Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2023 – 02:51 PM EDT

PDB ID	:	4P74
Title	:	PheRS in complex with compound 3a
Authors	:	Ferguson, A.D.
Deposited on	:	2014-03-25
Resolution	:	2.70 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:

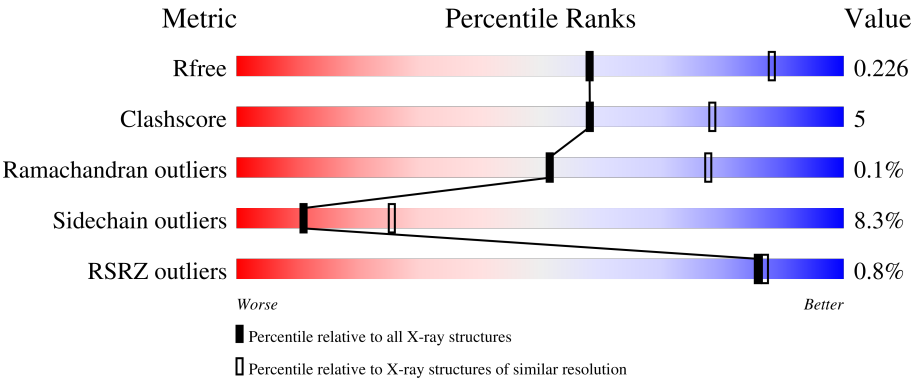
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	792	83% 16%
1	B	792	83% 15%
2	C	338	60% 9% 30%
2	D	338	59% 12% 28%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16186 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.

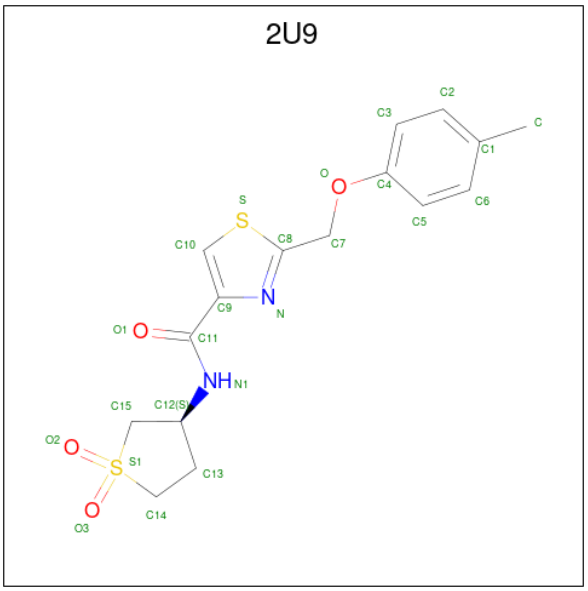
- Molecule 1 is a protein called Phenylalanine–tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	791	Total	C	N	O	S	0	0	0
			6103	3854	1087	1141	21			
1	B	791	Total	C	N	O	S	0	0	0
			6103	3854	1087	1141	21			

- Molecule 2 is a protein called Phenylalanine–tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	235	Total	C	N	O	S	0	0	0
			1897	1203	335	345	14			
2	D	244	Total	C	N	O	S	0	0	0
			1954	1238	345	356	15			

- Molecule 3 is N-[(3S)-1,1-dioxidotetrahydrothiophen-3-yl]-2-[(4-methylphenoxy)methyl]-1,3-thiazole-4-carboxamide (three-letter code: 2U9) (formula: $C_{16}H_{18}N_2O_4S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			24	16	2	4	2		
3	D	1	Total	C	N	O	S	0	0
			24	16	2	4	2		

- Molecule 4 is water.

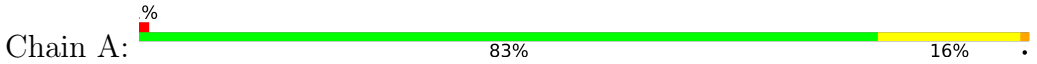
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	43	Total	O	0	0
			43	43		
4	C	3	Total	O	0	0
			3	3		
4	D	5	Total	O	0	0
			5	5		

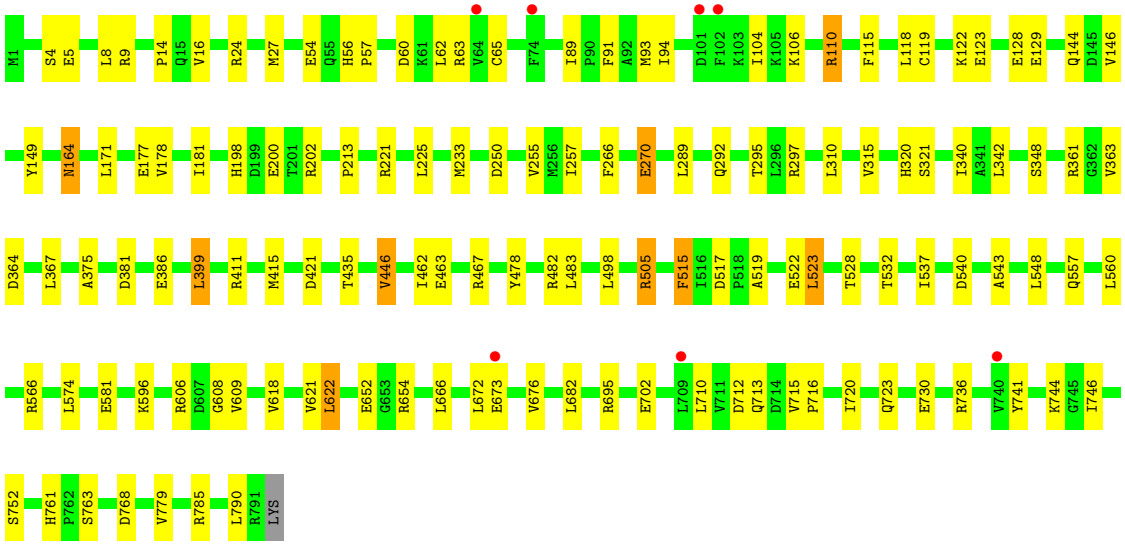
3 Residue-property plots (i)

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: Phenylalanine–tRNA ligase beta subunit

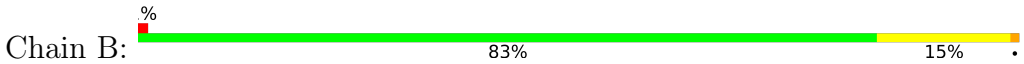
Chain A:

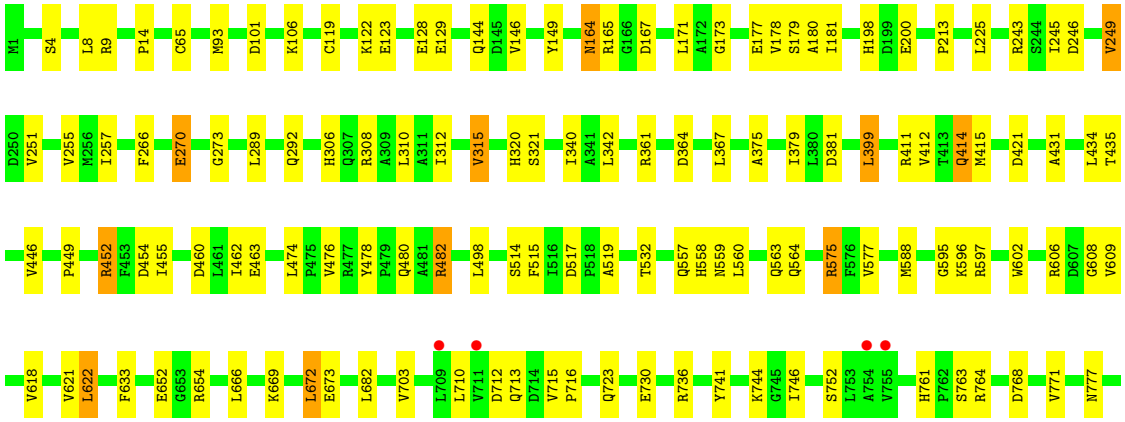


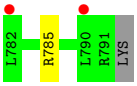


• Molecule 1: Phenylalanine–tRNA ligase beta subunit

Chain B:

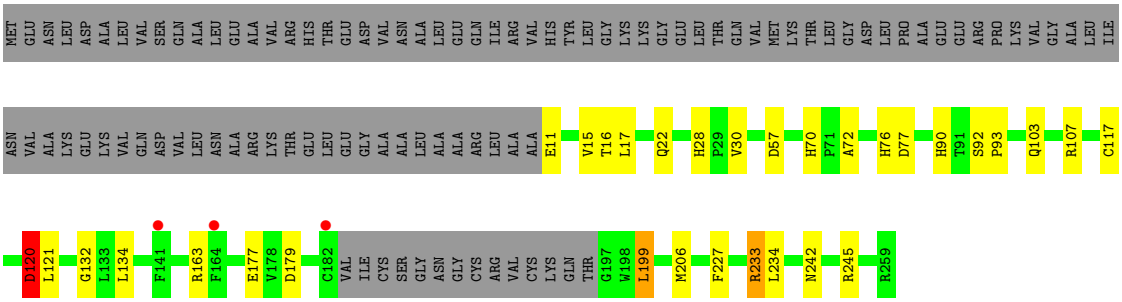






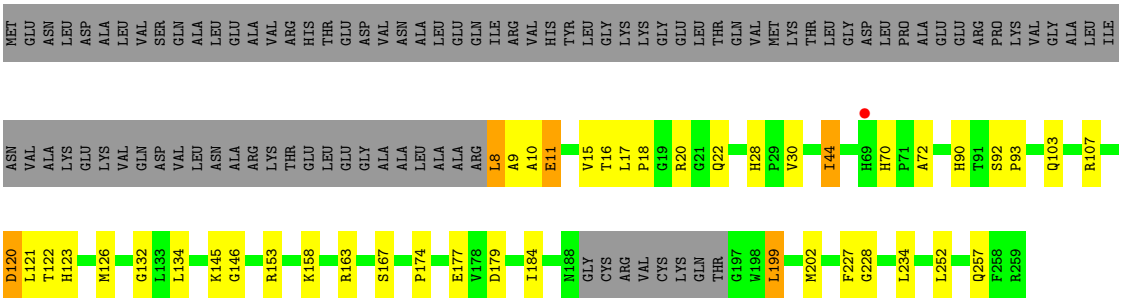
• Molecule 2: Phenylalanine–tRNA ligase alpha subunit

Chain C:



• Molecule 2: Phenylalanine–tRNA ligase alpha subunit

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	113.06Å 219.26Å 107.40Å 90.00° 101.88° 90.00°	Depositor
Resolution (Å)	60.98 – 2.70 55.55 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (60.98-2.70) 99.8 (55.55-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.183 , 0.217 0.190 , 0.226	Depositor DCC
R_{free} test set	3525 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	51.8	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16186	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: 2U9

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	0/6221	0.74	0/8450
1	B	0.51	0/6221	0.74	0/8450
2	C	0.51	0/1946	0.73	1/2628 (0.0%)
2	D	0.54	0/2003	0.75	1/2706 (0.0%)
All	All	0.52	0/16391	0.74	2/22234 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	103	GLN	CB-CG-CD	5.50	125.89	111.60
2	C	177	GLU	CB-CG-CD	5.05	127.83	114.20

There are no chirality outliers.

There are no planarity outliers.

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	6103	0	6136	58	0
1	B	6103	0	6136	64	0
2	C	1897	0	1821	21	0
2	D	1954	0	1881	37	0
3	C	24	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	24	0	18	0	0
4	A	30	0	0	0	0
4	B	43	0	0	1	0
4	C	3	0	0	0	0
4	D	5	0	0	0	0
All	All	16186	0	16010	154	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 (154) 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:559:ASN:HD21	2:D:252:LEU:H	1.23	0.86
1:A:198:HIS:HD2	1:A:200:GLU:H	1.23	0.86
1:B:198:HIS:HD2	1:B:200:GLU:H	1.24	0.83
1:A:761:HIS:HD2	1:A:763:SER:H	1.28	0.81
1:B:761:HIS:HD2	1:B:763:SER:H	1.30	0.80
1:B:716:PRO:HA	2:C:15:VAL:HG21	1.62	0.79
1:A:695:ARG:H	2:D:257:GLN:HE22	1.30	0.78
1:A:716:PRO:HA	2:D:15:VAL:HG21	1.66	0.77
1:B:312:ILE:HG12	1:B:315:VAL:HG13	1.69	0.75
1:B:564:GLN:HG2	2:D:252:LEU:HD12	1.67	0.74
1:B:597:ARG:HA	1:B:609:VAL:HG13	1.72	0.70
1:A:415:MET:HG2	1:A:462:ILE:HG21	1.72	0.70
2:C:15:VAL:HG22	2:C:16:THR:H	1.58	0.69
2:D:15:VAL:HG22	2:D:16:THR:H	1.59	0.68
1:A:89:ILE:HD13	1:A:118:LEU:HD22	1.75	0.68
1:A:5:GLU:HG2	1:A:9:ARG:HD2	1.78	0.65
1:B:463:GLU:HG2	2:D:174:PRO:HB3	1.77	0.65
1:A:482:ARG:HD2	1:B:478:TYR:O	1.97	0.64
2:D:28:HIS:HD2	2:D:30:VAL:H	1.45	0.64
2:C:28:HIS:HD2	2:C:30:VAL:H	1.45	0.64
1:A:566:ARG:HH12	2:C:22:GLN:NE2	1.96	0.64
1:B:251:VAL:HG21	1:B:379:ILE:HG13	1.80	0.64
1:B:761:HIS:CD2	1:B:763:SER:H	2.16	0.64
2:C:70:HIS:HD2	2:C:72:ALA:H	1.47	0.63
1:A:557:GLN:HE21	1:A:672:LEU:HD13	1.63	0.63
1:B:164:ASN:HD22	1:B:164:ASN:H	1.45	0.63
1:A:566:ARG:HH12	2:C:22:GLN:HE22	1.45	0.62
2:D:167:SER:HB2	2:D:177:GLU:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:LEU:HB3	2:D:44:ILE:HG13	1.81	0.62
1:B:246:ASP:HB2	1:B:249:VAL:HG23	1.83	0.61
2:C:199:LEU:HD23	2:C:233:ARG:HH22	1.66	0.61
1:A:310:LEU:HD22	1:A:321:SER:HB3	1.83	0.60
2:D:70:HIS:HD2	2:D:72:ALA:H	1.49	0.59
1:B:564:GLN:HE21	2:D:252:LEU:HB2	1.68	0.59
1:A:164:ASN:H	1:A:164:ASN:HD22	1.48	0.59
1:B:415:MET:HG2	1:B:462:ILE:HG21	1.84	0.59
1:B:597:ARG:HA	1:B:609:VAL:CG1	2.32	0.59
1:A:702:GLU:H	1:B:563:GLN:HE22	1.51	0.58
1:B:310:LEU:HD22	1:B:321:SER:HB3	1.84	0.58
1:A:761:HIS:CD2	1:A:763:SER:H	2.15	0.57
1:B:514:SER:H	2:D:126:MET:HE1	1.69	0.57
1:B:514:SER:H	2:D:126:MET:CE	2.17	0.57
1:B:476:VAL:HG13	2:D:146:GLY:HA2	1.87	0.57
1:A:779:VAL:HG11	1:A:790:LEU:HD21	1.88	0.56
1:A:715:VAL:HG23	1:A:720:ILE:HD11	1.88	0.56
1:B:703:VAL:HG11	1:B:771:VAL:HG21	1.88	0.55
1:A:505:ARG:HH11	1:A:505:ARG:HG2	1.71	0.55
2:C:163:ARG:HB3	2:C:179:ASP:HB2	1.87	0.55
2:D:163:ARG:HB3	2:D:179:ASP:HB2	1.88	0.55
1:B:434:LEU:HD23	1:B:449:PRO:HD3	1.89	0.54
1:B:595:GLY:O	1:B:609:VAL:HG22	2.08	0.54
1:A:435:THR:O	1:A:446:VAL:HA	2.08	0.54
2:C:132:GLY:HA3	2:C:227:PHE:CZ	2.43	0.54
1:B:435:THR:O	1:B:446:VAL:HA	2.08	0.54
1:A:14:PRO:HB2	1:A:16:VAL:HG22	1.90	0.53
2:D:132:GLY:HA3	2:D:227:PHE:CZ	2.44	0.53
1:B:633:PHE:HB3	2:C:16:THR:HG21	1.91	0.53
1:A:56:HIS:HE1	1:A:110:ARG:HB2	1.73	0.53
1:B:414:GLN:HG3	1:B:415:MET:N	2.22	0.53
1:A:94:ILE:O	1:A:104:ILE:O	2.26	0.53
1:A:519:ALA:O	1:A:523:LEU:HD22	2.09	0.53
2:D:28:HIS:CD2	2:D:30:VAL:H	2.26	0.53
1:B:8:LEU:HD21	1:B:178:VAL:HG21	1.90	0.52
1:A:91:PHE:CE2	1:A:93:MET:HG2	2.44	0.52
1:A:270:GLU:HG2	1:A:320:HIS:O	2.10	0.52
2:C:76:HIS:HD2	2:C:77:ASP:OD1	1.92	0.52
1:B:312:ILE:HG12	1:B:315:VAL:CG1	2.39	0.51
1:B:517:ASP:OD2	1:B:519:ALA:HB3	2.10	0.51
2:D:121:LEU:O	2:D:122:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LEU:HD21	1:A:178:VAL:HG21	1.93	0.51
2:C:28:HIS:CD2	2:C:30:VAL:H	2.26	0.50
1:A:517:ASP:OD2	1:A:519:ALA:HB3	2.11	0.50
1:B:602:TRP:CD1	2:D:18:PRO:HD2	2.47	0.50
2:D:122:THR:HG23	2:D:123:HIS:CE1	2.46	0.50
1:B:270:GLU:HG2	1:B:320:HIS:O	2.11	0.50
1:B:273:GLY:O	1:B:306:HIS:CE1	2.65	0.50
1:B:575:ARG:HG3	1:B:588:MET:HG3	1.94	0.50
1:A:56:HIS:CE1	1:A:110:ARG:HB2	2.47	0.49
2:D:107:ARG:HG2	2:D:134:LEU:HD12	1.94	0.49
1:B:559:ASN:ND2	2:D:252:LEU:H	2.00	0.48
1:B:596:LYS:HA	1:B:608:GLY:HA2	1.94	0.48
2:D:179:ASP:HA	2:D:199:LEU:O	2.14	0.48
1:A:56:HIS:HD2	1:A:57:PRO:HD2	1.79	0.48
1:A:106:LYS:HE3	1:A:115:PHE:CE1	2.49	0.48
1:B:575:ARG:HD2	1:B:577:VAL:HG23	1.96	0.48
1:A:198:HIS:HD2	1:A:200:GLU:N	2.01	0.47
1:B:364:ASP:HB3	1:B:367:LEU:HB2	1.96	0.47
1:A:596:LYS:HA	1:A:608:GLY:HA2	1.95	0.47
1:B:498:LEU:HD22	1:B:621:VAL:HG13	1.96	0.47
1:A:478:TYR:O	1:B:482:ARG:HG3	2.14	0.47
1:B:476:VAL:HG13	2:D:146:GLY:CA	2.45	0.47
2:D:92:SER:N	2:D:93:PRO:HD2	2.29	0.47
1:A:233:MET:CE	1:A:250:ASP:HB3	2.45	0.47
2:D:9:ALA:C	2:D:11:GLU:H	2.18	0.47
1:A:695:ARG:N	2:D:257:GLN:HE22	2.08	0.46
1:A:498:LEU:HD22	1:A:621:VAL:HG13	1.96	0.46
2:C:107:ARG:HG2	2:C:134:LEU:HD12	1.96	0.46
2:D:153:ARG:HG3	2:D:158:LYS:O	2.14	0.46
1:B:452:ARG:HG3	1:B:454:ASP:OD1	2.16	0.46
2:C:92:SER:N	2:C:93:PRO:HD2	2.31	0.46
1:A:266:PHE:HD1	1:A:321:SER:HB2	1.81	0.45
2:C:179:ASP:HA	2:C:199:LEU:O	2.16	0.45
1:B:474:LEU:HB2	2:D:145:LYS:HE2	1.99	0.45
1:B:198:HIS:HD2	1:B:200:GLU:N	2.03	0.45
2:C:15:VAL:CG1	2:C:17:LEU:HG	2.47	0.45
1:A:177:GLU:O	1:A:181:ILE:HG13	2.16	0.45
1:B:712:ASP:O	1:B:715:VAL:HG12	2.17	0.44
1:B:9:ARG:HG2	1:B:14:PRO:HD2	1.99	0.44
1:B:255:VAL:HG21	1:B:375:ALA:HB2	1.99	0.44
1:B:652:GLU:HB2	1:B:654:ARG:HH21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:SER:OG	2:D:126:MET:HE1	2.18	0.43
2:D:167:SER:CB	2:D:177:GLU:HG3	2.48	0.43
1:B:177:GLU:O	1:B:181:ILE:HG12	2.18	0.43
1:B:741:TYR:HB3	1:B:752:SER:HB3	2.00	0.43
1:A:741:TYR:HB3	1:A:752:SER:HB3	2.01	0.43
1:B:144:GLN:HE21	1:B:149:TYR:HB2	1.83	0.43
1:B:180:ALA:HA	1:B:431:ALA:HB1	2.00	0.43
1:B:266:PHE:HD1	1:B:321:SER:HB2	1.83	0.43
1:B:575:ARG:HD2	1:B:577:VAL:CG2	2.48	0.43
1:A:213:PRO:HB2	1:A:399:LEU:HD13	2.00	0.43
1:A:505:ARG:HH11	1:A:505:ARG:CG	2.31	0.42
1:B:165:ARG:HH22	1:B:177:GLU:CD	2.23	0.42
1:A:618:VAL:HG12	1:A:622:LEU:HD22	2.00	0.42
1:A:652:GLU:HB2	1:A:654:ARG:HH21	1.82	0.42
1:A:415:MET:SD	2:C:206:MET:HG3	2.59	0.42
1:A:505:ARG:HG2	1:A:505:ARG:NH1	2.32	0.42
1:B:434:LEU:HD23	1:B:449:PRO:CD	2.49	0.42
1:B:455:ILE:HD13	1:B:460:ASP:HB3	2.01	0.42
2:C:120:ASP:HB3	2:C:121:LEU:H	1.45	0.42
2:D:8:LEU:HD12	2:D:10:ALA:HB3	2.01	0.42
1:A:5:GLU:O	1:A:9:ARG:HG3	2.20	0.42
1:A:537:ILE:HD13	2:C:117:CYS:O	2.19	0.42
1:B:558:HIS:HB2	4:B:825:HOH:O	2.19	0.42
2:C:15:VAL:HG13	2:C:17:LEU:HG	2.02	0.42
2:D:15:VAL:CG1	2:D:17:LEU:HG	2.50	0.42
1:B:618:VAL:HG12	1:B:622:LEU:HD22	2.00	0.42
1:A:200:GLU:OE1	1:A:221:ARG:HD3	2.19	0.41
1:A:297:ARG:NH1	1:A:348:SER:HB2	2.34	0.41
1:B:167:ASP:O	1:B:173:GLY:HA3	2.21	0.41
1:B:213:PRO:HB2	1:B:399:LEU:HD13	2.01	0.41
2:D:122:THR:HG23	2:D:123:HIS:ND1	2.35	0.41
1:A:566:ARG:HD2	1:A:596:LYS:O	2.20	0.41
1:A:364:ASP:HB3	1:A:367:LEU:HB2	2.02	0.41
1:A:297:ARG:HH12	1:A:348:SER:CB	2.33	0.41
1:A:144:GLN:HE21	1:A:149:TYR:HB2	1.85	0.41
1:A:202:ARG:HA	1:A:202:ARG:HD3	1.92	0.41
1:B:557:GLN:HE21	1:B:672:LEU:HD12	1.85	0.41
2:D:15:VAL:HG13	2:D:17:LEU:HG	2.03	0.41
2:D:202:MET:HB2	2:D:228:GLY:O	2.20	0.41
1:A:515:PHE:HA	1:A:543:ALA:O	2.21	0.41
1:A:712:ASP:HB3	1:A:715:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:VAL:HG21	1:A:375:ALA:HB2	2.02	0.40
2:C:199:LEU:HD23	2:C:233:ARG:NH2	2.32	0.40
1:B:514:SER:N	2:D:126:MET:HE1	2.34	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	789/792 (100%)	769 (98%)	20 (2%)	0	100	100
1	B	789/792 (100%)	768 (97%)	21 (3%)	0	100	100
2	C	231/338 (68%)	218 (94%)	12 (5%)	1 (0%)	34	60
2	D	240/338 (71%)	224 (93%)	15 (6%)	1 (0%)	34	60
All	All	2049/2260 (91%)	1979 (97%)	68 (3%)	2 (0%)	51	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	120	ASP
2	D	120	ASP

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	645/646 (100%)	582 (90%)	63 (10%)	8 18
1	B	645/646 (100%)	587 (91%)	58 (9%)	9 22
2	C	205/287 (71%)	195 (95%)	10 (5%)	25 52
2	D	211/287 (74%)	201 (95%)	10 (5%)	26 54
All	All	1706/1866 (91%)	1565 (92%)	141 (8%)	11 25

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	24	ARG
1	A	27	MET
1	A	54	GLU
1	A	60	ASP
1	A	62	LEU
1	A	63	ARG
1	A	65	CYS
1	A	110	ARG
1	A	119	CYS
1	A	122	LYS
1	A	123	GLU
1	A	128	GLU
1	A	129	GLU
1	A	146	VAL
1	A	164	ASN
1	A	171	LEU
1	A	225	LEU
1	A	257	ILE
1	A	270	GLU
1	A	289	LEU
1	A	292	GLN
1	A	295	THR
1	A	315	VAL
1	A	340	ILE
1	A	342	LEU
1	A	361	ARG
1	A	363	VAL
1	A	381	ASP
1	A	386	GLU
1	A	399	LEU
1	A	411	ARG
1	A	421	ASP

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Mol	Chain	Res	Type
1	A	446	VAL
1	A	463	GLU
1	A	467	ARG
1	A	505	ARG
1	A	515	PHE
1	A	522	GLU
1	A	523	LEU
1	A	528	THR
1	A	532	THR
1	A	540	ASP
1	A	548	LEU
1	A	560	LEU
1	A	574	LEU
1	A	581	GLU
1	A	606	ARG
1	A	609	VAL
1	A	622	LEU
1	A	666	LEU
1	A	673	GLU
1	A	676	VAL
1	A	682	LEU
1	A	710	LEU
1	A	713	GLN
1	A	723	GLN
1	A	730	GLU
1	A	736	ARG
1	A	744	LYS
1	A	746	ILE
1	A	768	ASP
1	A	785	ARG
1	B	4	SER
1	B	65	CYS
1	B	93	MET
1	B	101	ASP
1	B	106	LYS
1	B	119	CYS
1	B	122	LYS
1	B	123	GLU
1	B	128	GLU
1	B	129	GLU
1	B	146	VAL
1	B	164	ASN

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Mol	Chain	Res	Type
1	B	171	LEU
1	B	179	SER
1	B	225	LEU
1	B	243	ARG
1	B	245	ILE
1	B	249	VAL
1	B	257	ILE
1	B	270	GLU
1	B	289	LEU
1	B	292	GLN
1	B	308	ARG
1	B	315	VAL
1	B	340	ILE
1	B	342	LEU
1	B	361	ARG
1	B	381	ASP
1	B	399	LEU
1	B	411	ARG
1	B	412	VAL
1	B	414	GLN
1	B	421	ASP
1	B	452	ARG
1	B	480	GLN
1	B	482	ARG
1	B	515	PHE
1	B	532	THR
1	B	560	LEU
1	B	575	ARG
1	B	606	ARG
1	B	622	LEU
1	B	666	LEU
1	B	669	LYS
1	B	672	LEU
1	B	673	GLU
1	B	682	LEU
1	B	710	LEU
1	B	713	GLN
1	B	723	GLN
1	B	730	GLU
1	B	736	ARG
1	B	744	LYS
1	B	746	ILE

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Mol	Chain	Res	Type
1	B	764	ARG
1	B	768	ASP
1	B	777	ASN
1	B	785	ARG
2	C	11	GLU
2	C	57	ASP
2	C	90	HIS
2	C	103	GLN
2	C	120	ASP
2	C	199	LEU
2	C	233	ARG
2	C	234	LEU
2	C	242	ASN
2	C	245	ARG
2	D	8	LEU
2	D	11	GLU
2	D	20	ARG
2	D	22	GLN
2	D	44	ILE
2	D	90	HIS
2	D	120	ASP
2	D	184	ILE
2	D	199	LEU
2	D	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	66	GLN
1	A	75	GLN
1	A	144	GLN
1	A	164	ASN
1	A	198	HIS
1	A	261	GLN
1	A	264	HIS
1	A	690	HIS
1	A	713	GLN
1	A	761	HIS
1	B	144	GLN
1	B	164	ASN
1	B	198	HIS

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Mol	Chain	Res	Type
1	B	261	GLN
1	B	264	HIS
1	B	430	GLN
1	B	559	ASN
1	B	563	GLN
1	B	564	GLN
1	B	645	GLN
1	B	713	GLN
1	B	761	HIS
2	C	22	GLN
2	C	28	HIS
2	C	70	HIS
2	C	76	HIS
2	D	28	HIS
2	D	70	HIS
2	D	257	GLN

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

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	$\#\|Z\|>2$
3	2U9	D	301	-	23,26,26	2.03	1 (4%)	24,37,37	0.70	0
3	2U9	C	301	-	23,26,26	2.01	1 (4%)	24,37,37	0.55	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
3	2U9	D	301	-	-	1/7/24/24	0/3/3/3
3	2U9	C	301	-	-	1/7/24/24	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	2U9	C12-N1	-9.52	1.27	1.46
3	C	301	2U9	C12-N1	-9.36	1.27	1.46

There are no bond angle outliers.

There are no chirality outliers.

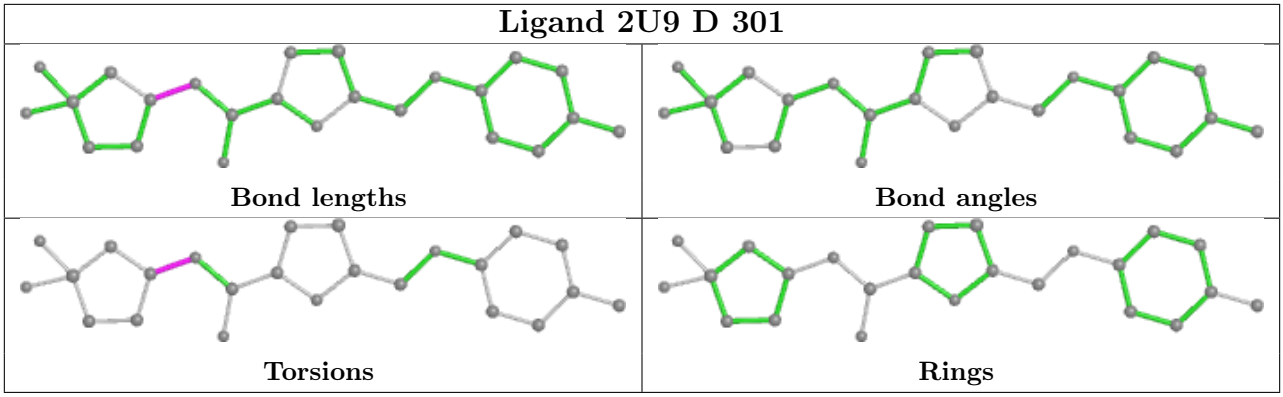
All (2) torsion outliers are listed below:

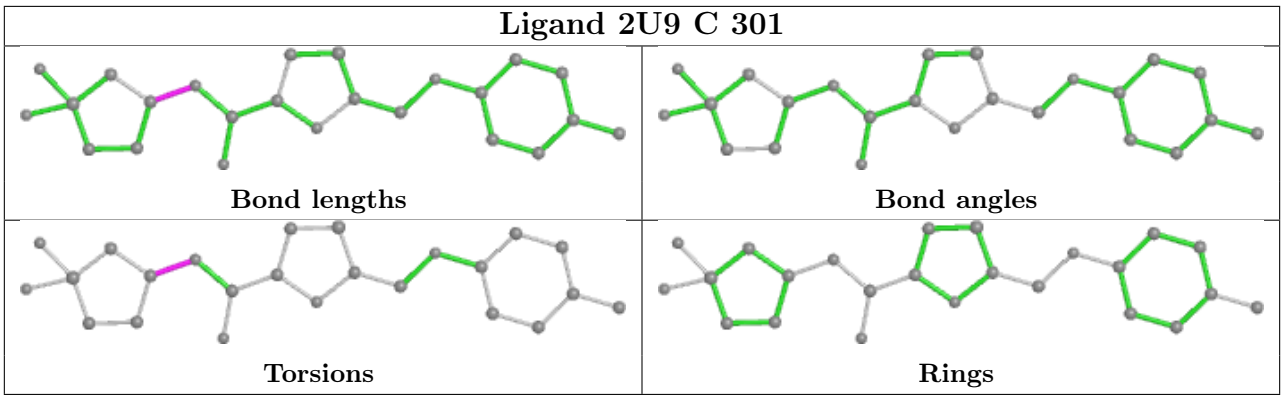
Mol	Chain	Res	Type	Atoms
3	C	301	2U9	C13-C12-N1-C11
3	D	301	2U9	C13-C12-N1-C11

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.





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, 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	791/792 (99%)	-0.01	7 (0%)	84	85	38, 57, 92, 115	0
1	B	791/792 (99%)	-0.10	6 (0%)	86	87	34, 55, 90, 116	0
2	C	235/338 (69%)	-0.11	3 (1%)	77	78	44, 57, 88, 118	0
2	D	244/338 (72%)	-0.03	1 (0%)	92	93	39, 54, 95, 123	0
All	All	2061/2260 (91%)	-0.06	17 (0%)	86	87	34, 56, 91, 123	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	782	LEU	3.7
1	A	101	ASP	3.5
1	A	102	PHE	3.4
1	B	790	LEU	3.3
1	B	709	LEU	2.8
1	B	711	VAL	2.7
2	D	69	HIS	2.5
1	A	709	LEU	2.5
1	B	755	VAL	2.5
1	A	74	PHE	2.3
1	A	64	VAL	2.2
2	C	182	CYS	2.2
1	A	673	GLU	2.1
2	C	141	PHE	2.0
2	C	164	PHE	2.0
1	B	754	ALA	2.0
1	A	740	VAL	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

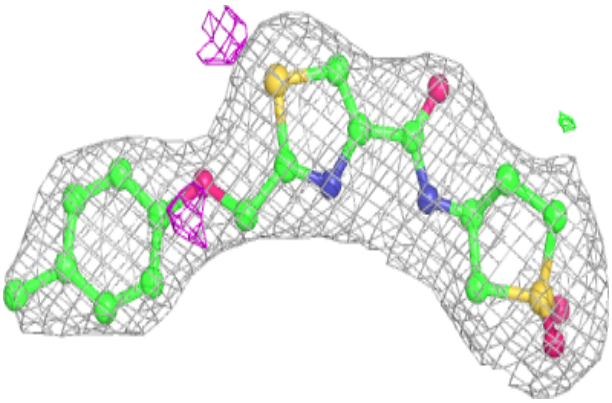
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

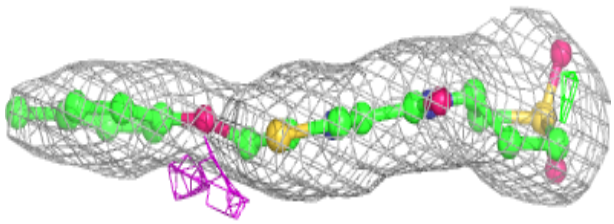
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	2U9	D	301	24/24	0.93	0.19	48,58,84,87	0
3	2U9	C	301	24/24	0.96	0.15	40,48,80,84	0

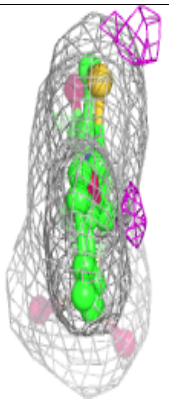
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2U9 D 301:

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

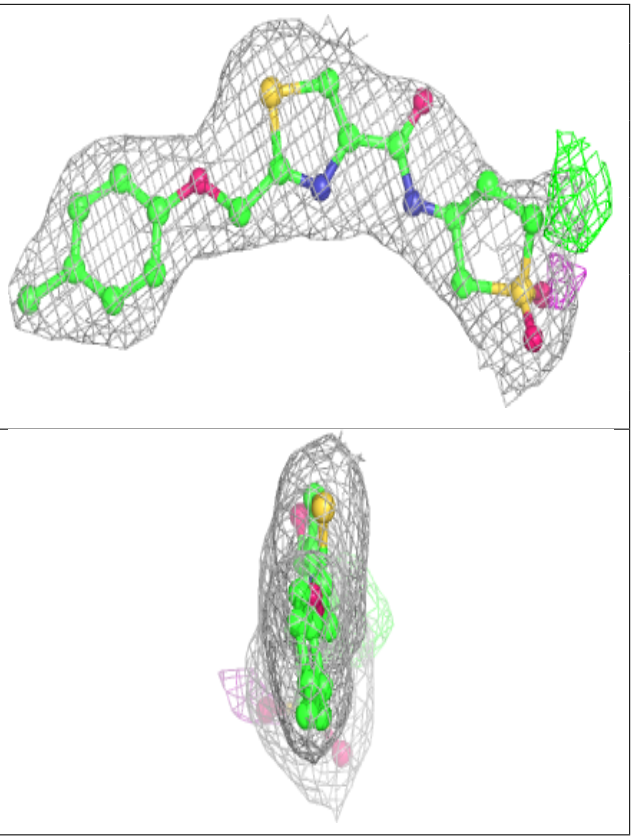






Electron density around 2U9 C 301:

$2mF_o$-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.