Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 09:33 PM EDT

PDB ID	:	3R7Q
Title	:	Structure-based design of thienobenzoxepin inhibitors of PI3- kinase
Authors	:	Murray, J.M.; Wiesmann, C.
Deposited on	:	2011-03-22
Resolution	:	2.50 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.
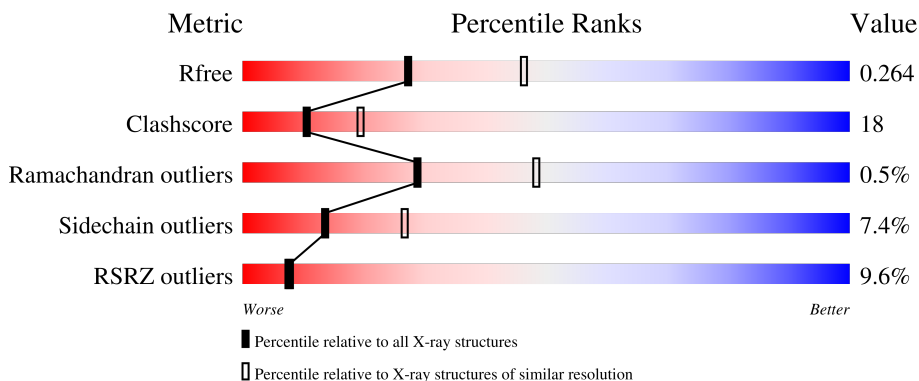

Full wwPDB X-ray Structure Validation Report

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 2.50 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	Percentile Ranks	Value
Rfree		0.264
Clashscore		18
Ramachandran outliers		0.5%
Sidechain outliers		7.4%
RSRZ outliers		9.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	966	8% 56% 27% • 13%

2 Entity composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 6800 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.
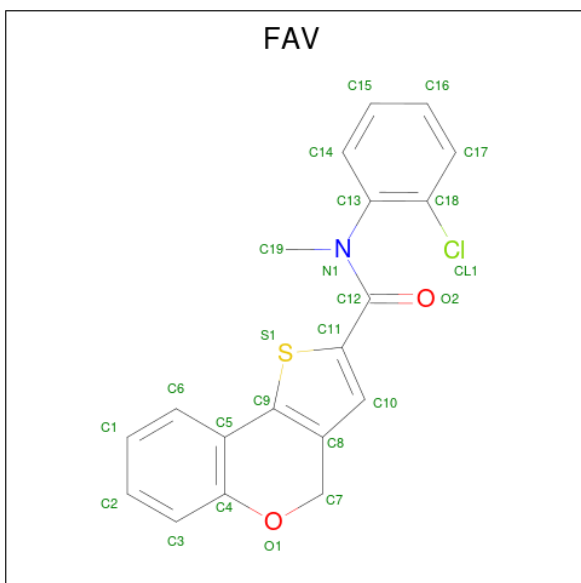
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	837	Total 6776	C 4354	N 1152	O 1234	S 36	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	initiating methionine	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	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

- Molecule 2 is N-(2-chlorophenyl)-N-methyl-4H-thieno[3,2-c]chromene-2-carboxamide (three-letter code: FAV) (formula: $C_{19}H_{14}ClNO_2S$).
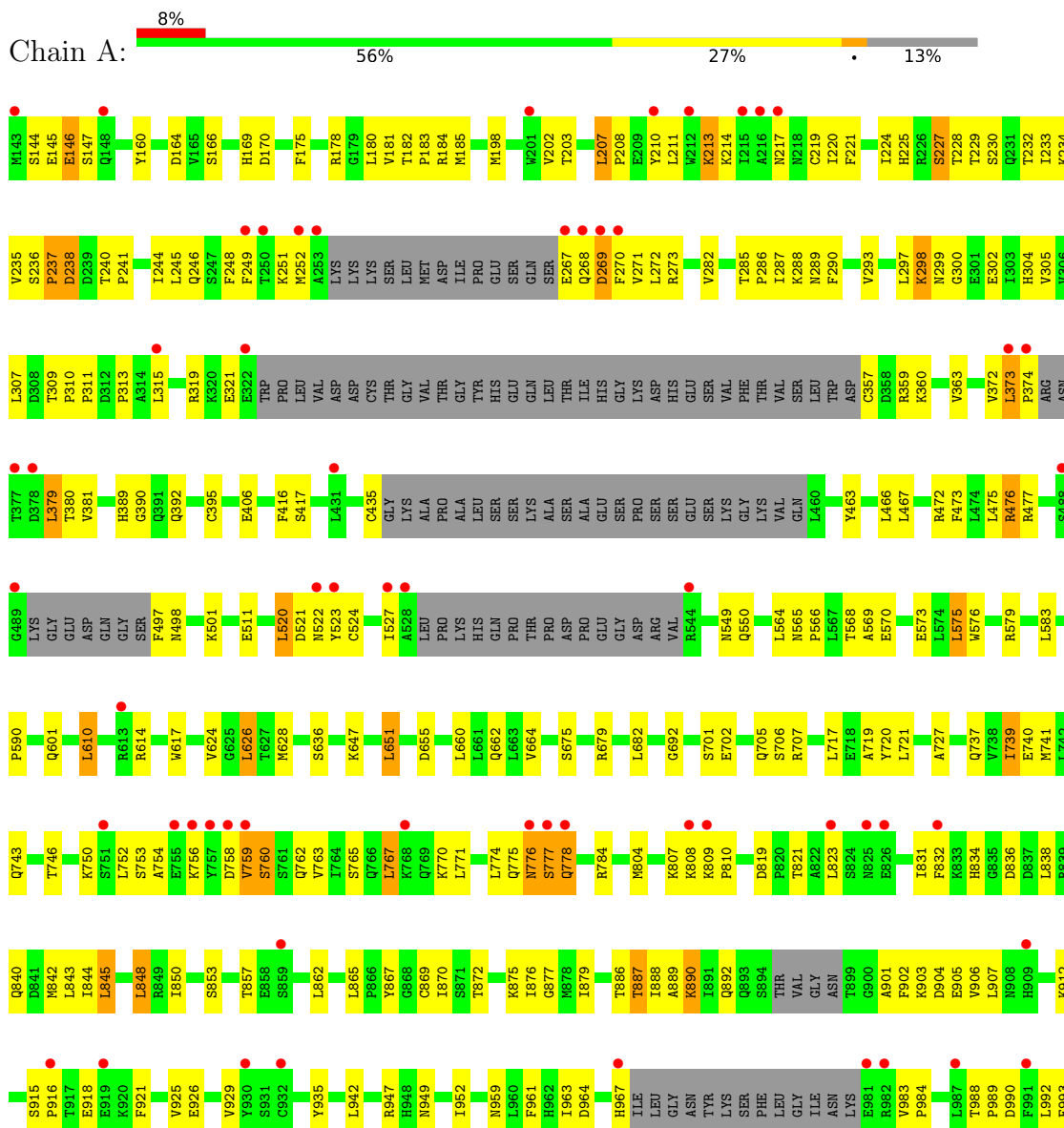

FAV

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
2	A	1	24	19	1	1	2	1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform

V994 M995 G996 T997 S998 G999 K1000 K1001 T1002 S1003 P1004 H1005 F1006 Q1007 K1008 F1009 I1012 K1015 A1016 Y1017 L1018 R1021 L1026 I1029 S1032 L1035 M1039 P1040 Q1041 L1042 T1043 S1044 K1045 E1046 D1047 I1048 E1049 Y1050 I1051 L1055 T1056 E1062 Y1067 F1068 Q1071 I1072 E1073

K1078 G1079 W1080 T1081 V1082 Q1083 F1084 N1085 W1086 F1087 L1088 H1089 L1090 V1091 LEU GLY ILE LYS GLN GLY GLU LYS HIS SER ALA HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.78Å 67.49Å 105.89Å 90.00° 96.43° 90.00°	Depositor
Resolution (Å)	19.93 – 2.50 19.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.93-2.50) 98.5 (19.93-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.50Å)	Xtriage
Refinement program	PHENIX dev_798, REFMAC	Depositor
R, R_{free}	0.216 , 0.269 0.211 , 0.264	Depositor DCC
R_{free} test set	1711 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 53.9	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6800	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.61	0/6922	0.85	5/9363 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	870	ILE	CG1-CB-CG2	-7.52	94.86	111.40
1	A	575	LEU	CA-CB-CG	7.47	132.47	115.30
1	A	651	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	160	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	A	160	TYR	CB-CG-CD1	5.27	124.16	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	756	LYS	Peptide
1	A	776	ASN	Peptide
1	A	777	SER	Peptide

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	6776	0	6793	250	0
2	A	24	0	14	6	0
All	All	6800	0	6807	251	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 18.

All (251) 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:1035:LEU:HD12	1:A:1048:ILE:HD13	1.31	1.10
1:A:184:ARG:NH2	1:A:321:GLU:OE1	1.88	1.07
1:A:997:THR:HG23	1:A:1001:LYS:HB3	1.38	1.05
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.40	0.99
1:A:170:ASP:OD2	1:A:476:ARG:NH2	1.98	0.96
1:A:807:LYS:H	1:A:807:LYS:HD2	1.35	0.91
1:A:1000:LYS:NZ	1:A:1073:GLU:OE1	2.07	0.87
1:A:819:ASP:OD1	1:A:821:THR:OG1	1.94	0.84
1:A:372:VAL:C	1:A:374:PRO:HD2	1.96	0.84
1:A:804:MET:HE2	1:A:831:ILE:HG12	1.57	0.84
1:A:217:ASN:HD22	1:A:219:CYS:HB2	1.43	0.84
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.63	0.79
1:A:947:ARG:NH2	1:A:963:ILE:O	2.16	0.79
1:A:741:MET:HE1	1:A:778:GLN:HB2	1.66	0.77
1:A:217:ASN:ND2	1:A:219:CYS:HB2	2.01	0.76
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.31	0.75
1:A:164:ASP:OD2	1:A:166:SER:OG	2.04	0.74
1:A:182:THR:HB	1:A:183:PRO:HD3	1.71	0.73
1:A:759:VAL:HG12	1:A:760:SER:H	1.54	0.72
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.70	0.71
1:A:888:ILE:HD13	1:A:952:ILE:HG22	1.73	0.71
1:A:473:PHE:HD2	1:A:527:ILE:HD13	1.56	0.70
1:A:743:GLN:HG2	1:A:876:ILE:HD12	1.71	0.70
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.09	0.70
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:THR:HG22	1:A:890:LYS:H	1.56	0.69
1:A:759:VAL:HG12	1:A:760:SER:N	2.07	0.69
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.75	0.69
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.74	0.69
1:A:758:ASP:OD1	1:A:759:VAL:N	2.27	0.68
1:A:202:VAL:HG12	1:A:203:THR:N	2.08	0.67
1:A:373:LEU:HD21	1:A:406:GLU:HG3	1.77	0.67
1:A:760:SER:O	1:A:763:VAL:HG12	1.95	0.67
1:A:760:SER:HB3	1:A:763:VAL:HG12	1.78	0.66
1:A:181:VAL:HG12	1:A:185:MET:CE	2.26	0.66
1:A:202:VAL:CG1	1:A:203:THR:N	2.58	0.65
1:A:743:GLN:CG	1:A:876:ILE:HD12	2.28	0.64
1:A:219:CYS:HA	1:A:235:VAL:O	1.97	0.64
1:A:905:GLU:HG2	1:A:993:PHE:CZ	2.32	0.64
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.14	0.63
1:A:807:LYS:H	1:A:807:LYS:CD	2.10	0.63
1:A:888:ILE:CD1	1:A:952:ILE:HG22	2.28	0.63
1:A:1039:MET:CB	1:A:1040:PRO:HD2	2.20	0.63
1:A:807:LYS:HD2	1:A:807:LYS:N	2.11	0.63
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.81	0.63
1:A:287:ILE:HD12	1:A:288:LYS:N	2.14	0.62
1:A:1000:LYS:HA	1:A:1000:LYS:HE2	1.82	0.62
1:A:372:VAL:HB	1:A:374:PRO:HD2	1.82	0.62
1:A:1008:LYS:O	1:A:1012:ILE:HG13	1.99	0.62
1:A:886:THR:HG22	1:A:887:THR:H	1.64	0.61
1:A:888:ILE:HD13	1:A:952:ILE:CG2	2.30	0.61
1:A:879:ILE:HD12	2:A:1:FAV:CL1	2.37	0.61
1:A:746:THR:HG21	1:A:834:HIS:HB3	1.82	0.61
1:A:758:ASP:HB3	1:A:809:LYS:HE3	1.82	0.61
1:A:831:ILE:HG21	2:A:1:FAV:CL1	2.37	0.61
1:A:565:ASN:OD1	1:A:566:PRO:HD2	2.01	0.60
1:A:997:THR:HG23	1:A:1001:LYS:CB	2.24	0.60
1:A:241:PRO:O	1:A:244:ILE:HG12	2.01	0.60
1:A:244:ILE:HD11	1:A:272:LEU:CD1	2.31	0.60
1:A:251:LYS:O	1:A:251:LYS:HD3	2.01	0.59
1:A:576:TRP:CZ3	1:A:579:ARG:HD2	2.37	0.59
1:A:905:GLU:HG2	1:A:993:PHE:CE1	2.37	0.59
1:A:1056:THR:HG23	1:A:1056:THR:O	2.02	0.59
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.84	0.59
1:A:832:PHE:CZ	1:A:876:ILE:HD11	2.38	0.59
1:A:1086:TRP:CH2	1:A:1090:LEU:HD21	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:THR:HG22	1:A:998:SER:N	2.18	0.59
1:A:267:GLU:N	1:A:269:ASP:OD1	2.36	0.59
1:A:701:SER:O	1:A:705:GLN:HG2	2.03	0.58
1:A:804:MET:HE1	2:A:1:FAV:H9	1.84	0.58
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.84	0.58
1:A:808:LYS:HE3	1:A:836:ASP:OD1	2.04	0.57
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.87	0.57
1:A:475:LEU:HD21	1:A:522:ASN:HB3	1.87	0.57
1:A:1039:MET:HB3	1:A:1040:PRO:CD	2.26	0.57
1:A:845:LEU:HD23	1:A:869:CYS:HB3	1.86	0.57
1:A:624:VAL:O	1:A:628:MET:HG2	2.05	0.57
1:A:232:THR:C	1:A:233:ILE:HD12	2.25	0.56
1:A:379:LEU:HD13	1:A:380:THR:H	1.69	0.56
1:A:225:HIS:HE1	1:A:304:HIS:CD2	2.17	0.56
1:A:759:VAL:CG1	1:A:760:SER:H	2.15	0.56
1:A:901:ALA:O	1:A:902:PHE:CD1	2.59	0.56
1:A:298:LYS:HD2	1:A:299:ASN:OD1	2.06	0.56
1:A:886:THR:HG22	1:A:887:THR:N	2.21	0.56
1:A:286:PRO:O	1:A:289:ASN:HB2	2.05	0.55
1:A:1006:PHE:O	1:A:1009:PHE:HB3	2.06	0.55
1:A:804:MET:HE3	1:A:810:PRO:HG2	1.88	0.55
1:A:746:THR:O	1:A:750:LYS:HB2	2.06	0.55
1:A:804:MET:CE	1:A:831:ILE:HG12	2.32	0.55
1:A:271:VAL:HG23	1:A:282:VAL:HG12	1.88	0.55
1:A:225:HIS:CE1	1:A:304:HIS:CD2	2.95	0.55
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.88	0.55
1:A:373:LEU:N	1:A:374:PRO:HD2	2.22	0.55
1:A:921:PHE:O	1:A:925:VAL:HG23	2.06	0.54
1:A:853:SER:O	1:A:857:THR:HG23	2.07	0.54
1:A:389:HIS:O	1:A:392:GLN:HB3	2.08	0.54
1:A:360:LYS:HE2	1:A:417:SER:HA	1.89	0.54
1:A:903:LYS:O	1:A:906:VAL:HG23	2.08	0.53
1:A:1032:SER:HB3	1:A:1048:ILE:CG2	2.38	0.53
1:A:1042:LEU:HD13	1:A:1042:LEU:O	2.08	0.53
1:A:888:ILE:HD12	1:A:952:ILE:O	2.09	0.53
1:A:887:THR:HG22	1:A:889:ALA:N	2.23	0.53
1:A:273:ARG:NH2	1:A:821:THR:OG1	2.42	0.53
1:A:146:GLU:HB3	1:A:319:ARG:HH22	1.74	0.52
1:A:363:VAL:HG23	1:A:520:LEU:CD1	2.38	0.52
1:A:964:ASP:CB	2:A:1:FAV:H12	2.38	0.52
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:THR:O	1:A:230:SER:HB3	2.10	0.52
1:A:583:LEU:O	1:A:583:LEU:HD23	2.10	0.52
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.39	0.52
1:A:576:TRP:CH2	1:A:579:ARG:HD2	2.45	0.52
1:A:741:MET:CE	1:A:778:GLN:HB2	2.37	0.52
1:A:1043:THR:N	1:A:1047:ASP:OD2	2.41	0.52
1:A:144:SER:OG	1:A:146:GLU:HB2	2.09	0.51
1:A:220:ILE:O	1:A:235:VAL:N	2.43	0.51
1:A:497:PHE:HB2	1:A:1041:GLN:HG3	1.92	0.51
1:A:758:ASP:HB3	1:A:809:LYS:CE	2.40	0.51
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.75	0.51
1:A:875:LYS:HD3	1:A:875:LYS:N	2.25	0.51
2:A:1:FAV:S1	2:A:1:FAV:C13	2.98	0.51
1:A:213:LYS:HD3	1:A:214:LYS:N	2.25	0.51
1:A:752:LEU:O	1:A:753:SER:HB2	2.10	0.51
1:A:777:SER:CB	1:A:778:GLN:HA	2.40	0.51
1:A:1042:LEU:O	1:A:1042:LEU:HD22	2.11	0.51
1:A:233:ILE:HD12	1:A:233:ILE:N	2.26	0.51
1:A:311:PRO:O	1:A:313:PRO:HD3	2.12	0.50
1:A:912:LYS:NZ	1:A:918:GLU:OE2	2.41	0.50
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.94	0.50
1:A:887:THR:CG2	1:A:889:ALA:H	2.25	0.50
1:A:759:VAL:CG1	1:A:760:SER:N	2.72	0.50
1:A:902:PHE:HD2	1:A:1080:TRP:HB3	1.77	0.50
1:A:804:MET:CE	1:A:831:ILE:HG23	2.43	0.49
1:A:1042:LEU:CD1	1:A:1042:LEU:H	2.26	0.49
1:A:774:LEU:O	1:A:776:ASN:N	2.46	0.49
1:A:1002:THR:O	1:A:1003:SER:HB3	2.13	0.49
1:A:583:LEU:CD1	1:A:610:LEU:HD22	2.42	0.49
1:A:244:ILE:HD11	1:A:272:LEU:HD11	1.94	0.49
1:A:692:GLY:HA3	1:A:720:TYR:OH	2.13	0.48
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.76	0.48
1:A:804:MET:HE2	1:A:831:ILE:HG23	1.94	0.48
1:A:848:LEU:HD12	1:A:848:LEU:HA	1.63	0.48
1:A:285:THR:HG22	1:A:289:ASN:HB2	1.96	0.48
1:A:1032:SER:HB3	1:A:1048:ILE:HG21	1.95	0.48
1:A:1039:MET:CB	1:A:1040:PRO:CD	2.90	0.48
1:A:270:PHE:HB3	1:A:307:LEU:HD11	1.96	0.48
1:A:221:PHE:HB3	1:A:232:THR:HG22	1.96	0.48
1:A:887:THR:HG22	1:A:889:ALA:H	1.79	0.48
1:A:221:PHE:HE2	1:A:234:LYS:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:TYR:CE2	1:A:1021:ARG:HD2	2.49	0.47
1:A:1048:ILE:O	1:A:1051:ILE:HG22	2.14	0.47
1:A:293:VAL:O	1:A:297:LEU:HG	2.15	0.47
1:A:842:MET:HG2	1:A:869:CYS:O	2.14	0.47
1:A:472:ARG:O	1:A:473:PHE:HB2	2.14	0.47
1:A:753:SER:OG	1:A:754:ALA:N	2.46	0.47
1:A:767:LEU:HD22	1:A:771:LEU:HG	1.97	0.47
1:A:180:LEU:C	1:A:183:PRO:HD2	2.35	0.47
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.50	0.47
1:A:175:PHE:HA	1:A:178:ARG:NH1	2.30	0.46
1:A:988:THR:HB	1:A:989:PRO:HD2	1.96	0.46
1:A:214:LYS:NZ	1:A:297:LEU:HA	2.30	0.46
1:A:372:VAL:HB	1:A:374:PRO:CD	2.44	0.46
1:A:379:LEU:HD13	1:A:380:THR:HG22	1.98	0.46
1:A:1032:SER:HA	1:A:1048:ILE:HD12	1.98	0.46
1:A:202:VAL:CG1	1:A:203:THR:H	2.28	0.46
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.79	0.46
1:A:867:TYR:CE2	1:A:963:ILE:HG22	2.51	0.46
1:A:760:SER:C	1:A:762:GLN:N	2.68	0.46
1:A:1026:LEU:O	1:A:1029:ILE:HG22	2.15	0.45
1:A:925:VAL:O	1:A:929:VAL:HG23	2.16	0.45
1:A:1002:THR:HG22	1:A:1003:SER:H	1.81	0.45
1:A:721:LEU:HD23	1:A:721:LEU:HA	1.67	0.45
1:A:832:PHE:CE1	1:A:876:ILE:HD11	2.51	0.45
1:A:210:TYR:CE1	1:A:211:LEU:HG	2.51	0.45
1:A:876:ILE:HG21	1:A:876:ILE:HD13	1.64	0.45
1:A:207:LEU:HD23	1:A:208:PRO:HD2	1.99	0.45
1:A:210:TYR:O	1:A:213:LYS:HD2	2.17	0.45
1:A:220:ILE:N	1:A:235:VAL:O	2.48	0.45
1:A:660:LEU:O	1:A:664:VAL:HG23	2.16	0.45
1:A:929:VAL:HG22	1:A:995:MET:HG2	1.99	0.45
1:A:569:ALA:O	1:A:573:GLU:HG3	2.17	0.45
1:A:770:LYS:O	1:A:774:LEU:HG	2.17	0.45
1:A:213:LYS:NZ	1:A:214:LYS:HB2	2.32	0.45
1:A:236:SER:O	1:A:238:ASP:N	2.50	0.45
1:A:760:SER:HB3	1:A:763:VAL:CG1	2.47	0.45
1:A:804:MET:HB2	1:A:810:PRO:HG2	1.99	0.45
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.17	0.45
1:A:892:GLN:HE21	1:A:902:PHE:HD1	1.64	0.45
1:A:287:ILE:H	1:A:287:ILE:HG13	1.67	0.44
1:A:1018:LEU:HD23	1:A:1021:ARG:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:CYS:N	1:A:524:CYS:HG	2.16	0.44
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.53	0.44
1:A:904:ASP:O	1:A:990:ASP:HA	2.18	0.44
1:A:213:LYS:HD3	1:A:214:LYS:H	1.83	0.44
1:A:372:VAL:CB	1:A:374:PRO:HD2	2.45	0.44
1:A:737:GLN:O	1:A:741:MET:HG3	2.17	0.44
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.17	0.44
1:A:1045:LYS:O	1:A:1049:GLU:OE1	2.35	0.44
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.47	0.44
1:A:198:MET:SD	1:A:282:VAL:HG11	2.58	0.44
1:A:304:HIS:CG	1:A:823:LEU:HD21	2.53	0.43
1:A:997:THR:CG2	1:A:998:SER:N	2.81	0.43
1:A:990:ASP:N	1:A:990:ASP:OD1	2.51	0.43
1:A:739:ILE:HG13	1:A:740:GLU:N	2.33	0.43
1:A:1055:LEU:O	1:A:1056:THR:HG22	2.19	0.43
1:A:315:LEU:O	1:A:727:ALA:HB2	2.19	0.43
1:A:915:SER:HA	1:A:916:PRO:HD3	1.89	0.43
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.87	0.43
1:A:784:ARG:NH1	1:A:784:ARG:HG2	2.34	0.43
1:A:992:LEU:HD23	1:A:992:LEU:HA	1.88	0.43
1:A:1042:LEU:HD22	1:A:1042:LEU:C	2.39	0.43
1:A:1082:VAL:HA	1:A:1085:ASN:ND2	2.33	0.43
1:A:888:ILE:HG22	1:A:949:ASN:OD1	2.18	0.43
1:A:309:THR:HA	1:A:310:PRO:HD3	1.90	0.42
1:A:675:SER:O	1:A:679:ARG:HG3	2.19	0.42
1:A:777:SER:HB2	1:A:778:GLN:HA	2.00	0.42
1:A:221:PHE:HA	1:A:233:ILE:O	2.19	0.42
1:A:373:LEU:N	1:A:374:PRO:CD	2.83	0.42
1:A:390:GLY:N	1:A:636:SER:OG	2.45	0.42
1:A:774:LEU:C	1:A:776:ASN:N	2.72	0.42
1:A:246:GLN:C	1:A:248:PHE:H	2.21	0.42
1:A:590:PRO:HD3	1:A:626:LEU:HD21	2.02	0.42
1:A:498:ASN:OD1	1:A:498:ASN:C	2.57	0.42
1:A:270:PHE:HB3	1:A:307:LEU:CD1	2.49	0.42
1:A:1068:PHE:O	1:A:1071:GLN:HB2	2.20	0.42
1:A:235:VAL:HG12	1:A:236:SER:N	2.35	0.42
1:A:467:LEU:O	1:A:476:ARG:HD2	2.20	0.42
1:A:583:LEU:HD12	1:A:610:LEU:HD22	2.01	0.42
1:A:662:GLN:HE22	1:A:850:ILE:CD1	2.33	0.42
1:A:862:LEU:CD2	1:A:862:LEU:N	2.83	0.42
1:A:207:LEU:CD2	1:A:208:PRO:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LEU:CD1	1:A:380:THR:H	2.32	0.41
1:A:359:ARG:HA	1:A:359:ARG:HD3	1.92	0.41
1:A:702:GLU:O	1:A:706:SER:HB3	2.21	0.41
1:A:887:THR:CG2	1:A:889:ALA:HB3	2.50	0.41
1:A:224:ILE:HA	1:A:305:VAL:O	2.20	0.41
1:A:942:LEU:HD23	1:A:942:LEU:HA	1.84	0.41
1:A:214:LYS:O	1:A:214:LYS:HG2	2.21	0.41
1:A:476:ARG:HB3	1:A:520:LEU:HD23	2.03	0.41
1:A:249:PHE:CD1	1:A:268:GLN:OE1	2.74	0.41
1:A:373:LEU:CD2	1:A:406:GLU:HG3	2.49	0.41
1:A:808:LYS:O	1:A:810:PRO:HD3	2.21	0.41
1:A:1032:SER:HB3	1:A:1048:ILE:HG23	2.03	0.41
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.91	0.41
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.86	0.41
1:A:227:SER:C	1:A:229:THR:H	2.24	0.40
1:A:169:HIS:CE1	1:A:466:LEU:CD1	3.04	0.40
1:A:304:HIS:CE1	1:A:823:LEU:HD21	2.57	0.40
1:A:964:ASP:CG	2:A:1:FAV:H12	2.41	0.40
1:A:182:THR:CB	1:A:183:PRO:HD3	2.45	0.40
1:A:840:GLN:O	1:A:844:ILE:HG12	2.21	0.40
1:A:184:ARG:HD3	1:A:719:ALA:O	2.22	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	819/966 (85%)	775 (95%)	40 (5%)	4 (0%)	29	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	775	GLN
1	A	759	VAL
1	A	1040	PRO
1	A	237	PRO

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	748/864 (87%)	693 (93%)	55 (7%)	13	27

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	146	GLU
1	A	147	SER
1	A	207	LEU
1	A	213	LYS
1	A	227	SER
1	A	228	THR
1	A	238	ASP
1	A	252	MET
1	A	269	ASP
1	A	298	LYS
1	A	373	LEU
1	A	379	LEU
1	A	381	VAL
1	A	435	CYS
1	A	476	ARG
1	A	477	ARG
1	A	511	GLU
1	A	520	LEU
1	A	521	ASP
1	A	523	TYR
1	A	549	ASN
1	A	550	GLN

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Mol	Chain	Res	Type
1	A	568	THR
1	A	570	GLU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	626	LEU
1	A	647	LYS
1	A	682	LEU
1	A	707	ARG
1	A	717	LEU
1	A	739	ILE
1	A	760	SER
1	A	765	SER
1	A	767	LEU
1	A	778	GLN
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	865	LEU
1	A	887	THR
1	A	890	LYS
1	A	907	LEU
1	A	926	GLU
1	A	959	ASN
1	A	967	HIS
1	A	1026	LEU
1	A	1042	LEU
1	A	1051	ILE
1	A	1078	LYS
1	A	1086	TRP
1	A	1088	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	HIS
1	A	304	HIS
1	A	778	GLN
1	A	1085	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	FAV	A	1	-	22,27,27	1.34	2 (9%)	30,39,39	1.62	5 (16%)

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	FAV	A	1	-	-	0/8/21/21	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	FAV	C11-S1	4.96	1.78	1.72
2	A	1	FAV	C13-N1	-2.38	1.41	1.44

All (5) bond angle outliers are listed below:

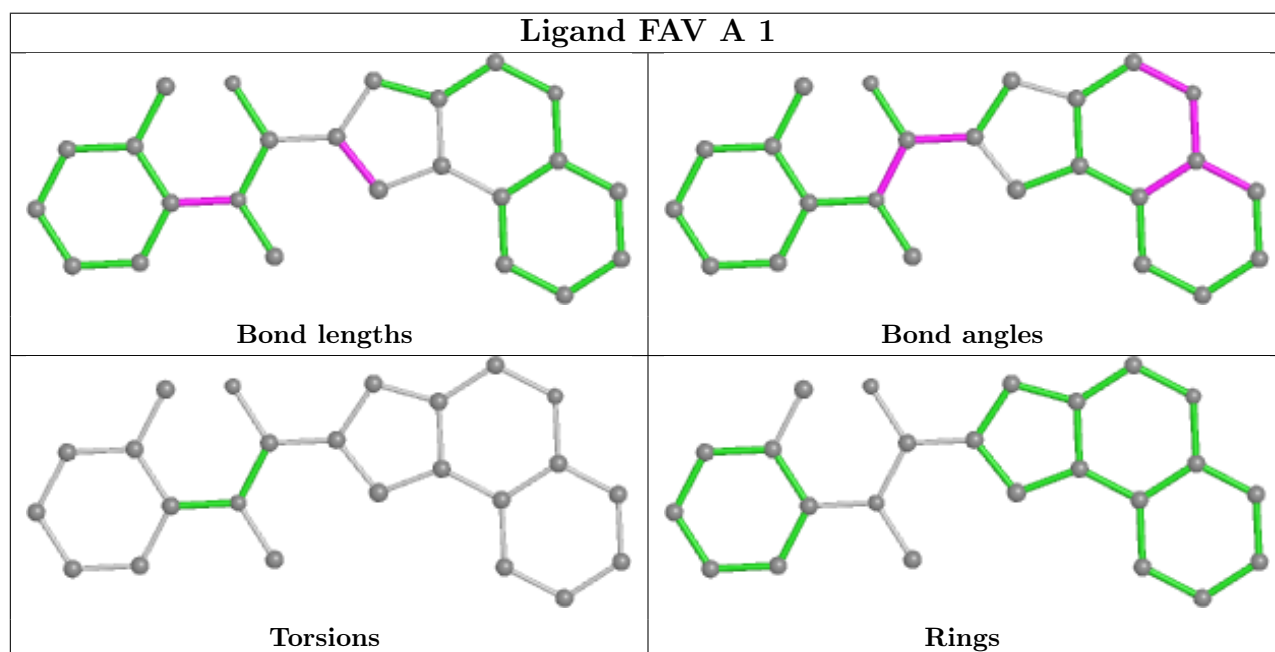| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	FAV	C7-O1-C4	4.69	124.67	112.99
2	A	1	FAV	O1-C4-C3	2.90	121.58	116.88
2	A	1	FAV	O1-C4-C5	2.48	120.89	118.51
2	A	1	FAV	C11-C12-N1	2.45	124.33	118.50
2	A	1	FAV	C3-C4-C5	-2.07	117.53	121.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	FAV	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FAV A 1

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	837/966 (86%)	0.38	80 (9%)	8	7	43, 85, 155, 227	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	ALA	16.5
1	A	1089	HIS	11.5
1	A	322	GLU	9.9
1	A	1086	TRP	8.6
1	A	756	LYS	8.3
1	A	544	ARG	8.1
1	A	143	MET	7.7
1	A	1000	LYS	7.5
1	A	1045	LYS	7.0
1	A	374	PRO	6.8
1	A	1044	SER	6.4
1	A	378	ASP	6.4
1	A	1091	VAL	6.3
1	A	377	THR	6.3
1	A	757	TYR	6.2
1	A	253	ALA	5.8
1	A	216	ALA	5.6
1	A	1046	GLU	5.4
1	A	148	GLN	4.7
1	A	758	ASP	4.7
1	A	981	GLU	4.6
1	A	1043	THR	4.5
1	A	999	GLY	4.5
1	A	982	ARG	4.3
1	A	250	THR	4.3
1	A	759	VAL	4.0
1	A	523	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	267	GLU	4.0
1	A	823	LEU	4.0
1	A	987	LEU	3.7
1	A	998	SER	3.5
1	A	919	GLU	3.5
1	A	1090	LEU	3.4
1	A	212	TRP	3.4
1	A	1084	PHE	3.3
1	A	1062	GLU	3.3
1	A	249	PHE	3.3
1	A	373	LEU	3.2
1	A	967	HIS	3.2
1	A	916	PRO	3.2
1	A	1041	GLN	3.2
1	A	991	PHE	3.1
1	A	488	SER	3.0
1	A	489	GLY	2.9
1	A	269	ASP	2.8
1	A	215	ILE	2.8
1	A	270	PHE	2.8
1	A	932	CYS	2.8
1	A	909	HIS	2.8
1	A	252	MET	2.7
1	A	1007	GLN	2.7
1	A	201	TRP	2.7
1	A	210	TYR	2.7
1	A	1040	PRO	2.6
1	A	809	LYS	2.6
1	A	1088	LEU	2.5
1	A	1015	LYS	2.5
1	A	1042	LEU	2.5
1	A	777	SER	2.5
1	A	859	SER	2.5
1	A	1082	VAL	2.4
1	A	778	GLN	2.4
1	A	930	TYR	2.4
1	A	826	GLU	2.4
1	A	751	SER	2.4
1	A	832	PHE	2.4
1	A	217	ASN	2.3
1	A	808	LYS	2.2
1	A	315	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	431	LEU	2.2
1	A	527	ILE	2.2
1	A	1004	PRO	2.2
1	A	776	ASN	2.1
1	A	1087	PHE	2.1
1	A	522	ASN	2.1
1	A	825	ASN	2.1
1	A	768	LYS	2.1
1	A	755	GLU	2.1
1	A	613	ARG	2.0
1	A	268	GLN	2.0

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

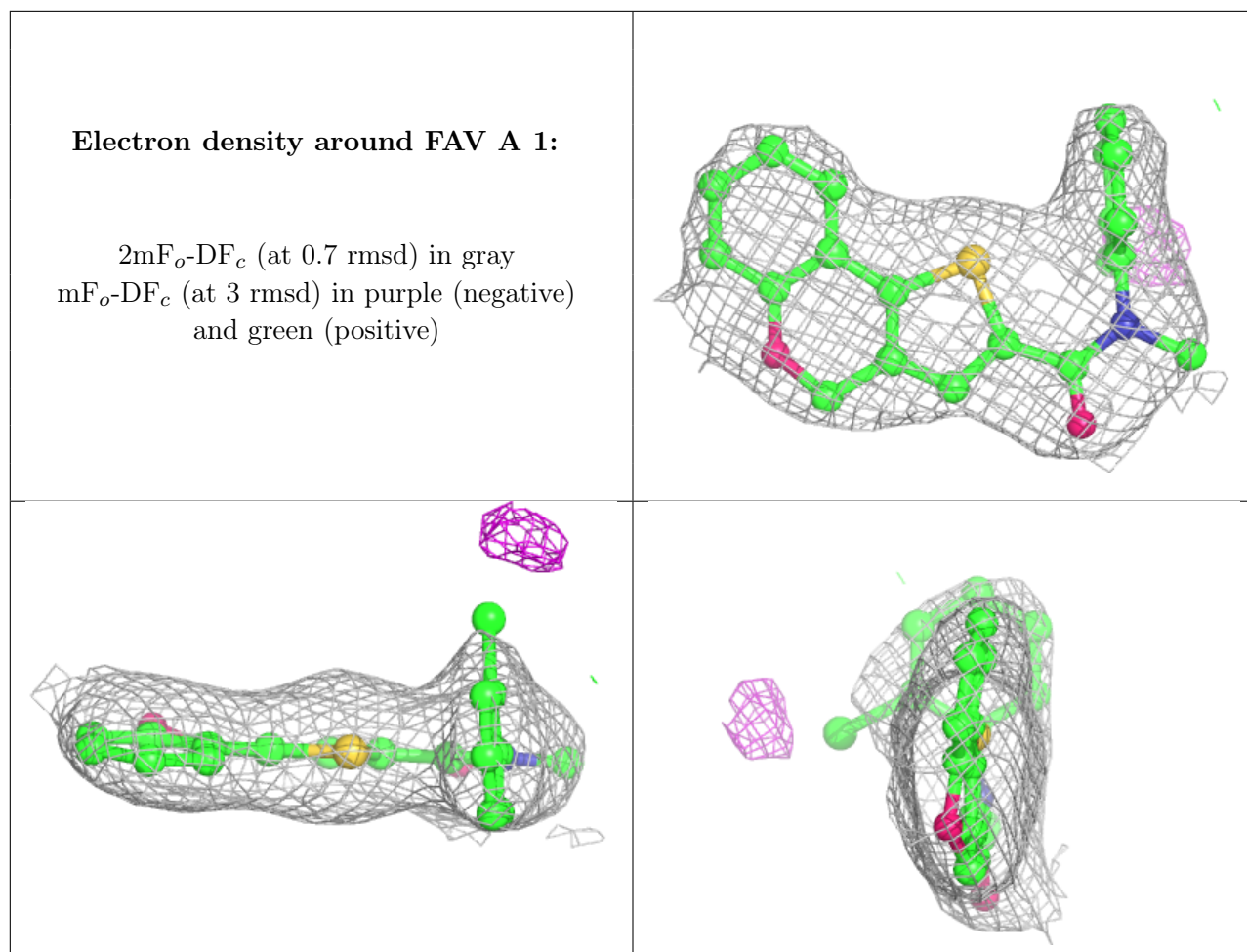There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	FAV	A	1	24/24	0.97	0.11	65,78,88,294	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 FAV A 1:

$2mF_o$-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.