



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:08 AM UTC

PDB ID : 7QA3 / pdb_00007qa3
Title : Crystal structure of PqsR (MvfR) ligand-binding domain in complex with compound N-((2-(4-phenoxyphenyl)thiazol-5-yl)methyl)-2-(trifluoromethyl)pyridin-4-amine
Authors : Schmelz, S.; Blankenfeldt, W.
Deposited on : 2021-11-15
Resolution : 2.67 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

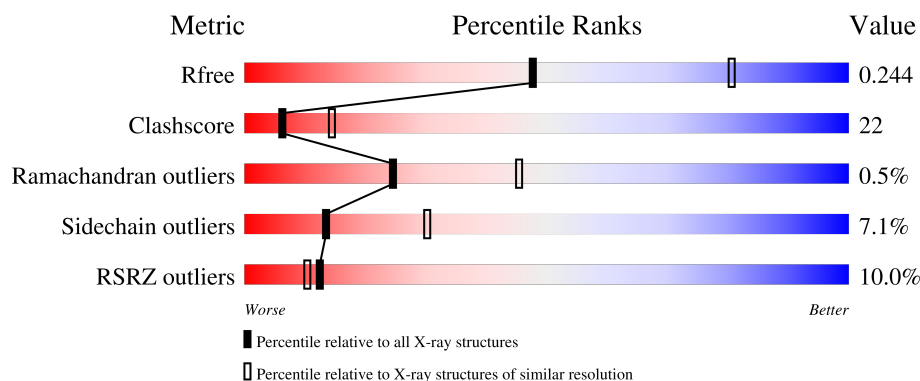
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	332	5% 41% 21% • 38%
1	B	332	8% 34% 24% • • 38%

2 Entry composition [i](#)

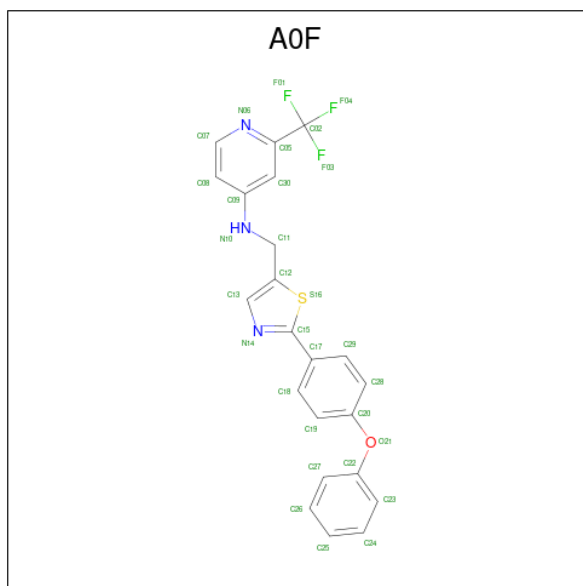
There are 3 unique types of molecules in this entry. The entry contains 6382 atoms, of which 3138 are hydrogens and 0 are deuteriums.

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 Multiple virulence factor regulator MvfR.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	206	Total	C	H	N	O	S		13	1	0
			3141	1010	1551	271	303	6				
1	B	206	Total	C	H	N	O	S		0	2	0
			3145	1011	1555	271	301	7				

- Molecule 2 is N-[[2-(4-phenoxyphenyl)-1,3-thiazol-5-yl]methyl]-2-(trifluoromethyl)pyridin-4-amine (CCD ID: A0F) (formula: C₂₂H₁₆F₃N₃OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	S	0	0
			46	22	3	16	3	1	1		
2	B	1	Total	C	F	H	N	O	S	0	0
			46	22	3	16	3	1	1		

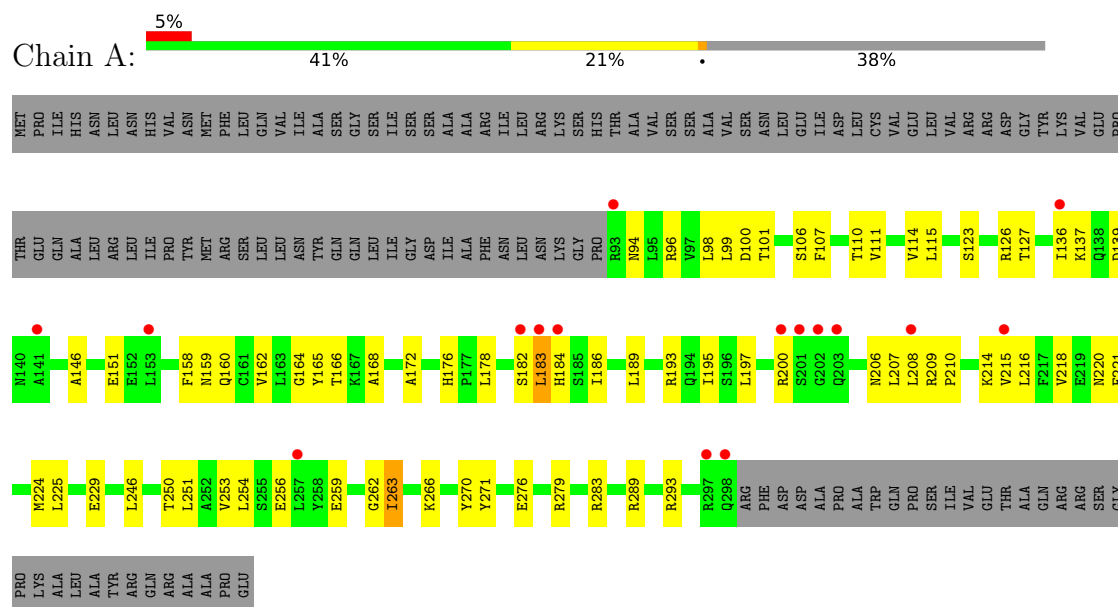
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	O 3	0	0
3	B	1	Total 1	O 1	0	0

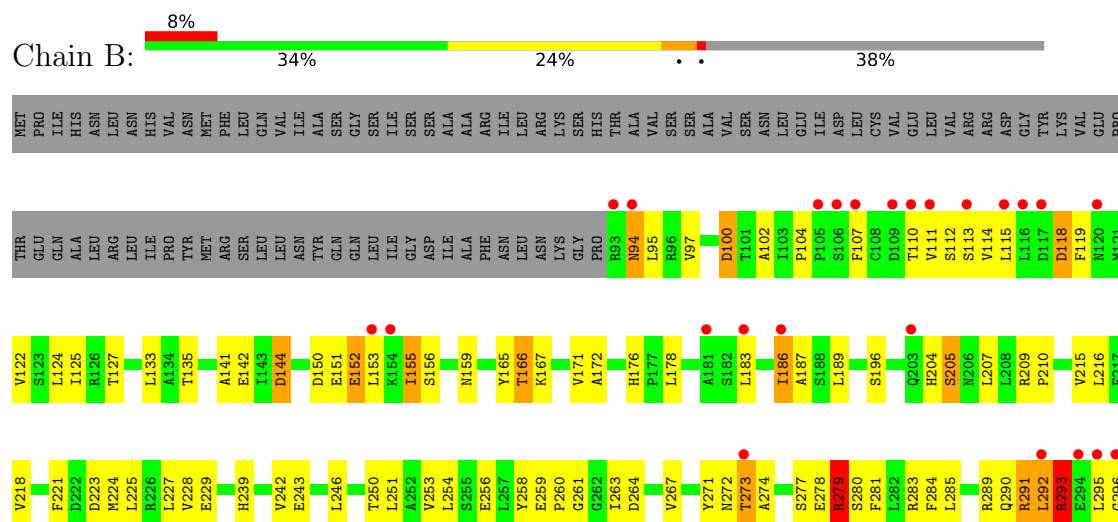
3 Residue-property plots

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: Multiple virulence factor regulator MvfR



• Molecule 1: Multiple virulence factor regulator MvfR



E297	ARG
Q298	PHE
	ASP
	ASP
	ALA
	PRO
	TRP
	GLN
	PRO
	SER
	ILE
	VAL
	GLU
	THR
	ALA
	GLN
	ARG
	ARG
	SER
	GLY
	PRO
	LYS
	ALA
	LEU
	ALA
	TYR
	ARG
	GLN
	ARG
	ALA
	ALA
	PRO
	GLU

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	113.02Å 122.61Å 112.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.86 – 2.67 53.86 – 2.67	Depositor EDS
% Data completeness (in resolution range)	63.8 (53.86-2.67) 59.5 (53.86-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.208 , 0.245 0.208 , 0.244	Depositor DCC
R_{free} test set	692 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6382	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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: A0F

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	0.51	0/1623	0.73	0/2210
1	B	0.60	2/1626 (0.1%)	0.83	5/2214 (0.2%)
All	All	0.56	2/3249 (0.1%)	0.78	5/4424 (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	1
1	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	186	ILE	CB-CG2	5.65	1.71	1.52
1	B	258	TYR	C-N	5.47	1.37	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	VAL	N-CA-C	-7.82	96.34	107.75
1	B	186	ILE	CG1-CB-CG2	6.09	128.97	110.70
1	B	186	ILE	CA-C-O	5.46	126.37	120.47
1	B	293	ARG	NH1-CZ-NH2	-5.22	112.51	119.30
1	B	279	ARG	N-CA-C	-5.17	99.79	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	ARG	Sidechain
1	B	279	ARG	Sidechain
1	B	293	ARG	Sidechain

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	1590	1551	1551	59	0
1	B	1590	1555	1555	84	0
2	A	30	16	0	1	0
2	B	30	16	0	2	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
All	All	3244	3138	3106	141	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 22.

All (141) 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:242[A]:VAL:HG13	1:B:251:LEU:HD23	1.60	0.82
1:A:207:LEU:HD23	1:A:208:LEU:HG	1.65	0.77
1:A:165:TYR:OH	1:B:259:GLU:OE2	2.03	0.76
1:B:224:MET:O	1:B:228:VAL:HG23	1.86	0.76
1:B:290:GLN:HA	1:B:293:ARG:HD2	1.73	0.70
1:B:111:VAL:HG22	1:B:284:PHE:HE1	1.58	0.69
1:A:276:GLU:HB3	1:B:183:LEU:HD22	1.76	0.67
1:A:96:ARG:HB2	1:A:96:ARG:NH1	2.11	0.66
1:B:110:THR:O	1:B:114:VAL:HG22	1.97	0.65
1:A:178:LEU:HD13	1:A:189:LEU:HD23	1.78	0.64
1:A:186:ILE:HD13	1:B:153:LEU:HB3	1.82	0.62
1:B:111:VAL:CG1	1:B:115:LEU:HD12	2.30	0.62
1:A:101:THR:HG23	1:A:127:THR:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:PHE:HD1	1:B:224:MET:HE3	1.66	0.60
1:B:95:LEU:HD12	1:B:115:LEU:HD22	1.82	0.60
1:B:171:VAL:HG11	1:B:242[A]:VAL:HG11	1.83	0.60
1:A:107:PHE:O	1:A:111:VAL:HG23	2.01	0.60
1:B:166:THR:HG22	1:B:267:VAL:HG23	1.83	0.59
1:A:176:HIS:CE1	1:A:178:LEU:HD12	2.37	0.59
1:A:271:TYR:HE1	1:A:276:GLU:HG2	1.67	0.59
1:B:151:GLU:OE1	1:B:152:GLU:N	2.35	0.59
1:A:225:LEU:O	1:A:229:GLU:HG3	2.02	0.58
1:B:115:LEU:O	1:B:119:PHE:HD1	1.86	0.58
1:B:281:PHE:CZ	1:B:285:LEU:HD11	2.38	0.58
1:B:111:VAL:HG13	1:B:115:LEU:HD12	1.86	0.57
1:B:100:ASP:OD1	1:B:100:ASP:C	2.47	0.57
1:A:98:LEU:C	1:A:99:LEU:HD12	2.30	0.56
1:A:209:ARG:HG3	1:A:209:ARG:HH11	1.69	0.56
1:B:242[A]:VAL:CG1	1:B:251:LEU:HD23	2.34	0.56
1:B:104:PRO:HG2	1:B:295:LEU:HD21	1.87	0.56
1:B:291:ARG:HG3	1:B:292:LEU:N	2.21	0.56
1:B:159:ASN:OD1	1:B:273:THR:HG22	2.06	0.56
1:B:189:LEU:HD21	1:B:254:LEU:HD12	1.88	0.56
1:A:189:LEU:HD21	1:A:254:LEU:HD23	1.88	0.55
1:B:221:PHE:CD1	1:B:224:MET:HE3	2.41	0.54
1:B:278:GLU:HG3	1:B:279:ARG:N	2.22	0.54
2:B:401:A0F:C08	2:B:401:A0F:C13	2.85	0.54
1:B:239:HIS:NE2	1:B:243:GLU:HG3	2.22	0.54
1:B:111:VAL:HG22	1:B:284:PHE:CE1	2.41	0.54
1:B:95:LEU:HD22	1:B:144:ASP:HB2	1.89	0.53
1:A:195:ILE:HD12	1:A:216:LEU:HB3	1.91	0.53
1:B:209:ARG:HG2	1:B:209:ARG:HH11	1.73	0.53
1:B:186:ILE:HG23	1:B:187:ALA:N	2.24	0.52
1:A:164:GLY:C	1:A:165:TYR:CD1	2.88	0.52
1:B:272:ASN:C	1:B:274:ALA:H	2.18	0.52
1:B:100:ASP:HA	1:B:127:THR:O	2.09	0.52
1:A:176:HIS:HE1	1:A:178:LEU:HD12	1.75	0.52
1:A:136:ILE:HG21	1:A:146:ALA:HB2	1.92	0.52
1:B:172:ALA:O	1:B:251:LEU:HD12	2.10	0.52
1:B:94:ASN:N	1:B:94:ASN:OD1	2.38	0.52
1:A:253:VAL:C	1:A:254:LEU:HD12	2.35	0.51
1:A:184:HIS:HB3	2:A:401:A0F:C26	2.40	0.51
1:A:172:ALA:O	1:A:251:LEU:HD12	2.11	0.50
1:B:176:HIS:CE1	1:B:178:LEU:HD12	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASP:C	1:A:100:ASP:OD1	2.54	0.50
1:A:229:GLU:OE1	1:A:250:THR:CG2	2.60	0.50
1:A:183:LEU:O	1:A:184:HIS:ND1	2.45	0.49
1:B:210:PRO:HB2	1:B:215:VAL:HG21	1.93	0.49
1:B:144:ASP:N	1:B:144:ASP:OD1	2.46	0.49
1:B:229:GLU:OE2	1:B:250:THR:HG21	2.12	0.49
1:A:209:ARG:HG3	1:A:209:ARG:NH1	2.28	0.49
1:B:205:SER:C	1:B:207:LEU:N	2.70	0.49
1:B:215:VAL:HG12	1:B:216:LEU:N	2.28	0.49
1:B:218:VAL:HG21	1:B:224:MET:HB2	1.94	0.49
1:A:246:LEU:HD23	1:A:251:LEU:O	2.13	0.49
1:B:165:TYR:CE2	1:B:264:ASP:HB3	2.48	0.48
1:A:151:GLU:OE1	1:A:160:GLN:NE2	2.46	0.48
1:A:195:ILE:HG22	1:A:224:MET:HG3	1.94	0.48
1:B:178:LEU:HD13	1:B:189:LEU:HD23	1.94	0.48
1:A:162:VAL:HG21	1:A:266:LYS:HE2	1.96	0.48
1:B:263:ILE:HG21	2:B:401:A0F:S16	2.54	0.48
1:A:164:GLY:C	1:A:165:TYR:HD1	2.22	0.48
1:B:246:LEU:HD23	1:B:251:LEU:O	2.14	0.48
1:B:242[A]:VAL:HG12	1:B:246:LEU:HG	1.95	0.47
1:A:207:LEU:HD23	1:A:208:LEU:CG	2.38	0.47
1:B:285:LEU:O	1:B:289:ARG:HG3	2.14	0.47
1:A:168:ALA:O	1:A:263:ILE:HG13	2.14	0.47
1:A:159:ASN:O	1:A:270:TYR:HA	2.15	0.47
1:B:271:TYR:CB	1:B:281:PHE:CZ	2.98	0.47
1:A:225:LEU:HD11	1:A:251:LEU:HD21	1.97	0.46
1:A:253:VAL:CG1	1:A:256:GLU:HG2	2.45	0.46
1:A:193:ARG:HA	1:A:214:LYS:O	2.16	0.46
1:B:95:LEU:CD1	1:B:115:LEU:HD22	2.46	0.46
1:A:197:LEU:HD11	1:A:221:PHE:CZ	2.51	0.45
1:A:96:ARG:HB2	1:A:96:ARG:HH11	1.82	0.45
1:A:210:PRO:HB2	1:A:215:VAL:HG21	1.99	0.45
1:B:133:LEU:CD1	1:B:150:ASP:HB3	2.47	0.45
1:B:111:VAL:HG12	1:B:115:LEU:HD12	1.97	0.45
1:A:215:VAL:HG12	1:A:216:LEU:N	2.32	0.44
1:B:111:VAL:HG13	1:B:115:LEU:CD1	2.47	0.44
1:B:111:VAL:HA	1:B:114:VAL:CG2	2.47	0.44
1:A:178:LEU:HD13	1:A:189:LEU:CD2	2.46	0.44
1:B:118:ASP:HB2	1:B:280:SER:OG	2.17	0.44
1:B:204:HIS:O	1:B:205:SER:C	2.61	0.43
1:B:250:THR:O	1:B:250:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ARG:HG3	1:B:280:SER:H	1.83	0.43
1:B:215:VAL:CG1	1:B:216:LEU:N	2.81	0.43
1:B:289:ARG:O	1:B:293:ARG:HD2	2.18	0.43
1:A:197:LEU:HD11	1:A:221:PHE:CE1	2.54	0.43
1:A:253:VAL:HG11	1:A:256:GLU:HG2	2.00	0.43
1:B:97:VAL:HB	1:B:124:LEU:HD23	2.01	0.43
1:A:98:LEU:C	1:A:98:LEU:HD23	2.44	0.43
1:B:223:ASP:O	1:B:227:LEU:HD13	2.19	0.43
1:B:271:TYR:CG	1:B:281:PHE:CZ	3.07	0.43
1:B:165:TYR:CD2	1:B:264:ASP:HB3	2.54	0.42
1:A:289:ARG:O	1:A:293:ARG:HG3	2.19	0.42
1:A:94:ASN:N	1:A:94:ASN:OD1	2.50	0.42
1:A:100:ASP:HA	1:A:127:THR:O	2.18	0.42
1:B:281:PHE:O	1:B:285:LEU:HD13	2.19	0.42
1:B:133:LEU:HD22	1:B:155:ILE:HD11	2.00	0.42
1:B:256:GLU:O	1:B:260:PRO:HG3	2.19	0.42
1:A:159:ASN:HB2	1:A:271:TYR:CE1	2.54	0.42
1:A:279:ARG:HD2	1:A:283:ARG:NH1	2.35	0.42
1:A:110:THR:O	1:A:114:VAL:HG23	2.19	0.42
1:A:218:VAL:HG21	1:A:224:MET:HB2	2.02	0.42
1:A:259:GLU:HG2	1:A:262:GLY:O	2.19	0.42
1:A:100:ASP:O	1:A:126:ARG:NH1	2.53	0.42
1:B:95:LEU:HD23	1:B:95:LEU:HA	1.75	0.42
1:B:107:PHE:CE1	1:B:292:LEU:HD22	2.54	0.42
1:B:167:LYS:CD	1:B:261:GLY:O	2.68	0.42
1:B:107:PHE:HA	1:B:291:ARG:HD2	2.02	0.41
1:A:253:VAL:CG1	1:A:253:VAL:O	2.68	0.41
1:B:205:SER:C	1:B:207:LEU:H	2.27	0.41
1:B:107:PHE:CD1	1:B:292:LEU:HD22	2.55	0.41
1:A:101:THR:HG23	1:A:127:THR:C	2.45	0.41
1:A:220:ASN:OD1	1:A:220:ASN:C	2.62	0.41
1:B:141:ALA:O	1:B:142:GLU:C	2.64	0.41
1:B:253:VAL:O	1:B:253:VAL:HG23	2.20	0.41
1:A:136:ILE:HD12	1:A:158:PHE:CD2	2.56	0.41
1:B:281:PHE:CE2	1:B:285:LEU:HD11	2.57	0.40
1:A:206:ASN:ND2	1:A:209:ARG:HH21	2.19	0.40
1:B:100:ASP:OD1	1:B:102:ALA:N	2.48	0.40
1:B:221:PHE:O	1:B:225:LEU:HD23	2.21	0.40
1:B:242[A]:VAL:HG13	1:B:251:LEU:CD2	2.41	0.40
1:B:167:LYS:HD3	1:B:261:GLY:O	2.22	0.40
1:A:136:ILE:HG13	1:A:137:LYS:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:SER:O	1:B:114:VAL:C	2.63	0.40
1:B:271:TYR:HB3	1:B:281:PHE:CZ	2.57	0.40
1:B:279:ARG:O	1:B:283:ARG:HG2	2.22	0.40
1:B:296:GLY:O	1:B:297:ARG:C	2.65	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	205/332 (62%)	192 (94%)	13 (6%)	0	100	100
1	B	206/332 (62%)	189 (92%)	15 (7%)	2 (1%)	12	28
All	All	411/664 (62%)	381 (93%)	28 (7%)	2 (0%)	24	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	THR
1	B	279	ARG

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/288 (59%)	163 (95%)	8 (5%)	23	47
1	B	172/288 (60%)	156 (91%)	16 (9%)	8	19
All	All	343/576 (60%)	319 (93%)	24 (7%)	13	31

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	A	115	LEU
1	A	123	SER
1	A	139	ASP
1	A	166	THR
1	A	182	SER
1	A	183	LEU
1	A	263	ILE
1	B	94	ASN
1	B	100	ASP
1	B	112	SER
1	B	118	ASP
1	B	125	ILE
1	B	135	THR
1	B	144	ASP
1	B	152	GLU
1	B	155	ILE
1	B	156	SER
1	B	166	THR
1	B	196	SER
1	B	205	SER
1	B	277	SER
1	B	291	ARG
1	B	292	LEU

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	159	ASN
1	B	160	GLN
1	B	176	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A0F	B	401	-	33,33,33	1.83	5 (15%)	42,46,46	2.85	16 (38%)
2	A0F	A	401	-	33,33,33	2.05	6 (18%)	42,46,46	2.20	14 (33%)

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	A0F	B	401	-	-	1/19/19/19	0/4/4/4
2	A0F	A	401	-	-	3/19/19/19	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	A0F	C13-N14	6.12	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	A0F	C15-S16	-4.74	1.63	1.74
2	A	401	A0F	C12-S16	-4.72	1.58	1.73
2	A	401	A0F	C17-C15	4.43	1.54	1.47
2	A	401	A0F	C15-S16	-4.30	1.64	1.74
2	B	401	A0F	C12-S16	-4.20	1.60	1.73
2	B	401	A0F	C17-C15	4.11	1.53	1.47
2	B	401	A0F	C13-N14	4.02	1.45	1.37
2	B	401	A0F	C09-N10	2.87	1.46	1.38
2	A	401	A0F	C09-N10	2.60	1.46	1.38
2	A	401	A0F	C15-N14	2.31	1.40	1.32

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	A0F	S16-C15-N14	-6.90	107.96	113.97
2	B	401	A0F	C18-C17-C15	6.28	130.29	120.75
2	B	401	A0F	C29-C17-C15	-6.21	111.30	120.75
2	A	401	A0F	S16-C15-N14	-5.97	108.77	113.97
2	B	401	A0F	C17-C15-S16	5.86	133.93	122.09
2	B	401	A0F	C17-C15-N14	-5.47	118.06	123.85
2	A	401	A0F	C18-C17-C15	4.73	127.94	120.75
2	B	401	A0F	C11-C12-C13	-4.63	122.60	128.12
2	B	401	A0F	F04-C02-C05	-4.20	105.04	112.43
2	A	401	A0F	C29-C17-C15	-4.15	114.43	120.75
2	B	401	A0F	F01-C02-C05	-4.14	105.14	112.43
2	B	401	A0F	C08-C09-C30	-4.03	114.78	119.66
2	A	401	A0F	C17-C15-S16	3.89	129.94	122.09
2	A	401	A0F	C08-C09-C30	-3.72	115.16	119.66
2	A	401	A0F	C12-C13-N14	-3.55	110.33	117.00
2	B	401	A0F	C11-C12-S16	3.53	128.62	120.70
2	A	401	A0F	F04-C02-C05	-3.52	106.24	112.43
2	A	401	A0F	O21-C20-C19	3.15	130.32	119.36
2	B	401	A0F	C12-C13-N14	-2.99	111.38	117.00
2	B	401	A0F	F03-C02-F01	2.86	116.10	105.77
2	A	401	A0F	C19-C20-C28	-2.65	116.29	120.16
2	B	401	A0F	O21-C20-C19	2.54	128.22	119.36
2	B	401	A0F	C07-C08-C09	2.54	122.21	118.88
2	A	401	A0F	C29-C28-C20	2.45	122.53	119.73
2	A	401	A0F	C17-C15-N14	-2.42	121.28	123.85
2	B	401	A0F	C08-C07-N06	-2.37	121.08	123.97
2	A	401	A0F	C11-C12-C13	-2.34	125.33	128.12
2	A	401	A0F	F01-C02-C05	-2.30	108.39	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	A0F	O21-C20-C28	-2.17	111.81	119.36
2	A	401	A0F	C12-C11-N10	2.15	116.75	112.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

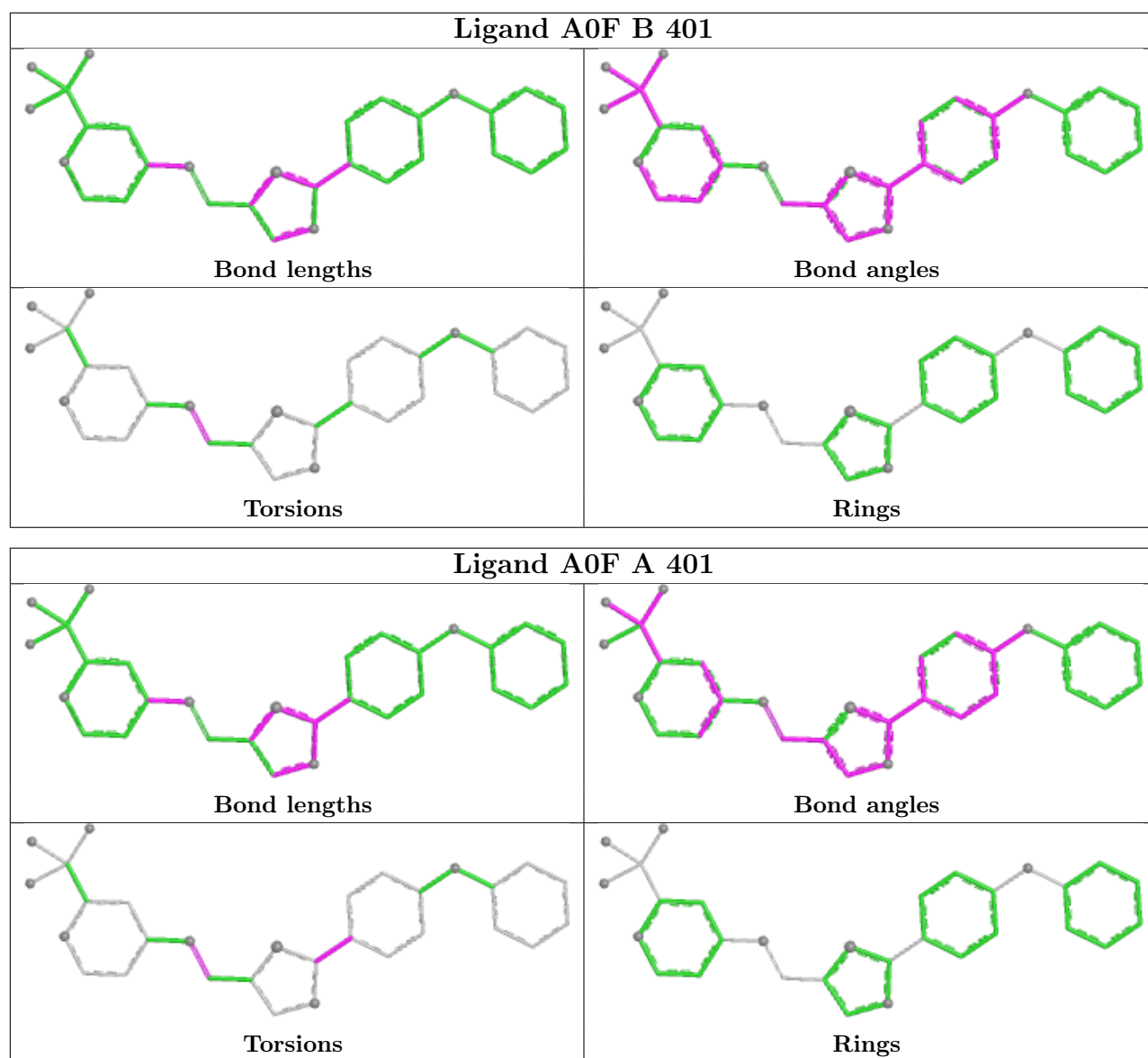
Mol	Chain	Res	Type	Atoms
2	A	401	A0F	C12-C11-N10-C09
2	B	401	A0F	C12-C11-N10-C09
2	A	401	A0F	N14-C15-C17-C18
2	A	401	A0F	N14-C15-C17-C29

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	A0F	2	0
2	A	401	A0F	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	206/332 (62%)	0.44	16 (7%) 19 16	31, 64, 108, 139	1 (0%)
1	B	206/332 (62%)	0.80	25 (12%) 8 7	40, 73, 125, 142	2 (0%)
All	All	412/664 (62%)	0.62	41 (9%) 12 10	31, 69, 119, 142	3 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	GLN	7.6
1	A	298	GLN	4.9
1	B	107	PHE	4.4
1	A	93	ARG	4.1
1	B	203	GLN	4.0
1	A	153	LEU	3.9
1	A	297	ARG	3.7
1	B	111	VAL	3.7
1	A	202	GLY	3.6
1	B	181	ALA	3.5
1	B	120	ASN	3.2
1	B	295	LEU	3.2
1	B	109	ASP	3.1
1	B	186	ILE	3.1
1	A	208	LEU	3.0
1	A	215	VAL	3.0
1	A	184	HIS	2.9
1	B	296	GLY	2.9
1	B	106	SER	2.9
1	B	94	ASN	2.9
1	B	153	LEU	2.8
1	B	93	ARG	2.8
1	A	200	ARG	2.5
1	B	117	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	2.4
1	B	294	GLU	2.4
1	A	201	SER	2.4
1	A	141	ALA	2.4
1	A	182	SER	2.3
1	A	183	LEU	2.3
1	A	136	ILE	2.2
1	B	292	LEU	2.2
1	B	273	THR	2.2
1	B	110	THR	2.2
1	B	183	LEU	2.2
1	B	297	ARG	2.1
1	A	257	LEU	2.1
1	B	154	LYS	2.1
1	B	116	LEU	2.1
1	B	105	PRO	2.1
1	B	113	SER	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

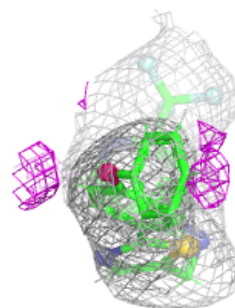
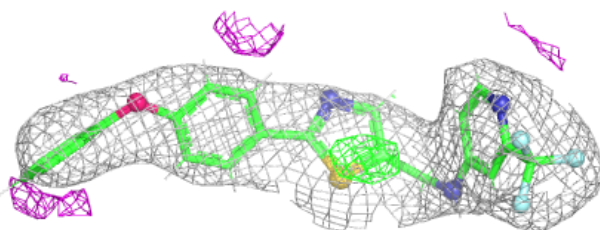
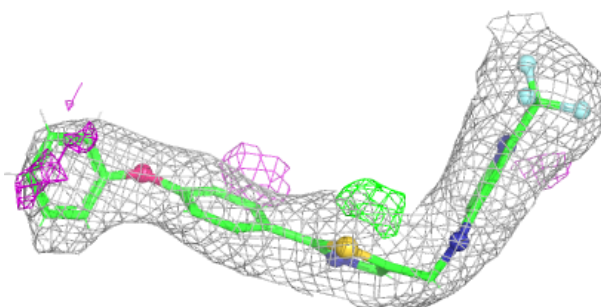
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A0F	A	401	30/30	0.96	0.11	19,49,71,87	0
2	A0F	B	401	30/30	0.96	0.09	32,43,63,77	0

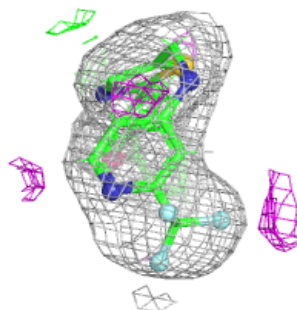
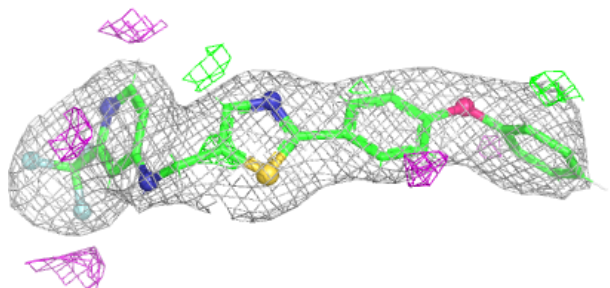
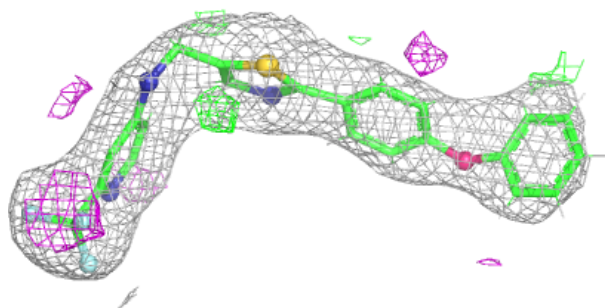
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A0F A 401:

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

**Electron density around A0F B 401:**

$2mF_o-DF_c$ (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.