Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 06:03 PM EST

PDB ID	:	3TT0
Title	:	Co-structure of Fibroblast Growth Factor Receptor 1 kinase domain with 3-(2,6-dichloro-3,5-dimethoxy-phenyl)-1-{6-[4-(4-ethyl-piperazin-1-yl)-phenylamino]-pyrimidin-4-yl}-1-methyl-urea (BGJ398)
Authors	:	Bussiere, D.E.; Murray, J.M.; Shu, W.
Deposited on	:	2011-09-13
Resolution	:	2.80 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:

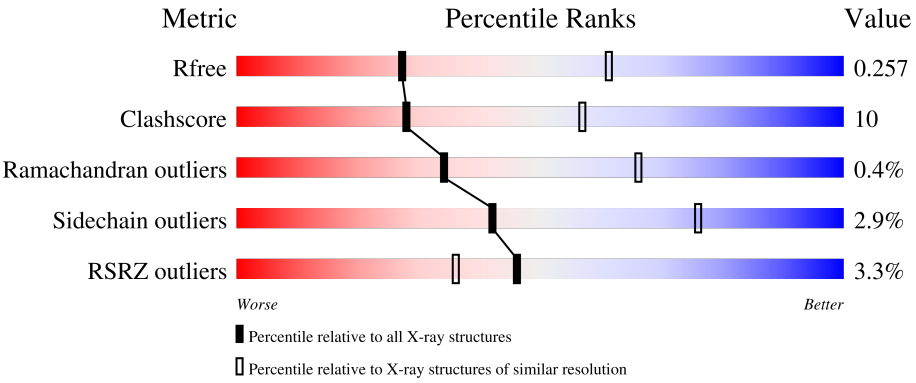
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	382	2% 66% 13% · 20%
1	B	382	3% 56% 14% · 29%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	791	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5056 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 Basic fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2409	1527	412	453	17			
1	B	272	Total	C	N	O	S	0	4	0
			2120	1347	358	396	19			

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	MET	-	expression tag	UNP P11362
A	409	GLY	-	expression tag	UNP P11362
A	410	TYR	-	expression tag	UNP P11362
A	411	TYR	-	expression tag	UNP P11362
A	412	HIS	-	expression tag	UNP P11362
A	413	HIS	-	expression tag	UNP P11362
A	414	HIS	-	expression tag	UNP P11362
A	415	HIS	-	expression tag	UNP P11362
A	416	HIS	-	expression tag	UNP P11362
A	417	HIS	-	expression tag	UNP P11362
A	418	ASP	-	expression tag	UNP P11362
A	419	TYR	-	expression tag	UNP P11362
A	420	ASP	-	expression tag	UNP P11362
A	421	ILE	-	expression tag	UNP P11362
A	422	PRO	-	expression tag	UNP P11362
A	423	THR	-	expression tag	UNP P11362
A	424	THR	-	expression tag	UNP P11362
A	425	GLU	-	expression tag	UNP P11362
A	426	ASN	-	expression tag	UNP P11362
A	427	LEU	-	expression tag	UNP P11362
A	428	TYR	-	expression tag	UNP P11362
A	429	PHE	-	expression tag	UNP P11362
A	430	ASN	-	expression tag	UNP P11362
A	431	GLY	-	expression tag	UNP P11362
A	432	MET	-	expression tag	UNP P11362

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Chain	Residue	Modelled	Actual	Comment	Reference
A	433	GLY	-	expression tag	UNP P11362
A	434	TYR	-	expression tag	UNP P11362
A	435	TYR	-	expression tag	UNP P11362
A	436	HIS	-	expression tag	UNP P11362
A	437	HIS	-	expression tag	UNP P11362
A	438	HIS	-	expression tag	UNP P11362
A	439	HIS	-	expression tag	UNP P11362
A	440	HIS	-	expression tag	UNP P11362
A	441	HIS	-	expression tag	UNP P11362
A	442	ASP	-	expression tag	UNP P11362
A	443	TYR	-	expression tag	UNP P11362
A	444	ASP	-	expression tag	UNP P11362
A	445	ILE	-	expression tag	UNP P11362
A	446	PRO	-	expression tag	UNP P11362
A	447	THR	-	expression tag	UNP P11362
A	448	THR	-	expression tag	UNP P11362
A	449	GLU	-	expression tag	UNP P11362
A	450	ASN	-	expression tag	UNP P11362
A	451	LEU	-	expression tag	UNP P11362
A	452	TYR	-	expression tag	UNP P11362
A	453	PHE	-	expression tag	UNP P11362
A	454	GLN	-	expression tag	UNP P11362
A	455	GLY	-	expression tag	UNP P11362
A	488	ALA	CYS	conflict	UNP P11362
A	584	SER	CYS	engineered mutation	UNP P11362
A	766	MET	-	expression tag	UNP P11362
A	767	GLY	-	expression tag	UNP P11362
A	768	TYR	-	expression tag	UNP P11362
A	769	TYR	-	expression tag	UNP P11362
A	770	HIS	-	expression tag	UNP P11362
A	771	HIS	-	expression tag	UNP P11362
A	772	HIS	-	expression tag	UNP P11362
A	773	HIS	-	expression tag	UNP P11362
A	774	HIS	-	expression tag	UNP P11362
A	775	HIS	-	expression tag	UNP P11362
A	776	ASP	-	expression tag	UNP P11362
A	777	TYR	-	expression tag	UNP P11362
A	778	ASP	-	expression tag	UNP P11362
A	779	ILE	-	expression tag	UNP P11362
A	780	PRO	-	expression tag	UNP P11362
A	781	THR	-	expression tag	UNP P11362
A	782	THR	-	expression tag	UNP P11362

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Chain	Residue	Modelled	Actual	Comment	Reference
A	783	GLU	-	expression tag	UNP P11362
A	784	ASN	-	expression tag	UNP P11362
A	785	LEU	-	expression tag	UNP P11362
A	786	TYR	-	expression tag	UNP P11362
A	787	PHE	-	expression tag	UNP P11362
A	788	ASN	-	expression tag	UNP P11362
A	789	GLY	-	expression tag	UNP P11362
B	408	MET	-	expression tag	UNP P11362
B	409	GLY	-	expression tag	UNP P11362
B	410	TYR	-	expression tag	UNP P11362
B	411	TYR	-	expression tag	UNP P11362
B	412	HIS	-	expression tag	UNP P11362
B	413	HIS	-	expression tag	UNP P11362
B	414	HIS	-	expression tag	UNP P11362
B	415	HIS	-	expression tag	UNP P11362
B	416	HIS	-	expression tag	UNP P11362
B	417	HIS	-	expression tag	UNP P11362
B	418	ASP	-	expression tag	UNP P11362
B	419	TYR	-	expression tag	UNP P11362
B	420	ASP	-	expression tag	UNP P11362
B	421	ILE	-	expression tag	UNP P11362
B	422	PRO	-	expression tag	UNP P11362
B	423	THR	-	expression tag	UNP P11362
B	424	THR	-	expression tag	UNP P11362
B	425	GLU	-	expression tag	UNP P11362
B	426	ASN	-	expression tag	UNP P11362
B	427	LEU	-	expression tag	UNP P11362
B	428	TYR	-	expression tag	UNP P11362
B	429	PHE	-	expression tag	UNP P11362
B	430	ASN	-	expression tag	UNP P11362
B	431	GLY	-	expression tag	UNP P11362
B	432	MET	-	expression tag	UNP P11362
B	433	GLY	-	expression tag	UNP P11362
B	434	TYR	-	expression tag	UNP P11362
B	435	TYR	-	expression tag	UNP P11362
B	436	HIS	-	expression tag	UNP P11362
B	437	HIS	-	expression tag	UNP P11362
B	438	HIS	-	expression tag	UNP P11362
B	439	HIS	-	expression tag	UNP P11362
B	440	HIS	-	expression tag	UNP P11362
B	441	HIS	-	expression tag	UNP P11362
B	442	ASP	-	expression tag	UNP P11362

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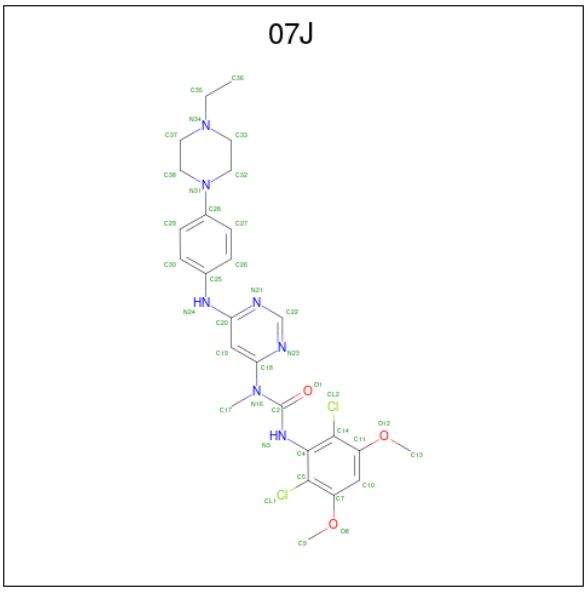
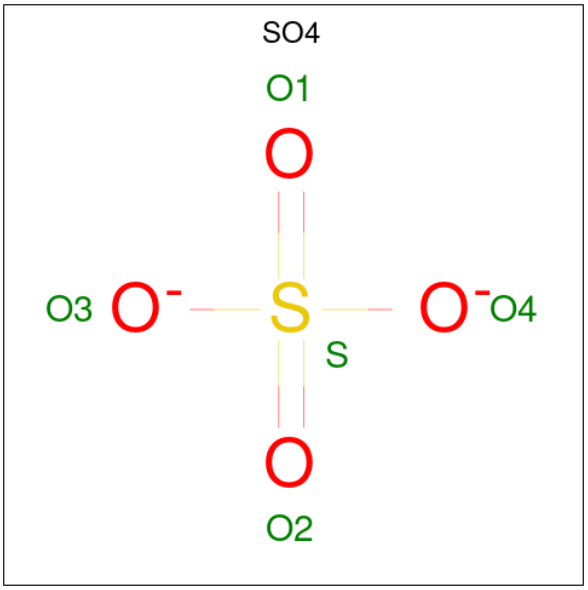
Chain	Residue	Modelled	Actual	Comment	Reference
B	443	TYR	-	expression tag	UNP P11362
B	444	ASP	-	expression tag	UNP P11362
B	445	ILE	-	expression tag	UNP P11362
B	446	PRO	-	expression tag	UNP P11362
B	447	THR	-	expression tag	UNP P11362
B	448	THR	-	expression tag	UNP P11362
B	449	GLU	-	expression tag	UNP P11362
B	450	ASN	-	expression tag	UNP P11362
B	451	LEU	-	expression tag	UNP P11362
B	452	TYR	-	expression tag	UNP P11362
B	453	PHE	-	expression tag	UNP P11362
B	454	GLN	-	expression tag	UNP P11362
B	455	GLY	-	expression tag	UNP P11362
B	488	ALA	CYS	conflict	UNP P11362
B	584	SER	CYS	engineered mutation	UNP P11362
B	766	MET	-	expression tag	UNP P11362
B	767	GLY	-	expression tag	UNP P11362
B	768	TYR	-	expression tag	UNP P11362
B	769	TYR	-	expression tag	UNP P11362
B	770	HIS	-	expression tag	UNP P11362
B	771	HIS	-	expression tag	UNP P11362
B	772	HIS	-	expression tag	UNP P11362
B	773	HIS	-	expression tag	UNP P11362
B	774	HIS	-	expression tag	UNP P11362
B	775	HIS	-	expression tag	UNP P11362
B	776	ASP	-	expression tag	UNP P11362
B	777	TYR	-	expression tag	UNP P11362
B	778	ASP	-	expression tag	UNP P11362
B	779	ILE	-	expression tag	UNP P11362
B	780	PRO	-	expression tag	UNP P11362
B	781	THR	-	expression tag	UNP P11362
B	782	THR	-	expression tag	UNP P11362
B	783	GLU	-	expression tag	UNP P11362
B	784	ASN	-	expression tag	UNP P11362
B	785	LEU	-	expression tag	UNP P11362
B	786	TYR	-	expression tag	UNP P11362
B	787	PHE	-	expression tag	UNP P11362
B	788	ASN	-	expression tag	UNP P11362
B	789	GLY	-	expression tag	UNP P11362

- Molecule 2 is 3-(2,6-dichloro-3,5-dimethoxyphenyl)-1-(6-{[4-(4-ethylpiperazin-1-yl)phenyl]amino}pyrimidin-4-yl)-1-methylurea (three-letter code: 07J) (formula: $C_{26}H_{31}Cl_2N_7O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			38	26	2	7	3		
2	B	1	Total	C	Cl	N	O	0	0
			38	26	2	7	3		

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



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

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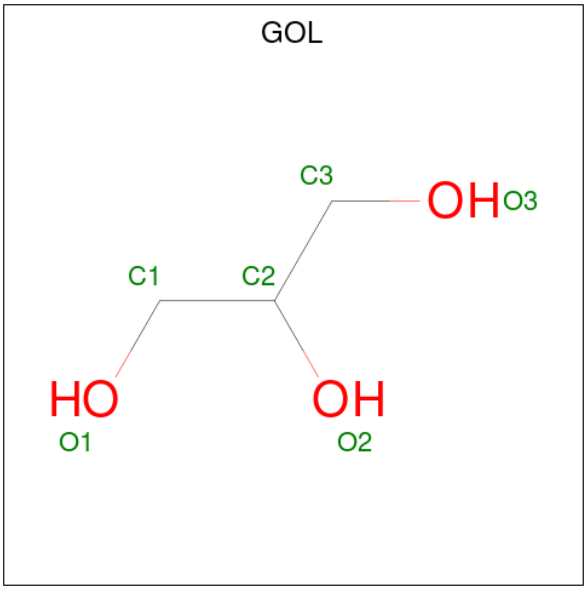
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

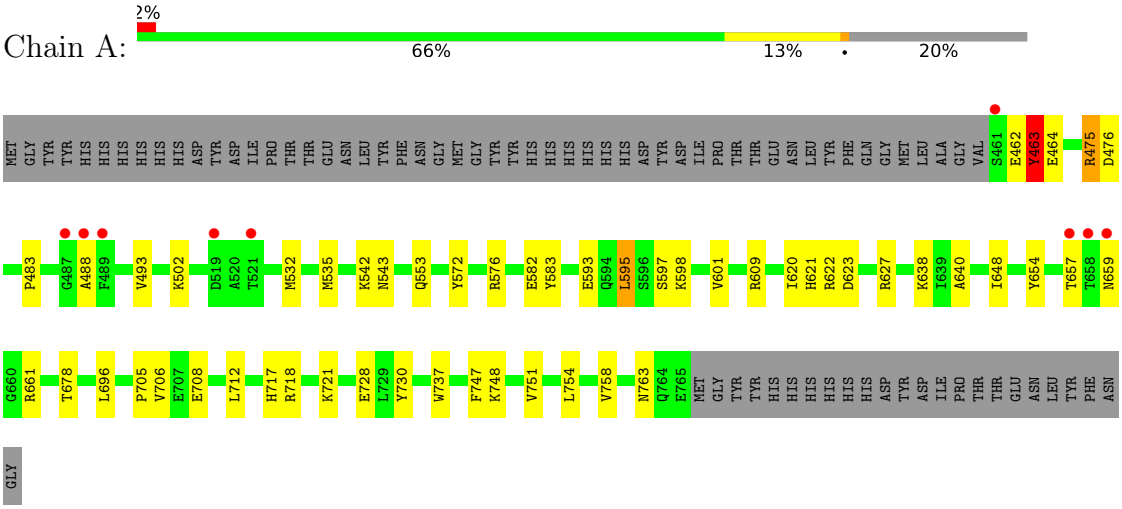
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	235	Total O 235 235	0	0
5	B	178	Total O 178 178	0	0

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.

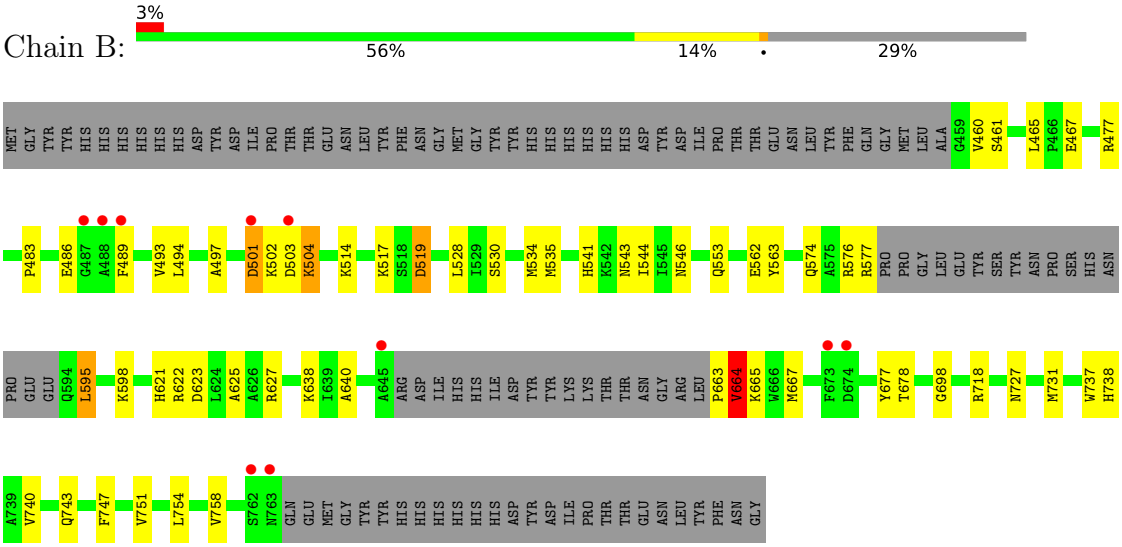
• Molecule 1: Basic fibroblast growth factor receptor 1

Chain A:



• Molecule 1: Basic fibroblast growth factor receptor 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	209.11Å 50.60Å 66.90Å 90.00° 107.27° 90.00°	Depositor
Resolution (Å)	25.86 – 2.80 25.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.86-2.80) 99.0 (25.92-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.204 , 0.261 0.201 , 0.257	Depositor DCC
R_{free} test set	976 reflections (5.89%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 62.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.027 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5056	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 07J, 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	0.33	0/2463	0.49	1/3340 (0.0%)
1	B	0.32	0/2172	0.51	0/2941
All	All	0.32	0/4635	0.50	1/6281 (0.0%)

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	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	463	TYR	N-CA-C	5.79	126.64	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	463	TYR	Peptide
1	A	475	ARG	Sidechain

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	2409	0	2365	40	0
1	B	2120	0	2097	47	0
2	A	38	0	31	2	0
2	B	38	0	31	6	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0
4	B	18	0	24	6	0
5	A	235	0	0	6	0
5	B	178	0	0	2	0
All	All	5056	0	4548	91	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 10.

All (91) 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:475:ARG:NH2	1:A:553:GLN:O	1.82	1.13
1:B:663:PRO:HA	1:B:664:VAL:HG22	1.36	1.06
1:A:542:LYS:NZ	1:A:609:ARG:HH11	1.70	0.89
1:B:727:ASN:O	1:B:731[A]:MET:HG3	1.75	0.86
1:A:542:LYS:HZ3	1:A:609:ARG:HH11	1.24	0.83
1:B:698:GLY:HA2	4:B:791:GOL:H2	1.60	0.82
2:B:1:07J:H29	5:B:284:HOH:O	1.78	0.82
1:A:620:ILE:HG22	1:A:622:ARG:HG3	1.62	0.80
1:B:461:SER:HB3	1:B:465:LEU:HD23	1.66	0.76
1:A:502:LYS:NZ	5:A:360:HOH:O	2.21	0.72
1:B:576:ARG:HE	4:B:790:GOL:H2	1.53	0.72
1:B:640:ALA:HB1	2:B:1:07J:CL2	2.28	0.71
1:A:627:ARG:NH1	1:A:659:ASN:HD22	1.89	0.70
1:B:663:PRO:HA	1:B:664:VAL:CG2	2.20	0.70
1:A:475:ARG:CZ	1:A:553:GLN:O	2.43	0.67
1:A:721:LYS:HG3	1:A:730:TYR:CG	2.30	0.67
1:B:663:PRO:CB	1:B:665:LYS:H	2.08	0.66
1:A:659:ASN:HB3	5:A:354:HOH:O	1.96	0.65
1:B:461:SER:HB3	1:B:465:LEU:CD2	2.27	0.64
1:B:501:ASP:O	1:B:502:LYS:CB	2.47	0.62
1:B:664:VAL:H	1:B:667:MET:HG3	1.64	0.61
1:B:574:GLN:HA	1:B:577:ARG:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:LEU:HG	1:A:717:HIS:HB2	1.85	0.59
1:A:721:LYS:HG3	1:A:730:TYR:HB2	1.85	0.59
1:B:577:ARG:NH1	4:B:791:GOL:O3	2.37	0.58
1:A:627:ARG:HH11	1:A:659:ASN:HD22	1.52	0.58
1:B:543:ASN:O	1:B:638:LYS:HA	2.04	0.57
1:B:460:VAL:HG12	1:B:460:VAL:O	2.05	0.57
1:A:620:ILE:HG22	1:A:622:ARG:CG	2.32	0.57
1:B:489:PHE:HE1	1:B:519:ASP:OD2	1.89	0.56
1:A:718:ARG:HD2	1:A:737:TRP:HB3	1.88	0.55
1:A:728:GLU:HB3	5:A:13:HOH:O	2.06	0.55
1:A:463:TYR:O	5:A:403:HOH:O	2.18	0.55
1:B:622:ARG:HG3	1:B:677:TYR:CD2	2.43	0.54
1:A:705:PRO:HD2	1:A:708:GLU:HG3	1.90	0.52
1:A:576:ARG:HG2	1:A:593:GLU:O	2.10	0.52
1:A:543:ASN:O	1:A:638:LYS:HA	2.10	0.52
1:B:577:ARG:NH2	4:B:791:GOL:O3	2.43	0.52
1:A:627:ARG:NH1	1:A:659:ASN:ND2	2.57	0.50
1:B:501:ASP:OD2	1:B:501:ASP:N	2.44	0.50
1:B:740:VAL:HB	1:B:743:GLN:HG3	1.93	0.50
1:A:721:LYS:HG3	1:A:730:TYR:CB	2.41	0.50
1:A:597:SER:O	1:A:601:VAL:HG23	2.13	0.49
1:A:598:LYS:HD2	1:A:763:ASN:HB3	1.96	0.48
1:B:477:ARG:O	1:B:497:ALA:HA	2.13	0.48
1:A:483:PRO:HA	1:A:493:VAL:HG12	1.96	0.48
2:B:1:07J:N23	2:B:1:07J:N3	2.52	0.48
1:A:488:ALA:HB1	5:A:316:HOH:O	2.13	0.48
1:B:541:HIS:HB3	1:B:544:ILE:HG12	1.95	0.48
1:B:718:ARG:HD2	1:B:737:TRP:HB3	1.95	0.48
1:B:530:SER:O	1:B:534:MET:HB2	2.14	0.47
1:B:460:VAL:O	1:B:461:SER:CB	2.62	0.47
2:B:1:07J:H12	2:B:1:07J:H9	1.69	0.46
1:B:494:LEU:HD13	1:B:563:TYR:CE1	2.50	0.46
1:B:625:ALA:HB3	1:B:627:ARG:HG2	1.97	0.46
1:A:654:TYR:CE1	1:A:706:VAL:HB	2.51	0.46
1:B:483:PRO:HA	1:B:493:VAL:HA	1.98	0.45
1:B:754:LEU:O	1:B:758:VAL:HG23	2.15	0.45
1:B:747:PHE:O	1:B:751:VAL:HG23	2.16	0.45
1:B:621:HIS:ND1	1:B:623:ASP:O	2.50	0.45
2:A:1:07J:H12	2:A:1:07J:H9	1.70	0.44
1:A:621:HIS:ND1	1:A:623:ASP:O	2.50	0.44
1:A:747:PHE:O	1:A:751:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:MET:HA	1:A:535:MET:HE3	2.00	0.44
1:A:621:HIS:CE1	1:A:623:ASP:O	2.71	0.44
1:A:542:LYS:HZ1	1:A:609:ARG:HH11	1.58	0.44
1:A:640:ALA:HB1	2:A:1:07J:CL2	2.55	0.44
1:A:659:ASN:OD1	1:A:661:ARG:N	2.51	0.44
1:A:462:GLU:HG3	5:A:403:HOH:O	2.17	0.43
1:B:577:ARG:HH22	4:B:791:GOL:C3	2.31	0.43
1:B:460:VAL:O	1:B:461:SER:HB2	2.18	0.43
1:B:663:PRO:HB3	1:B:665:LYS:H	1.80	0.43
1:B:486:GLU:OE1	1:B:517:LYS:HE2	2.17	0.43
1:A:754:LEU:O	1:A:758:VAL:HG23	2.18	0.43
1:B:514[A]:LYS:HG2	1:B:528:LEU:HD11	2.00	0.43
1:B:503:ASP:HA	1:B:504:LYS:HA	1.76	0.42
1:A:583:TYR:CG	1:A:696:LEU:HD12	2.55	0.42
1:B:621:HIS:CE1	1:B:623:ASP:O	2.72	0.42
1:A:627:ARG:CD	1:A:659:ASN:ND2	2.82	0.42
1:B:622:ARG:HD2	5:B:795:HOH:O	2.17	0.42
1:B:576:ARG:HB3	1:B:595:LEU:HD12	2.01	0.42
1:B:640:ALA:CB	2:B:1:07J:CL2	3.01	0.41
1:A:572:TYR:O	1:A:576:ARG:HD2	2.21	0.41
1:A:576:ARG:HB3	1:A:595:LEU:HD12	2.02	0.41
1:B:519:ASP:OD1	1:B:519:ASP:N	2.45	0.41
1:B:598:LYS:HE3	1:B:758:VAL:O	2.21	0.41
1:B:467[A]:GLU:HB3	1:B:553:GLN:NE2	2.36	0.40
1:B:535:MET:CE	2:B:1:07J:H3	2.51	0.40
1:A:462:GLU:HA	1:A:463:TYR:HB2	2.02	0.40
1:B:577:ARG:CZ	4:B:791:GOL:O3	2.69	0.40
1:B:546:ASN:HB2	1:B:562:GLU:CD	2.41	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	303/382 (79%)	296 (98%)	6 (2%)	1 (0%)	41 72
1	B	270/382 (71%)	259 (96%)	10 (4%)	1 (0%)	34 66
All	All	573/764 (75%)	555 (97%)	16 (3%)	2 (0%)	34 72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	GLU
1	B	664	VAL

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	260/337 (77%)	253 (97%)	7 (3%)	44 78
1	B	227/337 (67%)	220 (97%)	7 (3%)	40 74
All	All	487/674 (72%)	473 (97%)	14 (3%)	42 76

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	476	ASP
1	A	582	GLU
1	A	595	LEU
1	A	648	ILE
1	A	657	THR
1	A	678	THR
1	A	748	LYS
1	B	501	ASP
1	B	504	LYS
1	B	519	ASP
1	B	595	LEU
1	B	664	VAL
1	B	678	THR
1	B	738	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	679	HIS
1	A	749	GLN

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)

9 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	$\#\|Z\| > 2$
4	GOL	B	791	-	5,5,5	0.39	0	5,5,5	0.44	0
2	07J	B	1	-	40,41,41	1.39	1 (2%)	50,57,57	2.76	10 (20%)
3	SO4	A	2	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	A	790	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	A	4	-	4,4,4	0.14	0	6,6,6	0.06	0
4	GOL	B	790	-	5,5,5	0.36	0	5,5,5	0.19	0
2	07J	A	1	-	40,41,41	0.75	0	50,57,57	1.75	10 (20%)
3	SO4	B	3	-	4,4,4	0.15	0	6,6,6	0.04	0
4	GOL	B	2	-	5,5,5	0.38	0	5,5,5	0.32	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
4	GOL	B	791	-	-	2/4/4/4	-
2	07J	B	1	-	-	4/26/36/36	0/4/4/4
4	GOL	B	790	-	-	4/4/4/4	-
2	07J	A	1	-	-	2/26/36/36	0/4/4/4
4	GOL	B	2	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	07J	C33-N34	-7.43	1.26	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	07J	C37-N34-C33	9.88	131.06	108.83
2	B	1	07J	C33-N34-C35	-8.42	87.48	110.84
2	B	1	07J	C32-C33-N34	-8.04	94.14	110.64
2	B	1	07J	N23-C18-N16	7.07	121.06	115.28
2	A	1	07J	N23-C18-N16	6.41	120.53	115.28
2	A	1	07J	C9-O8-C7	-4.54	110.67	117.53
2	B	1	07J	C13-O12-C11	-4.42	110.86	117.53
2	A	1	07J	C13-O12-C11	-4.40	110.88	117.53
2	B	1	07J	C9-O8-C7	-4.23	111.15	117.53
2	B	1	07J	C19-C18-N16	-4.18	118.03	122.48
2	A	1	07J	C19-C18-N16	-3.81	118.42	122.48
2	B	1	07J	C38-N31-C32	3.02	118.18	111.52
2	A	1	07J	C38-N31-C32	2.97	118.08	111.52
2	A	1	07J	C32-N31-C28	-2.52	111.28	118.09
2	B	1	07J	C32-N31-C28	-2.33	111.78	118.09
2	A	1	07J	C37-N34-C33	2.29	113.98	108.83
2	A	1	07J	C38-N31-C28	-2.13	112.33	118.09
2	B	1	07J	C38-N31-C28	-2.13	112.34	118.09
2	A	1	07J	C29-C28-N31	-2.10	118.48	121.38
2	A	1	07J	C32-C33-N34	-2.08	106.36	110.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	790	GOL	O1-C1-C2-C3
4	B	2	GOL	O1-C1-C2-C3
4	B	791	GOL	O1-C1-C2-C3
4	B	2	GOL	O1-C1-C2-O2
4	B	791	GOL	O1-C1-C2-O2
2	B	1	07J	C27-C28-N31-C38
4	B	790	GOL	O1-C1-C2-O2
2	B	1	07J	C29-C28-N31-C38
2	B	1	07J	C36-C35-N34-C33
4	B	790	GOL	C1-C2-C3-O3
2	A	1	07J	C30-C25-N24-C20
4	B	790	GOL	O2-C2-C3-O3
2	A	1	07J	C26-C25-N24-C20
2	B	1	07J	C30-C25-N24-C20

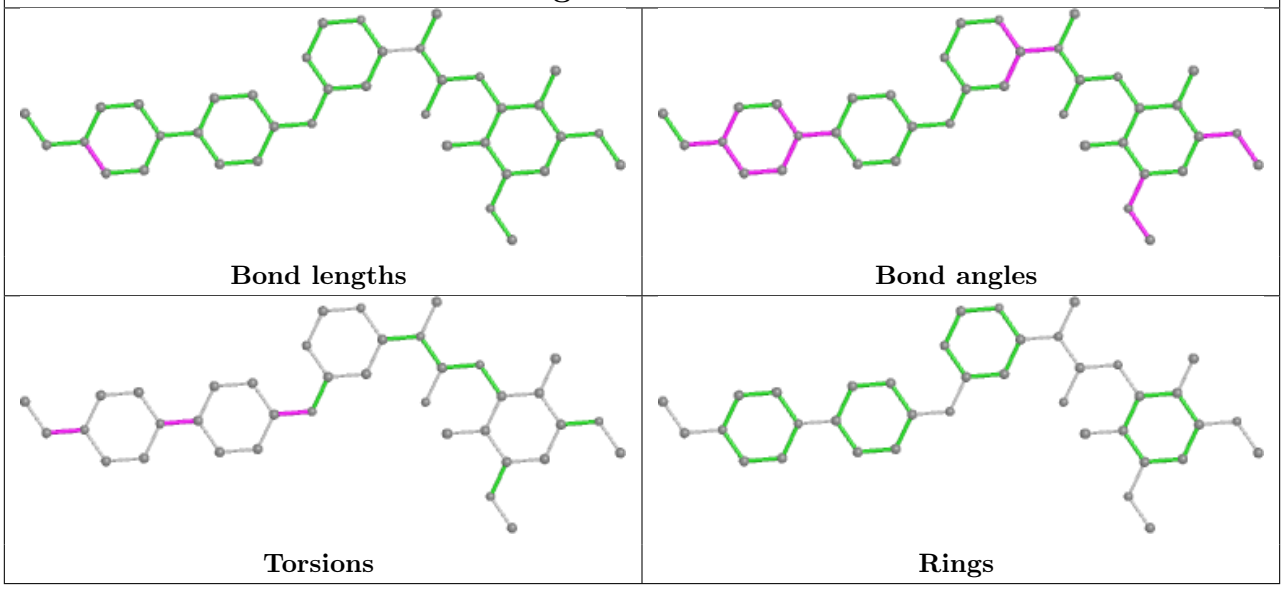
There are no ring outliers.

4 monomers are involved in 14 short contacts:

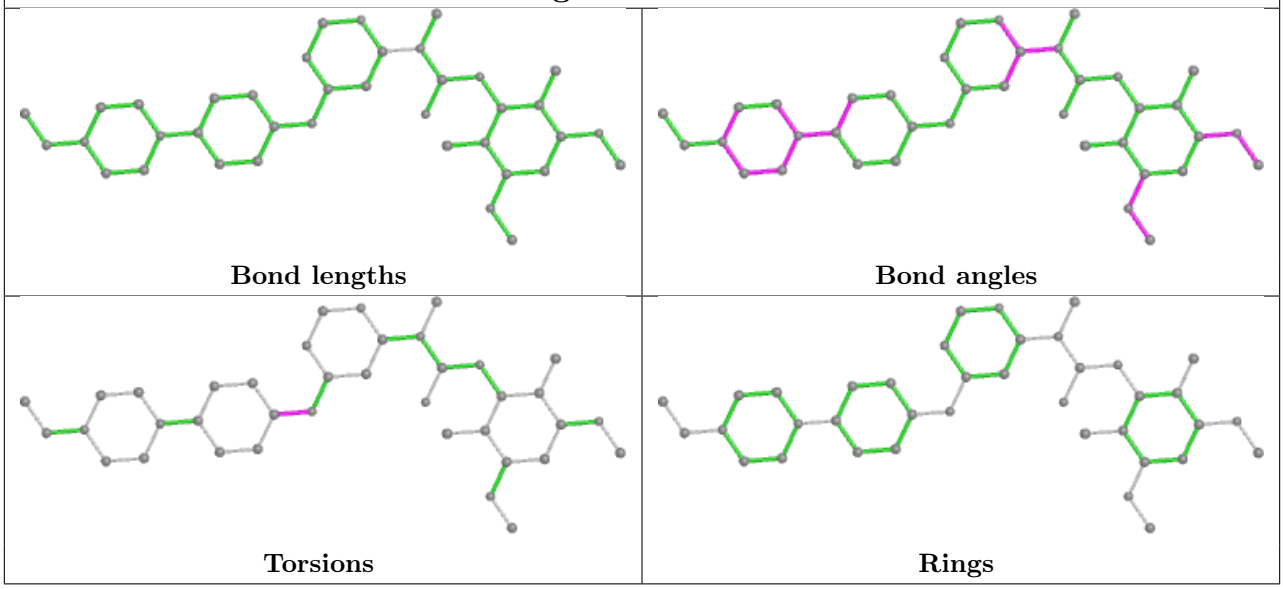
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	791	GOL	5	0
2	B	1	07J	6	0
4	B	790	GOL	1	0
2	A	1	07J	2	0

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 07J B 1



Ligand 07J A 1



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, 95^{th} 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	305/382 (79%)	-0.15	9 (2%) 50 40	17, 37, 71, 97	0
1	B	272/382 (71%)	-0.04	10 (3%) 41 31	17, 39, 72, 97	0
All	All	577/764 (75%)	-0.10	19 (3%) 46 36	17, 38, 72, 97	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	PHE	3.8
1	A	657	THR	3.6
1	B	488	ALA	3.5
1	A	658	THR	3.3
1	B	674	ASP	3.3
1	A	489	PHE	3.3
1	A	519	ASP	2.7
1	B	763	ASN	2.7
1	B	645	ALA	2.6
1	A	488	ALA	2.5
1	B	487	GLY	2.5
1	A	659	ASN	2.4
1	A	487	GLY	2.3
1	A	521	THR	2.3
1	B	673	PHE	2.3
1	B	501	ASP	2.2
1	A	461	SER	2.2
1	B	762	SER	2.1
1	B	503	ASP	2.1

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

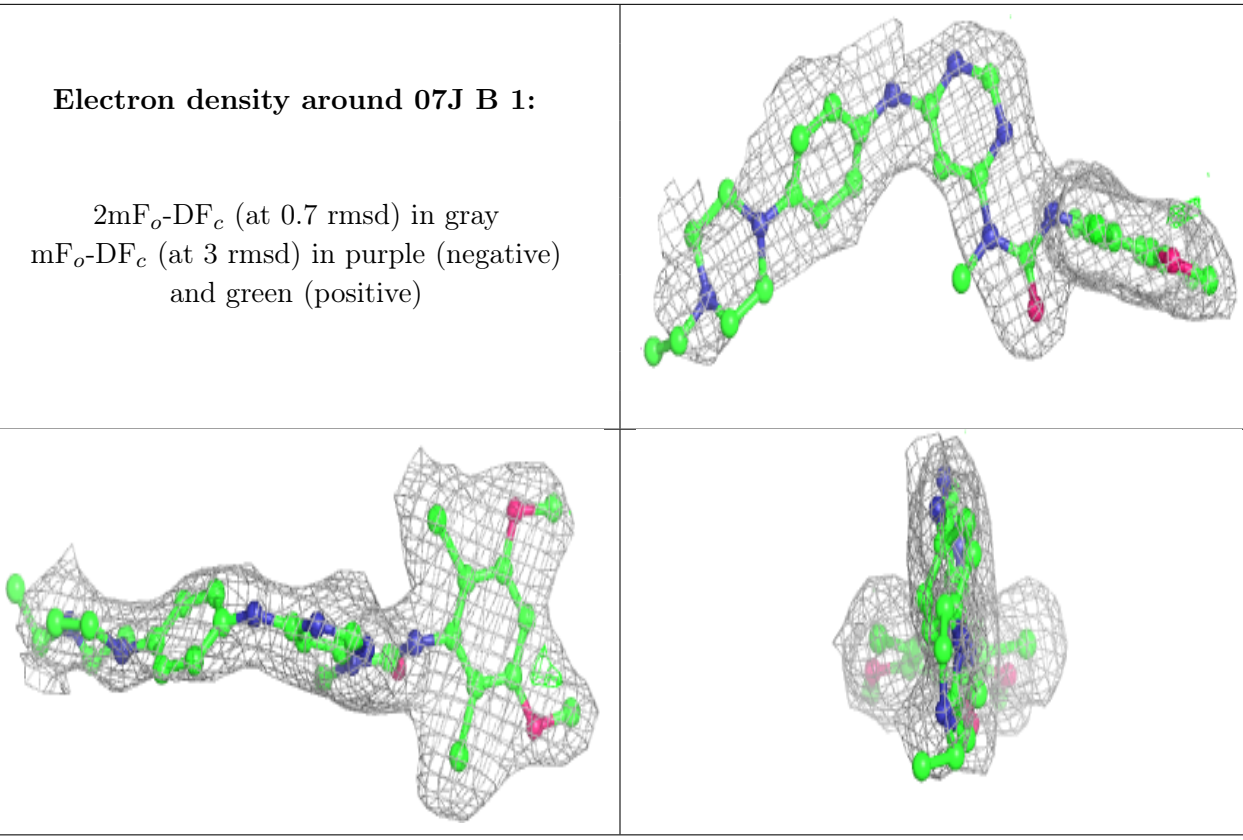
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	GOL	B	791	6/6	0.84	0.28	56,63,66,67	0
4	GOL	B	2	6/6	0.85	0.30	62,69,70,71	0
4	GOL	B	790	6/6	0.87	0.31	74,74,76,78	0
2	07J	B	1	38/38	0.89	0.22	34,50,87,91	0
3	SO4	A	4	5/5	0.90	0.29	135,135,136,138	0
2	07J	A	1	38/38	0.90	0.23	38,42,85,88	0
3	SO4	B	3	5/5	0.91	0.27	112,112,112,112	0
3	SO4	A	2	5/5	0.95	0.18	92,92,93,96	0
3	SO4	A	790	5/5	0.96	0.20	91,91,91,96	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.

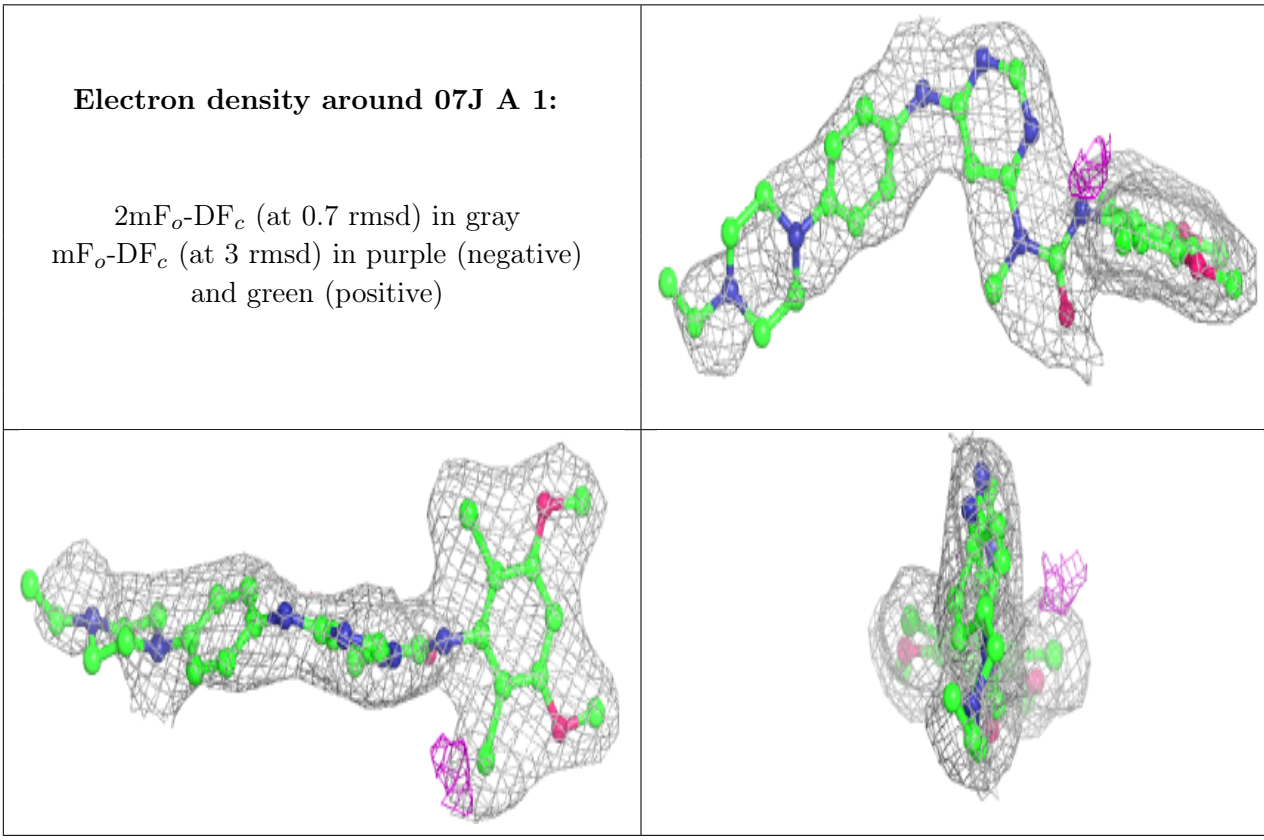
Electron density around 07J B 1:

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



Electron density around 07J 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.