (7%)	22 21	19, 53, 93, 134	6 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	492	PHE	7.1
1	D	651	ILE	5.3
1	D	764	THR	4.7
1	A	492	PHE	4.4
1	A	727	ASN	4.4
1	B	492	PHE	4.3
1	C	661	THR	4.2
1	C	492	PHE	4.0
1	B	506	ASP	3.8
1	C	506	ASP	3.6
1	D	491	ALA	3.6
1	B	764	THR	3.5
1	C	727	ASN	3.5
1	B	661	THR	3.5
1	D	763	LEU	3.5
1	A	656	TYR	3.4
1	D	713	PHE	3.4
1	D	727	ASN	3.3
1	C	578	ALA	3.2
1	A	661	THR	3.2
1	A	660	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	511	ALA	3.1
1	A	581	PRO	3.1
1	B	578	ALA	3.1
1	B	581	PRO	3.1
1	C	508	PRO	3.1
1	D	541	ILE	3.0
1	D	636	GLU	3.0
1	A	491	ALA	2.9
1	C	488	GLY	2.9
1	D	699	LEU	2.9
1	A	763	LEU	2.8
1	C	510	GLU	2.8
1	A	651	ILE	2.8
1	C	763	LEU	2.8
1	D	730	ASN	2.7
1	A	542	GLY	2.7
1	C	472	PRO	2.7
1	D	467	GLU	2.7
1	C	491	ALA	2.6
1	C	726	ALA	2.6
1	C	501	VAL	2.6
1	B	727	ASN	2.6
1	A	675	LEU	2.5
1	B	540	MET	2.5
1	D	720	HIS	2.5
1	C	487	LEU	2.5
1	D	677	ASP	2.5
1	A	710	GLU	2.5
1	D	505	LYS	2.5
1	C	493	GLY	2.4
1	C	764	THR	2.4
1	B	491	ALA	2.3
1	B	468	LEU	2.3
1	C	481	LEU	2.3
1	D	726	ALA	2.3
1	D	630	ARG	2.3
1	A	473	LYS	2.3
1	C	483	LEU	2.3
1	A	662	ASN	2.3
1	C	482	THR	2.3
1	D	743	VAL	2.3
1	D	488	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	503	ILE	2.2
1	B	490	GLY	2.2
1	C	509	LYS	2.1
1	B	489	GLU	2.1
1	A	663	GLY	2.1
1	B	763	LEU	2.1
1	D	675	LEU	2.1
1	D	741	HIS	2.1
1	A	541	ILE	2.1
1	B	660	THR	2.0
1	D	761	LEU	2.0
1	B	505	LYS	2.0
1	D	762	THR	2.0
1	D	507	LYS	2.0
1	D	601	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

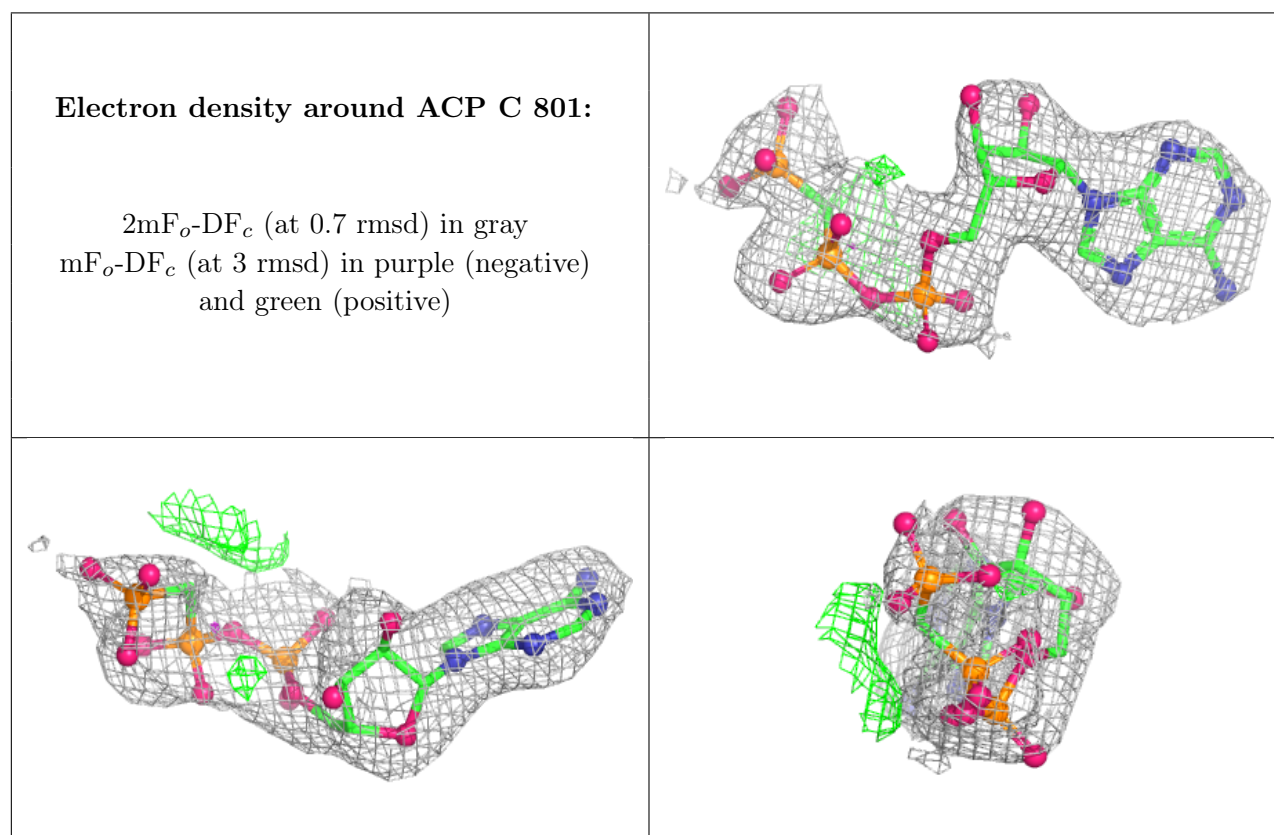
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	804	5/5	0.71	0.12	108,112,113,113	0
3	SO4	D	802	5/5	0.77	0.12	96,99,103,109	0
3	SO4	A	803	5/5	0.79	0.12	101,103,111,112	0
2	ACP	C	801	31/31	0.81	0.14	68,82,146,189	0
3	SO4	C	803	5/5	0.81	0.10	129,131,131,132	0
2	ACP	D	801	31/31	0.84	0.16	53,82,140,190	0
3	SO4	A	802	5/5	0.84	0.14	115,117,119,120	0
2	ACP	A	801	31/31	0.85	0.14	34,59,103,203	0

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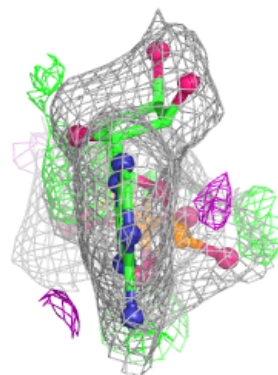
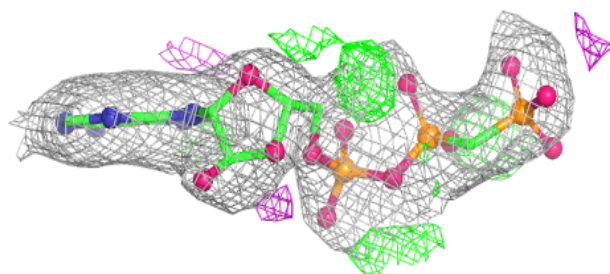
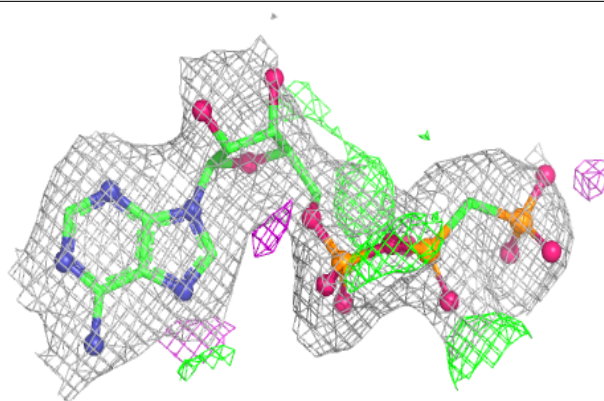
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACP	B	801	31/31	0.86	0.14	30,67,170,206	0
3	SO4	B	802	5/5	0.91	0.12	54,61,68,71	0
3	SO4	C	802	5/5	0.94	0.10	60,62,67,74	0

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.

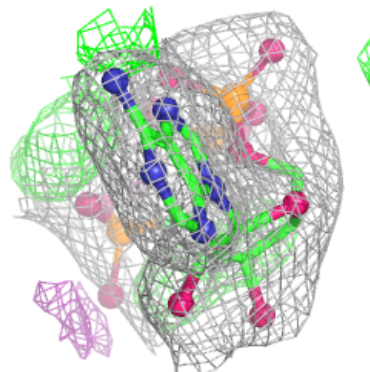
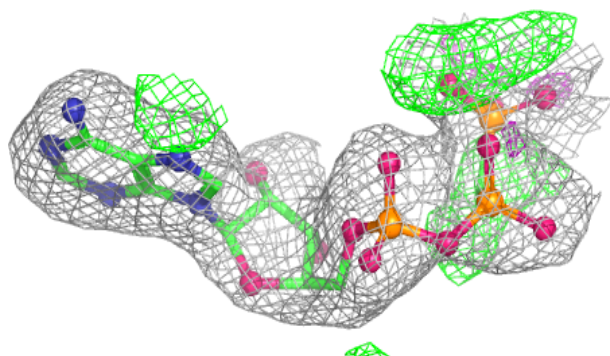
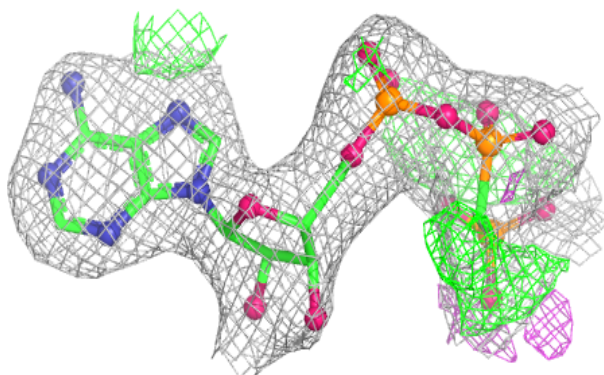


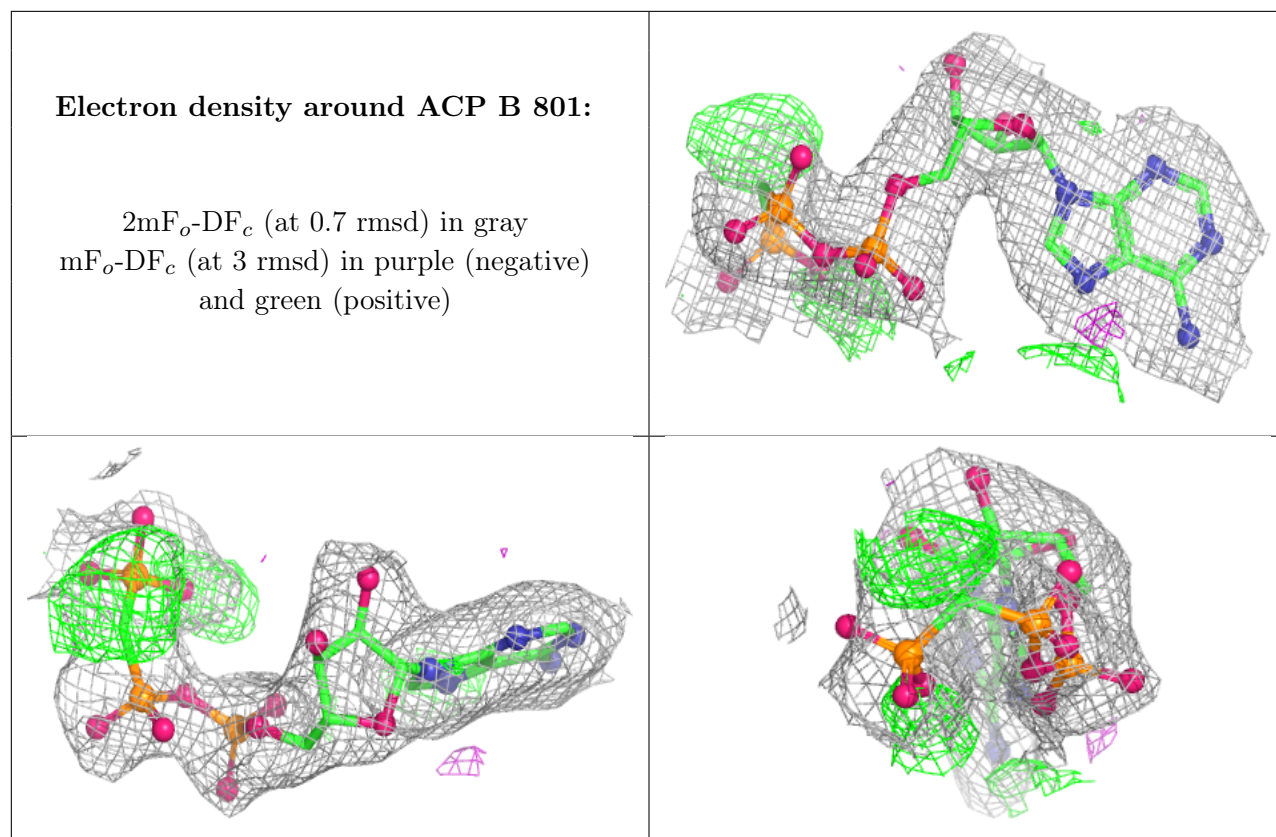
Electron density around ACP D 801:

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

**Electron density around ACP A 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 ⓘ

There are no such residues in this entry.