Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 10:20 AM EDT

PDB ID	:	6C1S
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 (i) 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 (i)) were used in the production of this report:

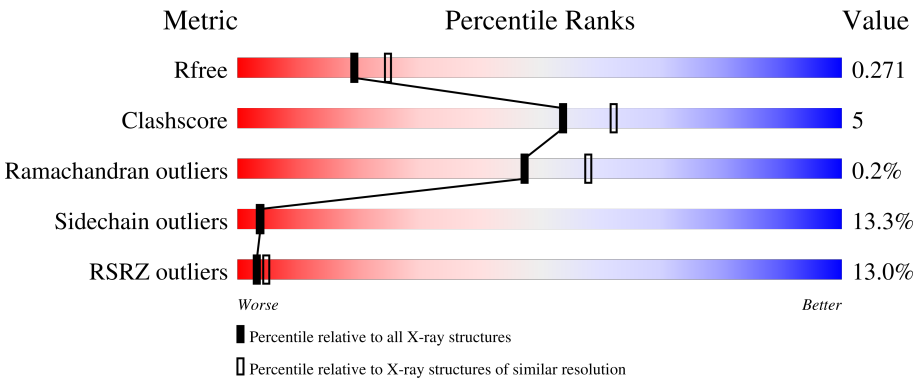
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (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 <=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	11% 66% 17% • 15%

2 Entry composition (i)

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.

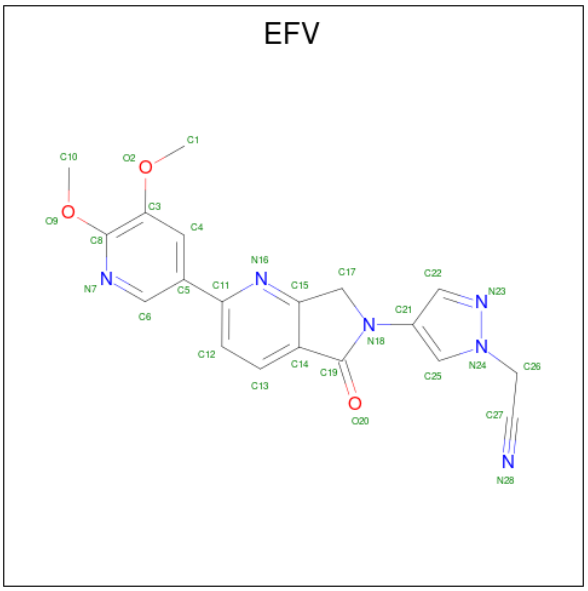
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

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

There are 12 discrepancies between the modelled and reference sequences:

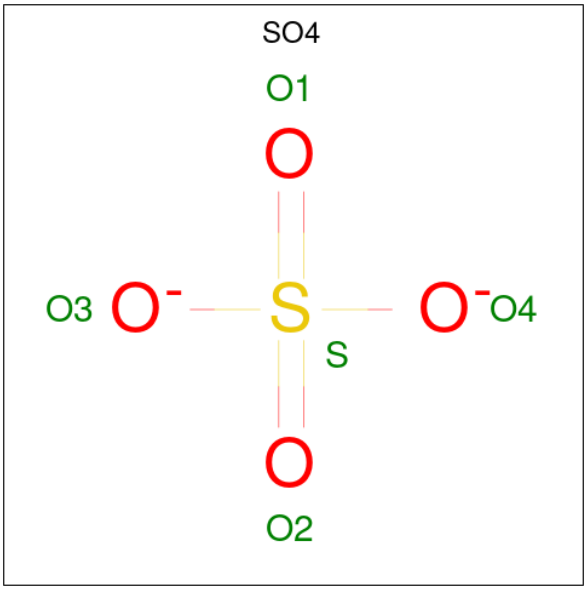
Chain	Residue	Modelled	Actual	Comment	Reference
A	140	MET	-	expression tag	UNP P48736
A	141	PRO	-	expression tag	UNP P48736
A	142	MET	-	expression tag	UNP P48736
A	143	ALA	-	expression tag	UNP P48736
A	1103	LEU	-	expression tag	UNP P48736
A	1104	GLU	-	expression tag	UNP P48736
A	1105	HIS	-	expression 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 (three-letter code: EFV) (formula: $C_{19}H_{16}N_6O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 4 is water.

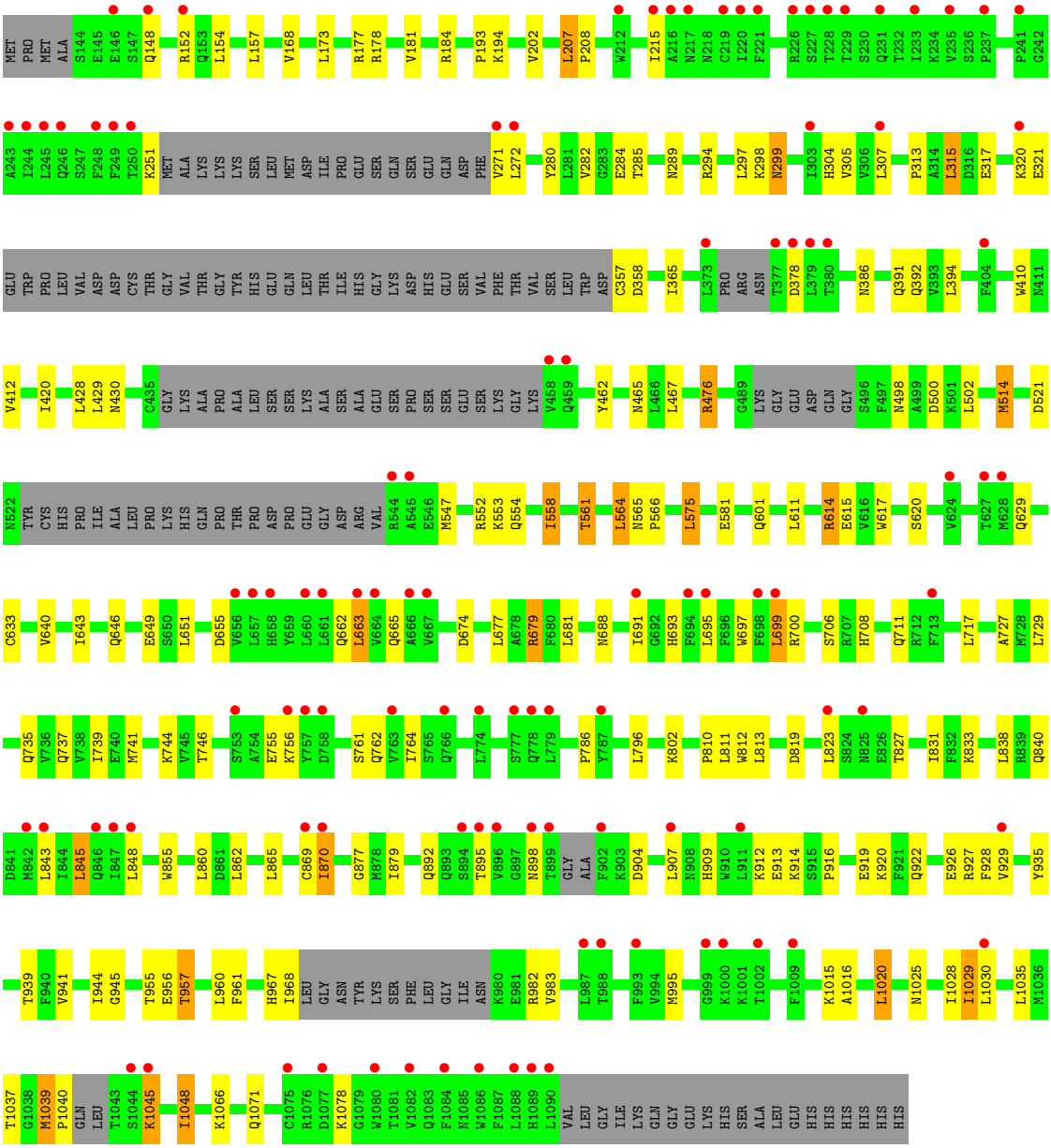
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	151	151	151	0	0

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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform

Chain A:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 67.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EFV, 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	0.50	0/6809	0.72	0/9212

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	6670	0	6675	71	0
2	A	28	0	0	0	0
3	A	20	0	0	0	0
4	A	151	0	0	3	0
All	All	6869	0	6675	71	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 (71) 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:840:GLN:HB3	1:A:1039:MET:HE3	1.88	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:955:THR:C	1:A:957:THR:H	2.22	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:552:ARG:HH12	1:A:581:GLU:CD	2.23	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
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:935:TYR:CE2	1:A:961:PHE:HA	2.56	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%)	47 58

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%)	638 (87%)	98 (13%)	4 4

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	152	ARG
1	A	154	LEU
1	A	157	LEU
1	A	168	VAL
1	A	177	ARG
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	299	ASN
1	A	307	LEU
1	A	315	LEU
1	A	317	GLU

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Mol	Chain	Res	Type
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	428	LEU
1	A	429	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	566	PRO
1	A	575	LEU
1	A	601	GLN
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	744	LYS
1	A	755	GLU
1	A	756	LYS
1	A	761	SER
1	A	762	GLN
1	A	764	ILE
1	A	796	LEU
1	A	813	LEU

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Mol	Chain	Res	Type
1	A	819	ASP
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	892	GLN
1	A	895	THR
1	A	898	ASN
1	A	904	ASP
1	A	907	LEU
1	A	909	HIS
1	A	912	LYS
1	A	913	GLU
1	A	914	LYS
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	1015	LYS
1	A	1020	LEU
1	A	1025	ASN
1	A	1029	ILE
1	A	1030	LEU
1	A	1039	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 (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	ASN

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Mol	Chain	Res	Type
1	A	299	ASN
1	A	388	GLN
1	A	391	GLN
1	A	430	ASN
1	A	465	ASN
1	A	577	HIS
1	A	665	GLN
1	A	688	ASN
1	A	693	HIS
1	A	710	GLN
1	A	735	GLN
1	A	762	GLN
1	A	769	GLN
1	A	840	GLN
1	A	1025	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 monosaccharides 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	1202	-	4,4,4	0.18	0	6,6,6	0.15	0
3	SO4	A	1204	-	4,4,4	0.25	0	6,6,6	0.17	0
3	SO4	A	1203	-	4,4,4	0.23	0	6,6,6	0.11	0
2	EFV	A	1201	-	28,31,31	1.12	2 (7%)	31,44,44	2.73	13 (41%)
3	SO4	A	1205	-	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
2	EFV	A	1201	-	-	3/8/27/27	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	N23-N24	3.56	1.40	1.35
2	A	1201	EFV	C14-C15	2.17	1.41	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	EFV	C14-C19-N18	5.35	111.03	106.23
2	A	1201	EFV	C25-N24-N23	-5.29	106.95	111.56
2	A	1201	EFV	C17-N18-C19	-5.16	107.99	112.28
2	A	1201	EFV	C11-N16-C15	4.64	122.38	118.35
2	A	1201	EFV	C10-O9-C8	4.49	121.66	117.21
2	A	1201	EFV	C22-N23-N24	4.31	108.72	104.23
2	A	1201	EFV	C17-N18-C21	4.00	125.64	121.20
2	A	1201	EFV	C15-C17-N18	3.65	106.12	102.34
2	A	1201	EFV	O20-C19-C14	-3.13	122.59	128.68
2	A	1201	EFV	C6-N7-C8	3.07	124.16	116.27
2	A	1201	EFV	C26-N24-N23	2.61	126.64	120.87
2	A	1201	EFV	C5-C6-N7	-2.59	120.05	124.32
2	A	1201	EFV	O2-C3-C4	-2.02	120.64	124.12

There are no chirality outliers.

All (3) torsion outliers are listed below:

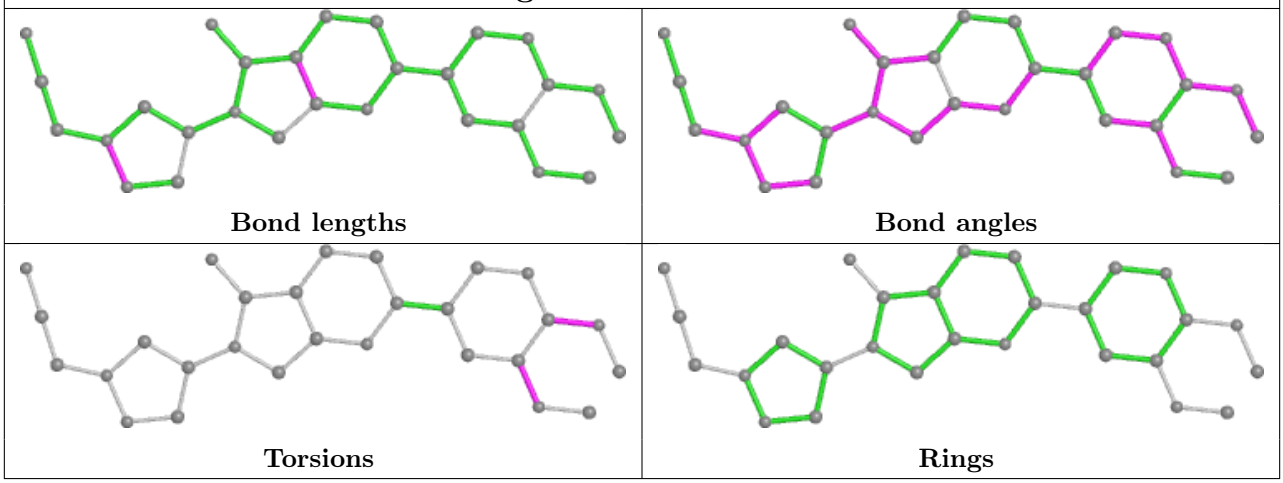
Mol	Chain	Res	Type	Atoms
2	A	1201	EFV	C8-C3-O2-C1
2	A	1201	EFV	C4-C3-O2-C1
2	A	1201	EFV	N7-C8-O9-C10

There are no ring outliers.

No monomer is involved in short contacts.

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 EFV A 1201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	826/971 (85%)	0.70	107 (12%) 3 5	38, 83, 146, 188	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	899	THR	10.2
1	A	220	ILE	6.3
1	A	907	LEU	6.1
1	A	896	VAL	6.1
1	A	757	TYR	6.0
1	A	911	LEU	5.8
1	A	379	LEU	5.6
1	A	228	THR	5.4
1	A	221	PHE	5.4
1	A	307	LEU	5.3
1	A	894	SER	5.0
1	A	404	PHE	5.0
1	A	373	LEU	5.0
1	A	249	PHE	4.8
1	A	895	THR	4.7
1	A	999	GLY	4.6
1	A	377	THR	4.6
1	A	902	PHE	4.6
1	A	226	ARG	4.4
1	A	229	THR	4.4
1	A	898	ASN	4.3
1	A	378	ASP	4.1
1	A	1000	LYS	4.0
1	A	248	PHE	4.0
1	A	660	LEU	4.0
1	A	545	ALA	3.9
1	A	219	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	778	GLN	3.9
1	A	244	ILE	3.9
1	A	993	PHE	3.6
1	A	1090	LEU	3.6
1	A	231	GLN	3.6
1	A	1086	TRP	3.5
1	A	698	PHE	3.5
1	A	152	ARG	3.4
1	A	869	CYS	3.4
1	A	272	LEU	3.3
1	A	320	LYS	3.3
1	A	216	ALA	3.3
1	A	661	LEU	3.3
1	A	1088	LEU	3.2
1	A	777	SER	3.2
1	A	1075	CYS	3.2
1	A	699	LEU	3.2
1	A	1002	THR	3.1
1	A	1077	ASP	3.1
1	A	664	VAL	3.1
1	A	233	ILE	3.1
1	A	148	GLN	3.1
1	A	1044	SER	3.1
1	A	656	VAL	3.0
1	A	237	PRO	3.0
1	A	758	ASP	2.9
1	A	245	LEU	2.9
1	A	774	LEU	2.9
1	A	1084	PHE	2.8
1	A	212	TRP	2.8
1	A	1045	LYS	2.8
1	A	246	GLN	2.8
1	A	241	PRO	2.7
1	A	271	VAL	2.7
1	A	756	LYS	2.7
1	A	227	SER	2.7
1	A	217	ASN	2.7
1	A	987	LEU	2.7
1	A	628	MET	2.7
1	A	787	TYR	2.6
1	A	235	VAL	2.6
1	A	657	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	146	GLU	2.6
1	A	215	ILE	2.6
1	A	779	LEU	2.6
1	A	663	LEU	2.6
1	A	458	VAL	2.6
1	A	842	MET	2.6
1	A	380	THR	2.6
1	A	459	GLN	2.5
1	A	848	LEU	2.5
1	A	988	THR	2.5
1	A	825	ASN	2.4
1	A	243	ALA	2.4
1	A	691	ILE	2.4
1	A	1009	PHE	2.4
1	A	870	ILE	2.4
1	A	753	SER	2.4
1	A	627	THR	2.3
1	A	847	ILE	2.3
1	A	763	VAL	2.3
1	A	1030	LEU	2.3
1	A	766	GLN	2.3
1	A	624	VAL	2.2
1	A	695	LEU	2.2
1	A	658	HIS	2.2
1	A	694	PHE	2.2
1	A	843	LEU	2.2
1	A	1082	VAL	2.1
1	A	1089	HIS	2.1
1	A	250	THR	2.1
1	A	1080	TRP	2.1
1	A	667	VAL	2.1
1	A	713	PHE	2.1
1	A	823	LEU	2.1
1	A	666	ALA	2.1
1	A	929	VAL	2.1
1	A	846	GLN	2.0
1	A	303	ILE	2.0
1	A	544	ARG	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)

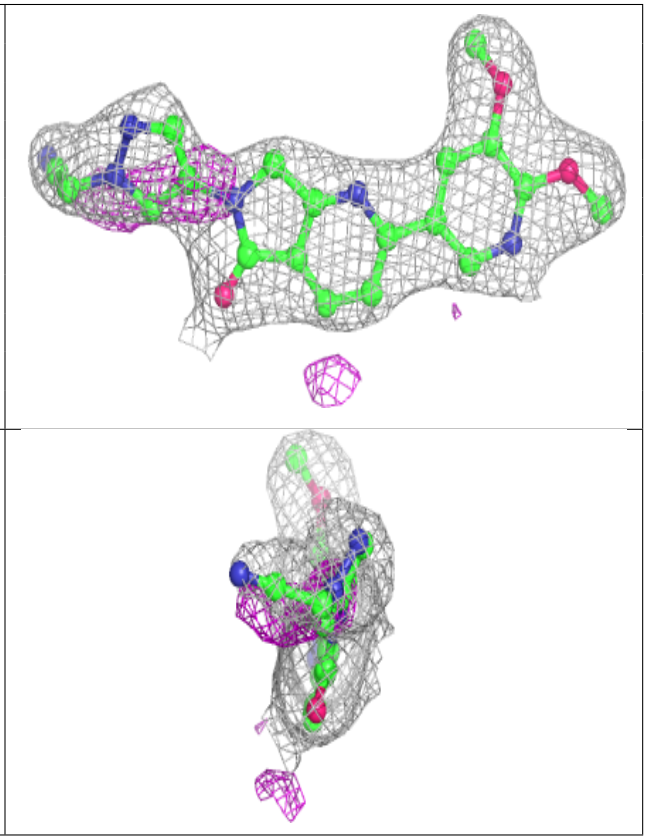
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	1202	5/5	0.93	0.16	133,133,133,135	0
3	SO4	A	1203	5/5	0.93	0.15	143,144,144,145	0
2	EFV	A	1201	28/28	0.94	0.14	53,68,83,83	0
3	SO4	A	1204	5/5	0.96	0.13	95,96,96,99	0
3	SO4	A	1205	5/5	0.97	0.26	117,117,117,118	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 EFV A 1201:

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.