



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:11 PM UTC

PDB ID : 6C1S / pdb_00006c1s
Title : Phosphoinositide 3-Kinase gamma bound to an pyrrolopyridinone Inhibitor
Authors : Jacobs, M.D.; Griffin, J.P.
Deposited on : 2018-01-05
Resolution : 2.31 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

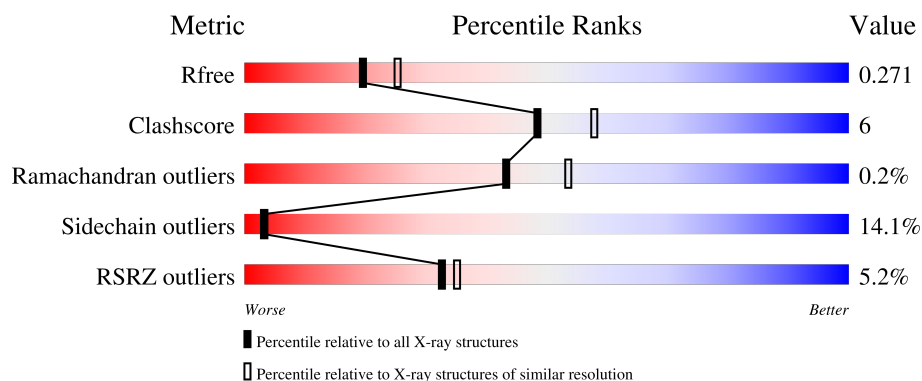
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	971	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6869 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.

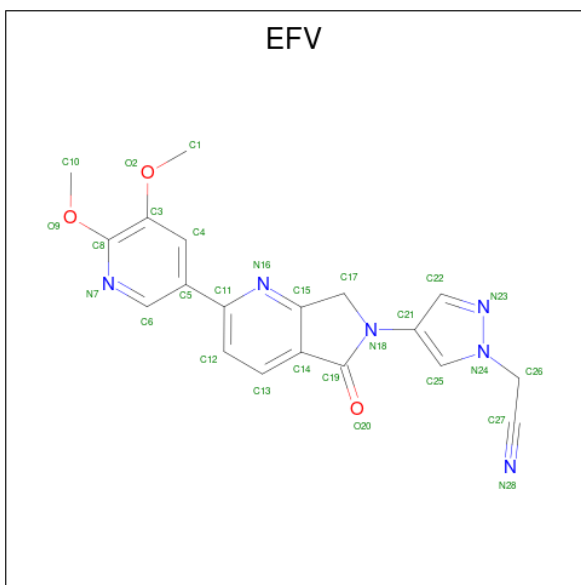
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	826	Total	C	N	O	S	0	0	0
			6670	4279	1136	1221	34			

There are 12 discrepancies between the modelled and reference sequences:

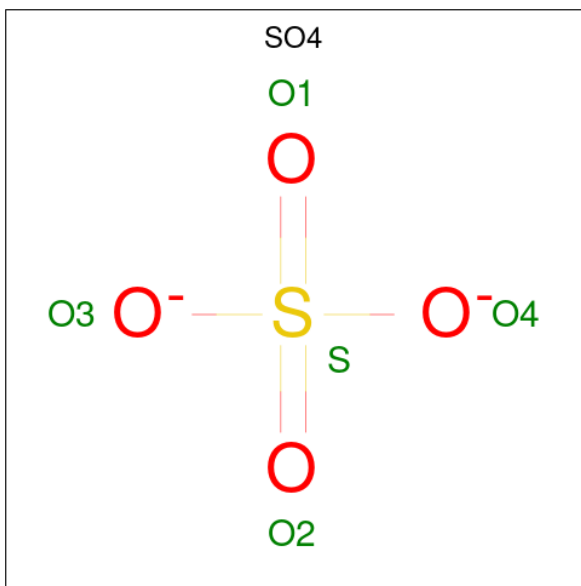
Chain	Residue	Modelled	Actual	Comment	Reference
A	140	MET	-	expression tag	UNP P48736
A	141	PRO	-	expression tag	UNP P48736
A	142	MET	-	expression tag	UNP P48736
A	143	ALA	-	expression tag	UNP P48736
A	1103	LEU	-	expression tag	UNP P48736
A	1104	GLU	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736
A	1109	HIS	-	expression tag	UNP P48736
A	1110	HIS	-	expression tag	UNP P48736

- Molecule 2 is {4-[2-(5,6-dimethoxypyridin-3-yl)-5-oxo-5,7-dihydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-1H-pyrazol-1-yl}acetonitrile (CCD ID: EFV) (formula: C₁₉H₁₆N₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	19	6	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.76Å 67.55Å 107.53Å 90.00° 95.53° 90.00°	Depositor
Resolution (Å)	41.12 – 2.31 41.12 – 2.31	Depositor EDS
% Data completeness (in resolution range)	73.4 (41.12-2.31) 73.4 (41.12-2.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.32Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.197 , 0.257 0.206 , 0.271	Depositor DCC
R_{free} test set	1650 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 77.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6869	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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: SO4, EFV

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	0.87	1/6809 (0.0%)	1.44	53/9212 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	842	MET	SD-CE	-6.35	1.63	1.79

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	593	PHE	CA-CB-CG	-7.88	105.92	113.80
1	A	904	ASP	CA-CB-CG	7.02	119.62	112.60
1	A	470	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	420	ILE	CA-C-N	6.55	129.36	120.38
1	A	420	ILE	C-N-CA	6.55	129.36	120.38
1	A	836	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	944	ILE	CA-C-N	6.50	127.02	119.94
1	A	944	ILE	C-N-CA	6.50	127.02	119.94
1	A	574	LEU	CA-C-N	6.28	128.61	120.44
1	A	574	LEU	C-N-CA	6.28	128.61	120.44
1	A	1035	LEU	CA-C-N	6.18	128.48	120.44
1	A	1035	LEU	C-N-CA	6.18	128.48	120.44
1	A	312	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	181	VAL	CA-C-N	5.79	127.96	120.44
1	A	181	VAL	C-N-CA	5.79	127.96	120.44
1	A	521	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	758	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	365	ILE	N-CA-CB	5.47	118.35	111.46
1	A	250	THR	N-CA-C	-5.42	105.45	111.36
1	A	856	GLU	CA-C-N	5.33	128.16	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	856	GLU	C-N-CA	5.33	128.16	120.38
1	A	790	GLY	CA-C-N	5.31	129.47	122.30
1	A	790	GLY	C-N-CA	5.31	129.47	122.30
1	A	509	ASP	CA-C-N	5.29	127.36	120.28
1	A	509	ASP	C-N-CA	5.29	127.36	120.28
1	A	904	ASP	CA-C-N	5.28	127.62	120.44
1	A	904	ASP	C-N-CA	5.28	127.62	120.44
1	A	513	SER	CA-C-N	5.25	128.93	121.42
1	A	513	SER	C-N-CA	5.25	128.93	121.42
1	A	756	LYS	CA-C-N	5.25	128.69	120.82
1	A	756	LYS	C-N-CA	5.25	128.69	120.82
1	A	842	MET	CA-C-N	5.25	127.31	120.28
1	A	842	MET	C-N-CA	5.25	127.31	120.28
1	A	750	LYS	CA-C-N	5.22	127.71	120.29
1	A	750	LYS	C-N-CA	5.22	127.71	120.29
1	A	949	ASN	CA-C-N	5.21	127.26	120.28
1	A	949	ASN	C-N-CA	5.21	127.26	120.28
1	A	199	HIS	O-C-N	-5.19	119.14	121.53
1	A	682	LEU	CA-C-N	5.18	127.22	120.28
1	A	682	LEU	C-N-CA	5.18	127.22	120.28
1	A	787	TYR	CA-C-N	5.18	126.84	122.28
1	A	787	TYR	C-N-CA	5.18	126.84	122.28
1	A	172	GLU	CB-CG-CD	5.17	121.39	112.60
1	A	688	ASN	CA-C-N	5.15	127.18	120.28
1	A	688	ASN	C-N-CA	5.15	127.18	120.28
1	A	163	THR	CA-C-N	5.15	128.08	120.82
1	A	163	THR	C-N-CA	5.15	128.08	120.82
1	A	504	SER	N-CA-C	-5.14	107.06	113.38
1	A	905	GLU	N-CA-C	5.06	116.61	111.14
1	A	283	GLY	N-CA-C	5.05	117.19	112.04
1	A	1011	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	929	VAL	N-CA-CB	5.02	117.37	110.54
1	A	378	ASP	CA-CB-CG	5.01	117.61	112.60

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	6670	0	6675	74	0
2	A	28	0	0	1	0
3	A	20	0	0	0	0
4	A	151	0	0	3	0
All	All	6869	0	6675	74	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 6.

All (74) 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:935:TYR:O	1:A:939:THR:HB	1.69	0.93
1:A:939:THR:CG2	1:A:945:GLY:HA2	2.04	0.86
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.73	0.70
1:A:178:ARG:O	1:A:181:VAL:HG12	1.95	0.67
1:A:386:ASN:HD22	1:A:430:ASN:HD22	1.43	0.66
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.77	0.66
1:A:558:ILE:HD11	1:A:575:LEU:HD13	1.78	0.65
1:A:564:LEU:HD22	1:A:1028:ILE:HG23	1.79	0.63
1:A:280:TYR:HB3	1:A:282:VAL:HG23	1.82	0.59
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.84	0.59
1:A:629:GLN:HG3	1:A:1029:ILE:HG13	1.86	0.57
1:A:926:GLU:HA	1:A:929:VAL:HG22	1.86	0.57
1:A:173:LEU:HD21	1:A:711:GLN:HB3	1.89	0.55
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.89	0.55
1:A:693:HIS:HE1	1:A:786:PRO:O	1.88	0.55
1:A:614:ARG:HH21	1:A:646:GLN:HE22	1.55	0.54
1:A:688:ASN:HD22	1:A:691:ILE:H	1.54	0.54
1:A:498:ASN:HD21	1:A:1040:PRO:HB3	1.74	0.53
1:A:304:HIS:HB2	1:A:823:LEU:HD11	1.90	0.53
1:A:467:LEU:O	1:A:476:ARG:HD2	2.08	0.53
1:A:944:ILE:HG22	1:A:968:ILE:HG12	1.92	0.52
1:A:802:LYS:HG2	1:A:812:TRP:HB3	1.92	0.52
1:A:786:PRO:HB2	1:A:870:ILE:HG21	1.92	0.51
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.92	0.51
1:A:840:GLN:HE21	1:A:1039:MET:HE3	1.75	0.50
1:A:614:ARG:HA	4:A:1314:HOH:O	2.11	0.49
1:A:430:ASN:HA	1:A:465:ASN:HD22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:THR:HG23	1:A:811:LEU:HD13	1.94	0.49
1:A:193:PRO:HB2	1:A:313:PRO:HB3	1.95	0.49
1:A:554:GLN:O	1:A:558:ILE:HG23	2.13	0.49
1:A:386:ASN:HD22	1:A:430:ASN:ND2	2.10	0.49
1:A:391:GLN:HE21	1:A:633:CYS:HB2	1.76	0.48
1:A:663:LEU:HB3	1:A:681:LEU:HD21	1.95	0.48
1:A:916:PRO:HD2	1:A:920:LYS:HD2	1.96	0.47
1:A:552:ARG:HH12	1:A:581:GLU:CD	2.23	0.47
1:A:810:PRO:HB3	1:A:833:LYS:HG3	1.96	0.47
1:A:928:PHE:HE1	1:A:960:LEU:HD13	1.80	0.47
1:A:1035:LEU:HA	1:A:1039:MET:HB2	1.97	0.47
1:A:665:GLN:HE21	1:A:1037:THR:HB	1.80	0.47
1:A:955:THR:C	1:A:957:THR:H	2.22	0.47
1:A:935:TYR:O	1:A:939:THR:CB	2.53	0.46
1:A:289:ASN:HD22	1:A:294:ARG:HH21	1.63	0.46
1:A:462:TYR:CZ	1:A:514:MET:HG3	2.50	0.46
1:A:862:LEU:HD21	1:A:1016:ALA:HB2	1.97	0.46
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.44	0.46
1:A:561:THR:HG23	1:A:565:ASN:HB3	1.98	0.45
1:A:368:ILE:HB	1:A:514:MET:HE1	1.98	0.45
1:A:564:LEU:HD21	1:A:1048:ILE:HG23	1.98	0.45
1:A:929:VAL:HG12	1:A:995:MET:HG2	1.99	0.45
1:A:855:TRP:NE1	1:A:1020:LEU:HD13	2.32	0.45
1:A:855:TRP:CD2	1:A:862:LEU:HD13	2.52	0.45
1:A:697:TRP:HE1	1:A:735:GLN:HE22	1.64	0.45
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.52	0.44
1:A:695:LEU:O	1:A:699:LEU:HB2	2.17	0.44
1:A:697:TRP:HE1	1:A:735:GLN:NE2	2.15	0.44
1:A:831:ILE:HB	1:A:879:ILE:HB	1.99	0.44
1:A:298:LYS:HG2	1:A:299:ASN:HD22	1.82	0.44
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.98	0.44
1:A:735:GLN:O	1:A:739:ILE:HD12	2.18	0.44
1:A:207:LEU:HD22	1:A:208:PRO:HD2	2.00	0.44
1:A:643:ILE:O	1:A:646:GLN:HG2	2.18	0.43
1:A:855:TRP:HE3	4:A:1370:HOH:O	2.02	0.42
1:A:737:GLN:O	1:A:741:MET:HG2	2.20	0.41
1:A:845:LEU:HD23	1:A:869:CYS:HB3	2.02	0.41
1:A:1045:LYS:HD3	1:A:1045:LYS:H	1.84	0.41
1:A:674:ASP:OD1	1:A:679:ARG:HD3	2.20	0.41
1:A:939:THR:HG21	4:A:1333:HOH:O	2.20	0.41
1:A:315:LEU:O	1:A:727:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:VAL:O	1:A:643:ILE:HG12	2.21	0.41
1:A:838:LEU:CD1	1:A:877:GLY:HA3	2.48	0.41
1:A:184:ARG:HH12	1:A:321:GLU:HG2	1.86	0.41
1:A:953:MET:HE1	2:A:1201:EFV:C21	2.51	0.41
1:A:935:TYR:CE2	1:A:961:PHE:HA	2.56	0.40
1:A:1029:ILE:HD12	1:A:1033:MET:HE3	2.02	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	806/971 (83%)	775 (96%)	29 (4%)	2 (0%)	43 53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	ASP
1	A	620	SER

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	736/868 (85%)	632 (86%)	104 (14%)	3 3

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	148	GLN
1	A	152	ARG
1	A	154	LEU
1	A	157	LEU
1	A	168	VAL
1	A	194	LYS
1	A	202	VAL
1	A	207	LEU
1	A	215	ILE
1	A	251	LYS
1	A	271	VAL
1	A	284	GLU
1	A	285	THR
1	A	297	LEU
1	A	298	LYS
1	A	307	LEU
1	A	315	LEU
1	A	317	GLU
1	A	320	LYS
1	A	357	CYS
1	A	358	ASP
1	A	365	ILE
1	A	392	GLN
1	A	394	LEU
1	A	420	ILE
1	A	421	LYS
1	A	428	LEU
1	A	429	LEU
1	A	461	LEU
1	A	467	LEU
1	A	476	ARG
1	A	502	LEU
1	A	514	MET
1	A	521	ASP
1	A	547	MET
1	A	553	LYS
1	A	558	ILE
1	A	561	THR
1	A	564	LEU
1	A	575	LEU
1	A	591	LYS

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Mol	Chain	Res	Type
1	A	601	GLN
1	A	610	LEU
1	A	611	LEU
1	A	614	ARG
1	A	615	GLU
1	A	649	GLU
1	A	662	GLN
1	A	663	LEU
1	A	677	LEU
1	A	679	ARG
1	A	699	LEU
1	A	700	ARG
1	A	706	SER
1	A	717	LEU
1	A	729	LEU
1	A	739	ILE
1	A	755	GLU
1	A	756	LYS
1	A	761	SER
1	A	762	GLN
1	A	764	ILE
1	A	768	LYS
1	A	796	LEU
1	A	813	LEU
1	A	827	THR
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	860	LEU
1	A	865	LEU
1	A	870	ILE
1	A	888	ILE
1	A	892	GLN
1	A	895	THR
1	A	898	ASN
1	A	904	ASP
1	A	907	LEU
1	A	909	HIS
1	A	911	LEU
1	A	912	LYS
1	A	913	GLU
1	A	914	LYS

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Mol	Chain	Res	Type
1	A	919	GLU
1	A	922	GLN
1	A	927	ARG
1	A	941	VAL
1	A	956	GLU
1	A	957	THR
1	A	967	HIS
1	A	982	ARG
1	A	983	VAL
1	A	992	LEU
1	A	1015	LYS
1	A	1020	LEU
1	A	1029	ILE
1	A	1030	LEU
1	A	1036	MET
1	A	1045	LYS
1	A	1048	ILE
1	A	1066	LYS
1	A	1071	GLN
1	A	1078	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	218	ASN
1	A	246	GLN
1	A	289	ASN
1	A	295	HIS
1	A	299	ASN
1	A	388	GLN
1	A	389	HIS
1	A	391	GLN
1	A	396	GLN
1	A	430	ASN
1	A	465	ASN
1	A	550	GLN
1	A	577	HIS
1	A	634	ASN
1	A	658	HIS
1	A	665	GLN
1	A	688	ASN

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Mol	Chain	Res	Type
1	A	693	HIS
1	A	710	GLN
1	A	735	GLN
1	A	840	GLN
1	A	846	GLN
1	A	1010	GLN
1	A	1025	ASN
1	A	1060	ASN
1	A	1085	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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	1204	-	4,4,4	0.36	0	6,6,6	0.21	0
3	SO4	A	1202	-	4,4,4	0.23	0	6,6,6	0.16	0
2	EFV	A	1201	-	28,31,31	1.09	2 (7%)	30,44,44	2.72	12 (40%)
3	SO4	A	1203	-	4,4,4	0.32	0	6,6,6	0.14	0
3	SO4	A	1205	-	4,4,4	0.25	0	6,6,6	0.10	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	EFV	A	1201	-	-	3/11/27/27	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	EFV	C19-N18	-3.00	1.36	1.39
2	A	1201	EFV	N24-N23	2.32	1.40	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	EFV	C14-C19-N18	6.96	111.03	105.88
2	A	1201	EFV	C11-N16-C15	4.78	122.38	118.37
2	A	1201	EFV	C10-O9-C8	4.77	121.66	117.20
2	A	1201	EFV	C17-N18-C21	4.26	125.64	119.18
2	A	1201	EFV	C3-C8-N7	-4.00	119.41	123.57
2	A	1201	EFV	C17-C15-C14	-3.41	106.74	110.15
2	A	1201	EFV	C6-N7-C8	3.17	124.16	116.51
2	A	1201	EFV	O20-C19-C14	-3.13	122.59	128.66
2	A	1201	EFV	C25-N24-N23	-3.08	106.95	112.01
2	A	1201	EFV	C21-C22-N23	-2.92	109.00	110.82
2	A	1201	EFV	C5-C6-N7	-2.66	120.05	124.28
2	A	1201	EFV	C22-N23-N24	2.65	108.72	104.68

There are no chirality outliers.

All (3) torsion outliers are listed below:

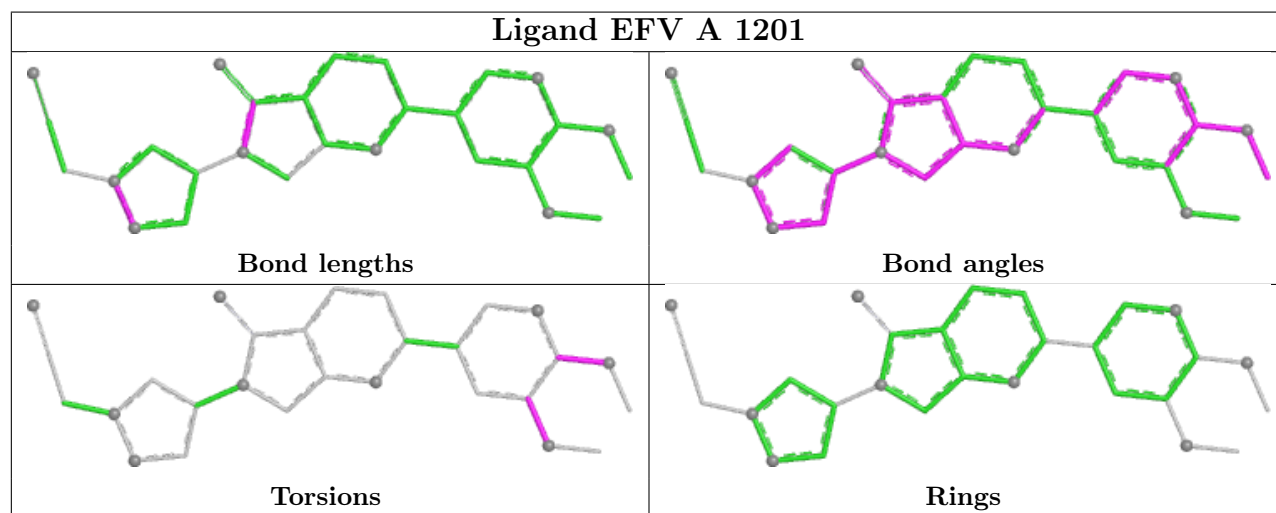
Mol	Chain	Res	Type	Atoms
2	A	1201	EFV	C8-C3-O2-C1
2	A	1201	EFV	C4-C3-O2-C1
2	A	1201	EFV	N7-C8-O9-C10

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	EFV	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 ⓘ

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	826/971 (85%)	0.52	43 (5%) 33 35	38, 83, 146, 188	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	545	ALA	3.4
1	A	379	LEU	3.3
1	A	435	CYS	3.3
1	A	1090	LEU	3.2
1	A	968	ILE	3.1
1	A	902	PHE	3.1
1	A	1048	ILE	3.1
1	A	1014	VAL	2.9
1	A	911	LEU	2.9
1	A	1089	HIS	2.8
1	A	898	ASN	2.8
1	A	489	GLY	2.6
1	A	297	LEU	2.6
1	A	292	TRP	2.5
1	A	271	VAL	2.5
1	A	220	ILE	2.5
1	A	418	ILE	2.5
1	A	1068	PHE	2.5
1	A	929	VAL	2.4
1	A	757	TYR	2.4
1	A	989	PRO	2.4
1	A	1044	SER	2.4
1	A	1040	PRO	2.4
1	A	599	GLY	2.3
1	A	381	VAL	2.3
1	A	754	ALA	2.3
1	A	219	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	749	ILE	2.3
1	A	373	LEU	2.2
1	A	896	VAL	2.3
1	A	1009	PHE	2.2
1	A	907	LEU	2.2
1	A	1002	THR	2.2
1	A	1087	PHE	2.2
1	A	154	LEU	2.1
1	A	753	SER	2.1
1	A	229	THR	2.1
1	A	949	ASN	2.1
1	A	181	VAL	2.1
1	A	899	THR	2.1
1	A	983	VAL	2.1
1	A	149	ALA	2.0
1	A	251	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.

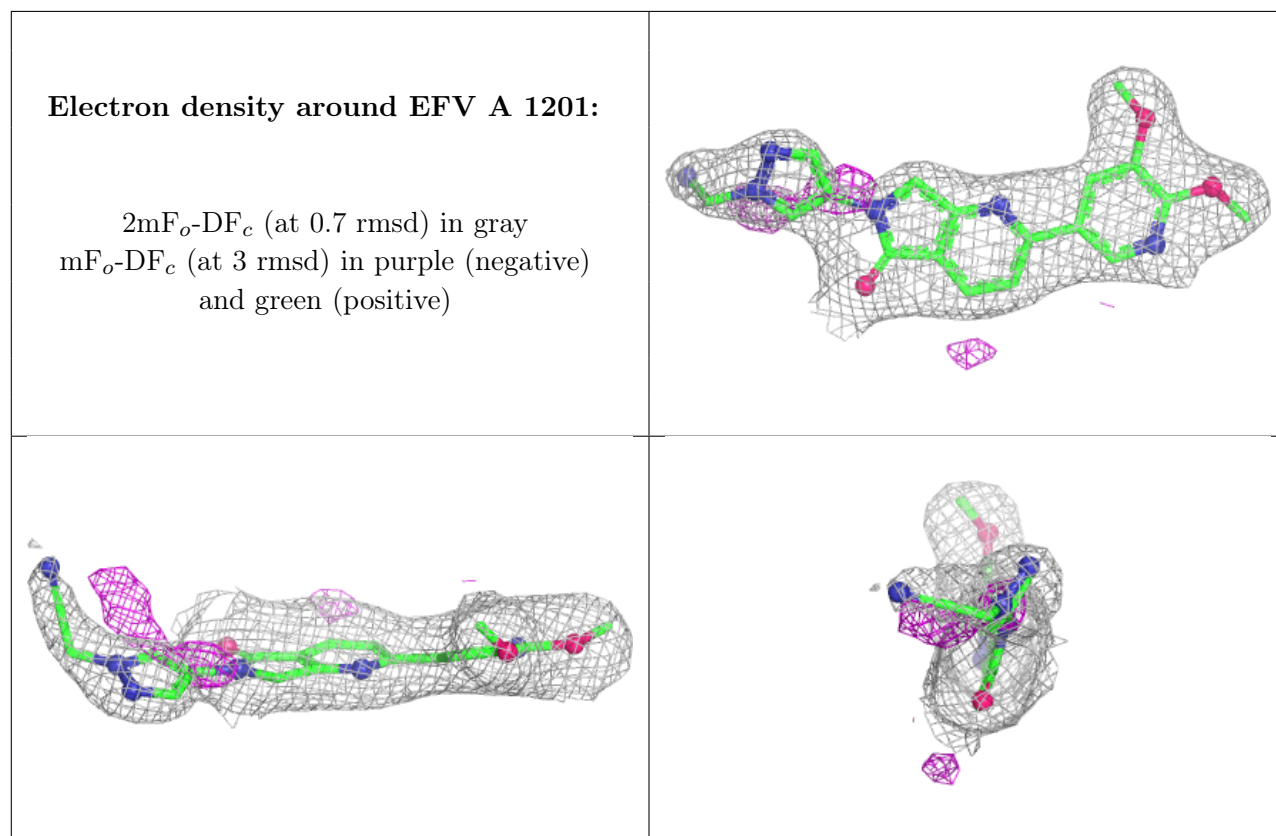
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	SO4	A	1203	5/5	0.63	0.16	143,144,144,145	0
3	SO4	A	1202	5/5	0.90	0.11	133,133,133,135	0
3	SO4	A	1204	5/5	0.92	0.08	95,96,96,99	0
3	SO4	A	1205	5/5	0.92	0.12	117,117,117,118	0
2	EFV	A	1201	28/28	0.95	0.08	53,68,83,83	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.