Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 06:30 PM EDT

PDB ID	:	3E8C
Title	:	Crystal structures of the kinase domain of PKA in complex with ATP-competitive inhibitors
Authors	:	Concha, N.O.; Elkins, P.A.; Smallwood, A.; Ward, P.
Deposited on	:	2008-08-19
Resolution	:	2.20 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:

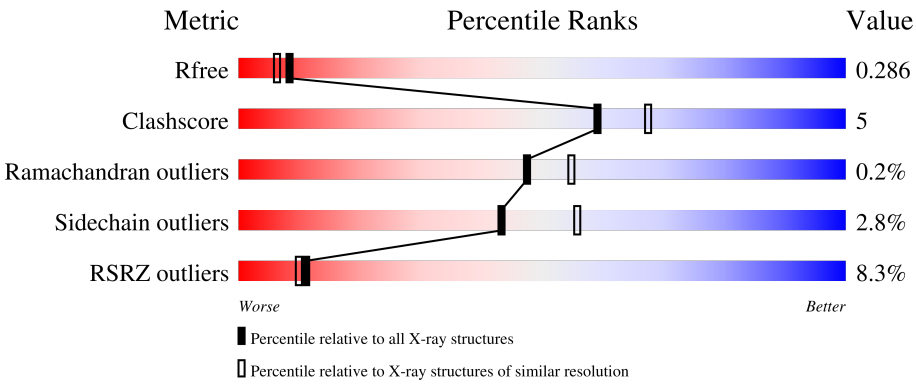
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	350	6% 89% 9% •
1	B	350	4% 89% 11% •
1	C	350	7% 85% 13% •
1	D	350	5% 86% 13% ••
1	E	350	8% 87% 9% • •

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Mol	Chain	Length	Quality of chain
1	F	350	15% 83% 15%
2	G	20	10% 85% 5% 10%
2	H	20	10% 90% 10%
2	I	20	20% 65% 35%
2	J	20	10% 55% 35% 5% 5%
2	K	20	15% 90% 10%
2	L	20	55% 60% 35% 5%

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
1	SEP	C	10	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18893 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.

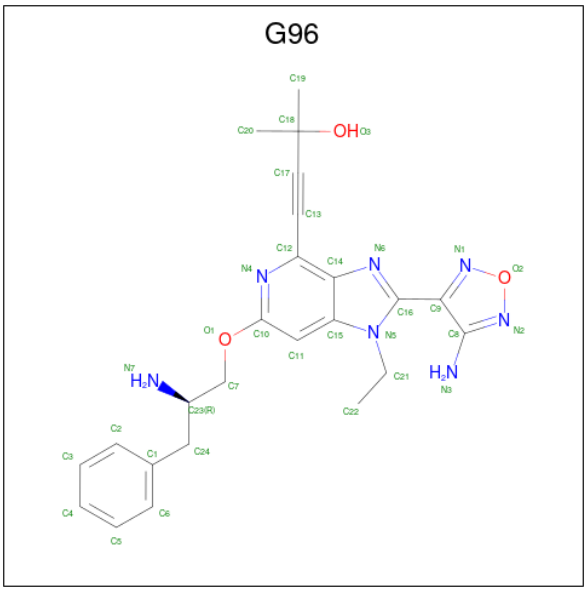
- Molecule 1 is a protein called cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	344	2845	1838	477	518	3	9	0	0	0
1	B	347	2860	1847	480	521	3	9	0	0	0
1	C	344	2844	1838	477	517	3	9	0	1	0
1	D	347	2842	1838	475	517	3	9	0	0	0
1	E	338	2785	1804	467	503	2	9	0	0	0
1	F	344	2845	1838	477	518	3	9	0	0	0

- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	G	18	138	84	28	26	0	0	0
2	H	20	157	94	32	31	0	0	0
2	I	20	157	94	32	31	0	0	0
2	J	19	148	90	31	27	0	0	0
2	K	20	157	94	32	31	0	0	0
2	L	19	149	90	30	29	0	0	0

- Molecule 3 is 4-[2-(4-amino-1,2,5-oxadiazol-3-yl)-6-{[(2R)-2-amino-3-phenylpropyl]oxy}-1-ethyl-1H-imidazo[4,5-c]pyridin-4-yl]-2-methylbut-3-yn-2-ol (three-letter code: G96) (formula: $C_{24}H_{27}N_7O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	34	24	7	3	0	0
3	B	1	34	24	7	3	0	0
3	C	1	34	24	7	3	0	0
3	D	1	34	24	7	3	0	0
3	E	1	34	24	7	3	0	0
3	F	1	34	24	7	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	130	130	130	0	0
4	B	160	160	160	0	0
4	C	122	122	122	0	0
4	D	106	106	106	0	0
4	E	95	95	95	0	0
4	F	103	103	103	0	0

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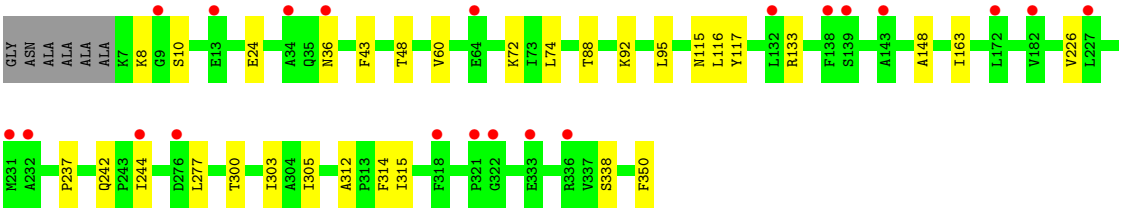
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	G	4	4	4	0	0
			Total	O		
4	H	12	12	12	0	0
			Total	O		
4	I	12	12	12	0	0
			Total	O		
4	J	6	6	6	0	0
			Total	O		
4	K	8	8	8	0	0
			Total	O		
4	L	4	4	4	0	0

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.

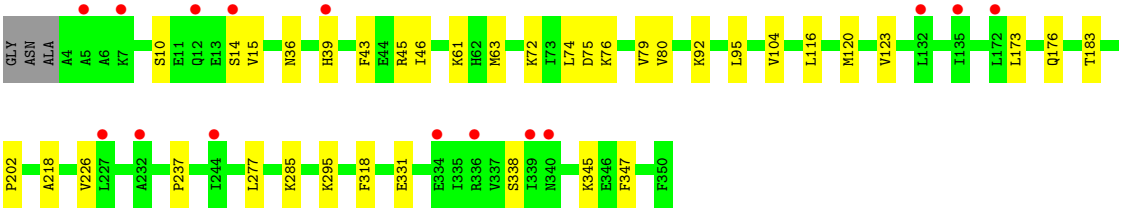
• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain A:



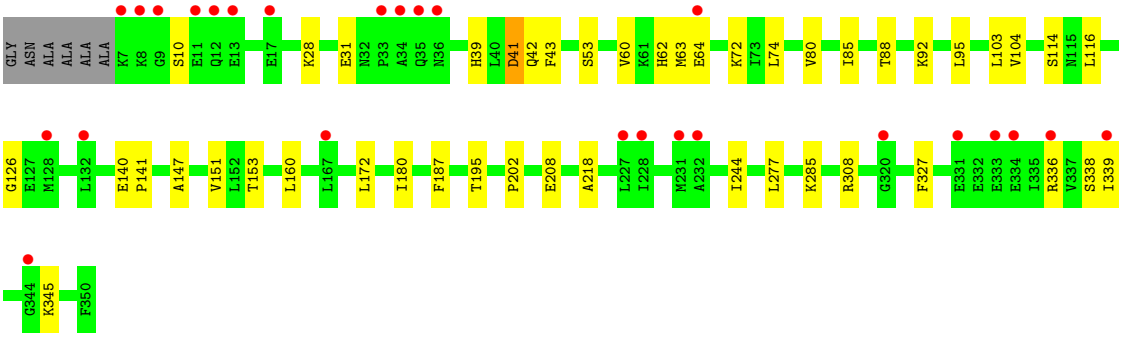
• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain B:



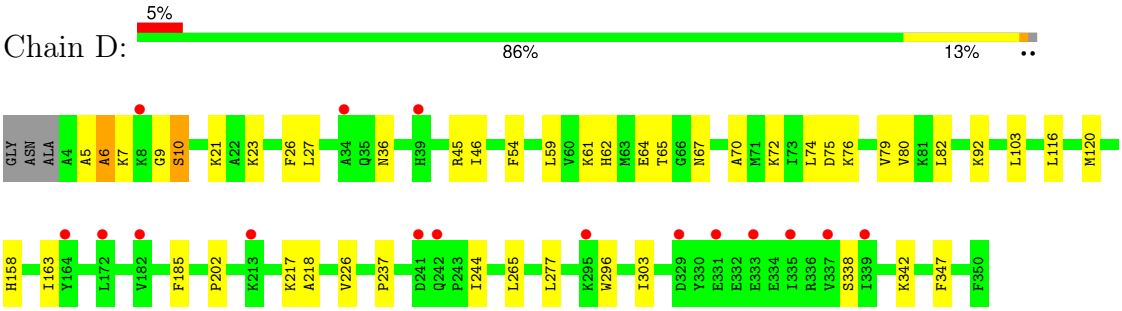
• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain C:



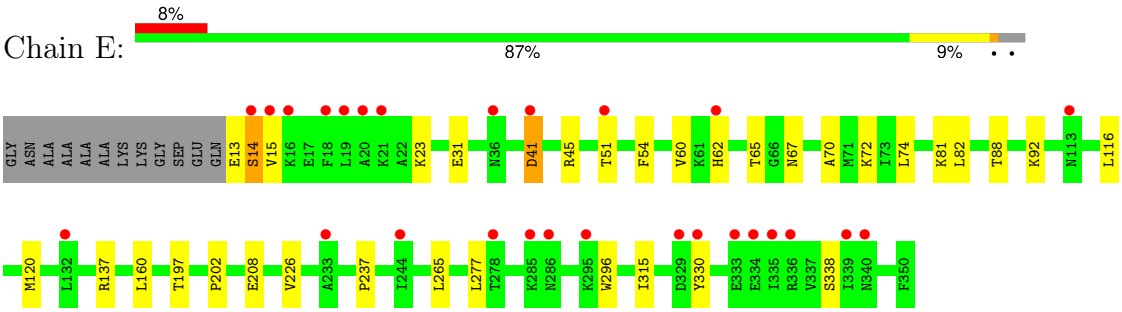
• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain D:



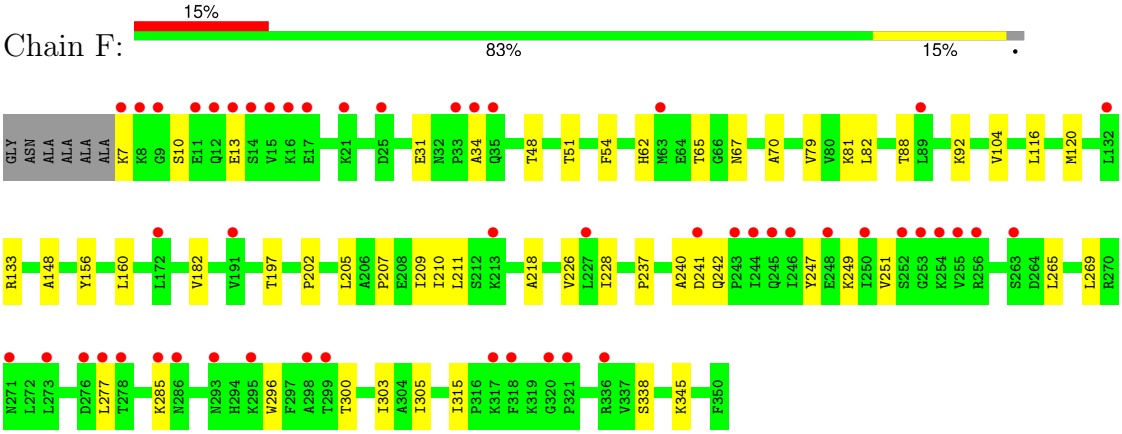
• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain E:



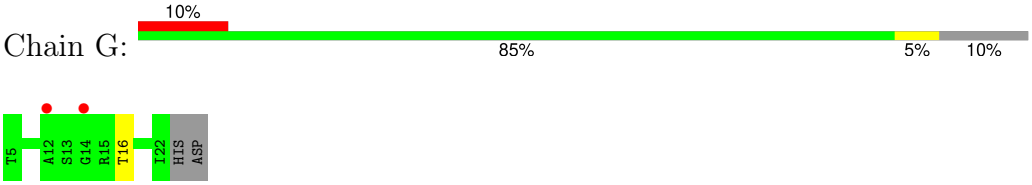
• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain F:



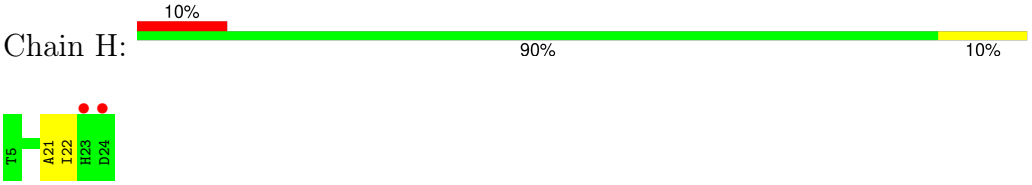
• Molecule 2: cAMP-dependent protein kinase inhibitor peptide

Chain G:



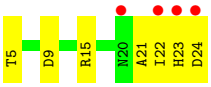
• Molecule 2: cAMP-dependent protein kinase inhibitor peptide

Chain H:



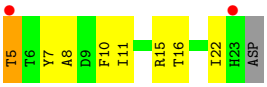
• Molecule 2: cAMP-dependent protein kinase inhibitor peptide

Chain I:



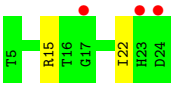
• Molecule 2: cAMP-dependent protein kinase inhibitor peptide

Chain J:



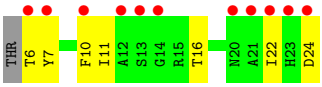
• Molecule 2: cAMP-dependent protein kinase inhibitor peptide

Chain K:



• Molecule 2: cAMP-dependent protein kinase inhibitor peptide

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.46Å 96.39Å 180.04Å 90.00° 102.66° 90.00°	Depositor
Resolution (Å)	46.93 – 2.20 43.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.8 (46.93-2.20) 95.8 (43.06-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.264 , 0.290 0.263 , 0.286	Depositor DCC
R_{free} test set	6759 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.001 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18893	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8220e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: G96, TPO, SEP

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	0.38	0/2884	0.57	0/3880
1	B	0.39	0/2899	0.58	0/3901
1	C	0.38	0/2886	0.57	1/3884 (0.0%)
1	D	0.37	0/2881	0.53	0/3880
1	E	0.35	0/2835	0.53	0/3820
1	F	0.36	0/2884	0.52	0/3880
2	G	0.61	0/139	0.69	0/186
2	H	0.44	0/159	0.68	0/212
2	I	0.43	0/159	0.66	0/212
2	J	0.40	0/150	0.64	0/201
2	K	0.40	0/159	0.63	0/212
2	L	0.42	0/150	0.59	0/197
All	All	0.38	0/18185	0.55	1/24465 (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	E	0	1

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	C	345	LYS	N-CA-CB	-5.03	101.55	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	15	VAL	Peptide

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	2845	0	2819	17	0
1	B	2860	0	2834	15	0
1	C	2844	0	2813	26	0
1	D	2842	0	2800	34	0
1	E	2785	0	2750	21	0
1	F	2845	0	2819	39	0
2	G	138	0	135	1	0
2	H	157	0	146	3	0
2	I	157	0	146	5	0
2	J	148	0	142	5	0
2	K	157	0	146	1	0
2	L	149	0	137	6	0
3	A	34	0	27	2	0
3	B	34	0	27	4	0
3	C	34	0	27	2	0
3	D	34	0	27	2	0
3	E	34	0	27	0	0
3	F	34	0	27	0	0
4	A	130	0	0	3	0
4	B	160	0	0	3	0
4	C	122	0	0	3	0
4	D	106	0	0	1	0
4	E	95	0	0	0	0
4	F	103	0	0	6	0
4	G	4	0	0	0	0
4	H	12	0	0	1	0
4	I	12	0	0	0	0
4	J	6	0	0	0	0
4	K	8	0	0	0	0
4	L	4	0	0	0	0
All	All	18893	0	17849	168	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 (168) 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:E:208:GLU:HG2	1:E:277:LEU:HD21	1.58	0.84
1:A:48:THR:HG23	4:A:408:HOH:O	1.83	0.79
1:C:180:ILE:O	4:C:467:HOH:O	2.00	0.78
2:J:5:THR:HG23	2:J:8:ALA:HB3	1.68	0.75
1:F:210:ILE:CD1	1:F:251:VAL:CG1	2.67	0.72
1:F:210:ILE:HD11	1:F:251:VAL:HG12	1.69	0.72
1:D:65:THR:HG23	1:D:67:ASN:H	1.54	0.71
1:F:65:THR:HG23	1:F:67:ASN:H	1.56	0.70
2:J:5:THR:HG23	2:J:8:ALA:CB	2.22	0.70
1:D:62:HIS:ND1	1:D:65:THR:HG22	2.06	0.69
1:F:62:HIS:CD2	1:F:65:THR:HG22	2.27	0.69
1:F:210:ILE:HD11	1:F:251:VAL:CG1	2.23	0.69
1:D:5:ALA:CA	1:D:6:ALA:HB3	2.23	0.68
1:F:218:ALA:HB3	1:F:277:LEU:HD11	1.74	0.67
1:A:95:LEU:HD11	3:A:351:G96:H19	1.75	0.67
1:D:5:ALA:N	1:D:6:ALA:HB3	2.11	0.66
1:E:65:THR:HG23	1:E:67:ASN:H	1.60	0.65
1:F:218:ALA:CB	1:F:277:LEU:HD11	2.26	0.65
1:E:62:HIS:CD2	1:E:65:THR:HG22	2.32	0.64
2:H:22:ILE:O	4:H:448:HOH:O	2.15	0.64
1:E:72:LYS:HE2	1:E:74:LEU:HD11	1.79	0.63
1:F:62:HIS:HD2	1:F:65:THR:HG22	1.64	0.63
1:C:218:ALA:HB3	1:C:277:LEU:HD11	1.79	0.63
1:A:133:ARG:HD2	2:G:16:THR:O	1.99	0.62
1:D:5:ALA:HA	1:D:6:ALA:HB3	1.81	0.62
1:F:210:ILE:HD13	1:F:251:VAL:CG1	2.29	0.62
1:E:265:LEU:HD13	1:E:296:TRP:CE2	2.35	0.60
1:B:218:ALA:HB3	1:B:277:LEU:HD11	1.84	0.59
1:F:202:PRO:HD3	2:L:22:ILE:HG23	1.84	0.59
2:L:6:THR:C	2:L:7:TYR:CA	2.71	0.59
1:D:218:ALA:HB3	1:D:277:LEU:HD11	1.85	0.58
1:D:72:LYS:HE2	1:D:74:LEU:HD11	1.86	0.57
1:A:88:THR:HG21	1:A:116:LEU:CD1	2.34	0.57
1:D:226:VAL:HG13	1:D:237:PRO:HD2	1.85	0.57
1:B:202:PRO:HD3	2:H:22:ILE:HG23	1.89	0.55
2:J:10:PHE:CE2	2:J:16:THR:HG22	2.42	0.54
2:J:7:TYR:CE2	2:J:11:ILE:HD11	2.42	0.54
1:E:54:PHE:HB3	1:E:82:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:VAL:HG13	1:E:237:PRO:HD2	1.89	0.54
1:D:62:HIS:CE1	1:D:64:GLU:HG2	2.42	0.54
1:B:218:ALA:CB	1:B:277:LEU:HD11	2.38	0.54
1:F:207:PRO:O	1:F:210:ILE:HD12	2.08	0.54
1:D:244:ILE:HD12	1:D:244:ILE:H	1.73	0.54
1:F:205:LEU:HD22	1:F:209:ILE:HG21	1.90	0.53
1:A:244:ILE:HG23	4:A:445:HOH:O	2.08	0.53
1:C:88:THR:HG21	1:C:116:LEU:CD1	2.39	0.53
1:B:72:LYS:HE2	1:B:74:LEU:HD21	1.90	0.53
1:F:88:THR:HG21	1:F:116:LEU:CD1	2.38	0.53
3:B:351:G96:N1	3:B:351:G96:H21	2.24	0.52
1:D:23:LYS:O	1:D:27:LEU:HD23	2.10	0.52
1:F:48:THR:HG21	4:F:448:HOH:O	2.08	0.52
1:F:148:ALA:HB3	4:F:457:HOH:O	2.09	0.52
1:D:54:PHE:HB3	1:D:82:LEU:HD12	1.91	0.52
1:E:208:GLU:CG	1:E:277:LEU:HD11	2.39	0.52
1:A:24:GLU:OE2	1:C:244:ILE:HD12	2.11	0.51
1:F:300:THR:HG23	1:F:305:ILE:HD11	1.93	0.51
1:D:202:PRO:HD3	2:J:22:ILE:HG23	1.92	0.51
1:F:54:PHE:HB3	1:F:82:LEU:HD12	1.93	0.51
1:F:210:ILE:HD13	1:F:251:VAL:HG11	1.92	0.51
1:D:26:PHE:HD2	1:D:27:LEU:HD22	1.75	0.50
1:B:226:VAL:HG13	1:B:237:PRO:HD2	1.94	0.50
1:C:95:LEU:CD1	3:C:351:G96:H20	2.42	0.50
3:B:351:G96:H19A	4:B:752:HOH:O	2.11	0.50
1:F:7:LYS:NZ	1:F:303:ILE:HD13	2.27	0.49
1:D:74:LEU:HD22	1:D:74:LEU:N	2.27	0.49
1:D:120:MET:SD	3:D:351:G96:H20B	2.52	0.49
3:D:351:G96:H21	3:D:351:G96:N1	2.28	0.49
1:E:51:THR:HG22	1:E:330:TYR:CE2	2.47	0.49
1:C:103:LEU:HD21	1:C:153:THR:CG2	2.43	0.49
1:E:208:GLU:HG3	1:E:277:LEU:HD11	1.93	0.49
1:F:228:ILE:CG2	1:F:269:LEU:HD11	2.43	0.48
2:I:5:THR:O	2:I:9:ASP:OD2	2.31	0.48
4:B:516:HOH:O	2:H:21:ALA:HB2	2.14	0.48
1:C:187:PHE:CE2	2:I:21:ALA:HB1	2.49	0.48
1:D:103:LEU:HD22	1:D:185:PHE:HZ	1.77	0.48
3:A:351:G96:H21	3:A:351:G96:N1	2.29	0.48
1:F:300:THR:HG23	1:F:305:ILE:CD1	2.44	0.48
1:B:95:LEU:CD1	3:B:351:G96:H20	2.43	0.48
1:A:88:THR:HG21	1:A:116:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:THR:HG23	1:A:305:ILE:CD1	2.43	0.47
1:B:46:ILE:HD11	1:B:61:LYS:HB2	1.94	0.47
1:C:147:ALA:O	1:C:151:VAL:HG23	2.13	0.47
1:F:247:TYR:O	1:F:251:VAL:HG22	2.14	0.47
1:A:303:ILE:HD13	4:A:451:HOH:O	2.14	0.47
1:D:5:ALA:N	1:D:6:ALA:CB	2.77	0.47
1:F:226:VAL:HG13	1:F:237:PRO:HD2	1.96	0.47
1:B:75:ASP:O	1:B:79:VAL:HG23	2.15	0.47
1:B:116:LEU:HD11	1:B:347:PHE:CD1	2.50	0.47
1:F:265:LEU:HD13	1:F:296:TRP:CE2	2.49	0.47
1:D:62:HIS:ND1	1:D:65:THR:CG2	2.76	0.47
1:F:133:ARG:HD2	2:L:16:THR:O	2.15	0.47
1:F:305:ILE:HG23	4:F:453:HOH:O	2.14	0.47
1:A:72:LYS:HE2	1:A:74:LEU:HD11	1.97	0.47
1:C:187:PHE:HE2	2:I:21:ALA:HB1	1.79	0.47
1:B:43:PHE:C	1:B:63:MET:HE2	2.35	0.47
1:C:39:HIS:CE1	1:C:42:GLN:HG3	2.50	0.47
2:I:23:HIS:CG	2:I:24:ASP:H	2.33	0.46
1:D:218:ALA:CB	1:D:277:LEU:HD11	2.44	0.46
1:A:226:VAL:HG13	1:A:237:PRO:HD2	1.98	0.46
1:A:312:ALA:HB3	1:A:315:ILE:HD11	1.98	0.46
1:C:88:THR:HG21	1:C:116:LEU:HD13	1.97	0.46
1:D:265:LEU:HD13	1:D:296:TRP:CE2	2.50	0.46
1:F:305:ILE:HD13	4:F:457:HOH:O	2.15	0.46
1:C:103:LEU:HD21	1:C:153:THR:HG23	1.97	0.46
1:C:339:ILE:HD12	1:C:339:ILE:H	1.81	0.46
2:L:6:THR:HG22	2:L:6:THR:O	2.15	0.45
1:F:34:ALA:HB3	4:F:455:HOH:O	2.15	0.45
1:D:46:ILE:HD11	1:D:61:LYS:HB2	1.97	0.45
1:C:172:LEU:HB3	1:C:180:ILE:HD12	1.98	0.45
1:A:92:LYS:HE2	1:A:350:PHE:HA	1.98	0.45
1:C:43:PHE:C	1:C:63:MET:HE2	2.37	0.45
1:D:103:LEU:HD22	1:D:185:PHE:CZ	2.51	0.45
1:C:202:PRO:HD3	2:I:22:ILE:HG23	1.99	0.45
1:E:265:LEU:HD13	1:E:296:TRP:CZ2	2.51	0.45
1:E:202:PRO:HD3	2:K:22:ILE:HG23	1.98	0.44
1:C:80:VAL:HG22	1:C:85:ILE:HD11	2.00	0.44
1:A:43:PHE:HB3	1:A:60:VAL:HG13	1.99	0.44
1:D:75:ASP:O	1:D:79:VAL:HG23	2.17	0.44
1:C:41:ASP:O	1:C:63:MET:HE3	2.18	0.44
2:L:10:PHE:CE2	2:L:16:THR:HG22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ALA:CA	1:D:6:ALA:CB	2.91	0.44
1:F:207:PRO:O	1:F:210:ILE:CD1	2.65	0.44
1:E:74:LEU:HD22	1:E:74:LEU:N	2.33	0.44
1:D:46:ILE:HD12	1:D:59:LEU:HG	2.00	0.43
1:B:95:LEU:HD11	3:B:351:G96:H20	1.99	0.43
1:E:88:THR:HG21	1:E:116:LEU:CD1	2.48	0.43
1:F:104:VAL:HG22	1:F:182:VAL:O	2.18	0.43
1:F:156:TYR:O	1:F:160:LEU:HD13	2.18	0.43
1:B:123:VAL:HB	1:B:173:LEU:HD13	2.00	0.43
1:C:308:ARG:NH2	4:C:467:HOH:O	2.51	0.43
1:F:34:ALA:HB2	4:F:378:HOH:O	2.18	0.43
1:F:210:ILE:HD12	1:F:211:LEU:HG	2.01	0.43
1:D:5:ALA:HA	1:D:7:LYS:H	1.83	0.43
1:C:218:ALA:CB	1:C:277:LEU:HD11	2.46	0.42
1:E:208:GLU:CG	1:E:277:LEU:HD21	2.40	0.42
1:C:72:LYS:HE2	1:C:74:LEU:HD11	2.01	0.42
1:D:54:PHE:CD2	1:D:79:VAL:HG22	2.54	0.42
1:C:104:VAL:HG22	4:C:479:HOH:O	2.18	0.42
1:E:13:GLU:O	1:E:14:SER:HB2	2.19	0.42
1:E:13:GLU:O	1:E:14:SER:CB	2.68	0.42
1:A:148:ALA:CB	1:A:305:ILE:HD13	2.50	0.42
1:C:62:HIS:CD2	1:C:64:GLU:HG2	2.55	0.42
1:C:140:GLU:N	1:C:141:PRO:CD	2.83	0.42
1:D:70:ALA:HB3	1:D:120:MET:HG3	2.01	0.42
1:F:207:PRO:HA	1:F:210:ILE:HD11	2.02	0.42
1:B:176:GLN:NE2	1:B:318:PHE:CE2	2.87	0.42
1:E:70:ALA:HB3	1:E:120:MET:HG2	2.02	0.42
1:E:315:ILE:HD12	1:E:315:ILE:N	2.35	0.42
1:F:70:ALA:HB3	1:F:120:MET:HG2	2.01	0.41
1:A:314:PHE:C	1:A:315:ILE:HD12	2.41	0.41
1:D:116:LEU:HD11	1:D:347:PHE:CD1	2.55	0.41
1:D:9:GLY:HA2	1:D:10:SEP:HB3	2.01	0.41
1:D:303:ILE:HD11	4:D:438:HOH:O	2.21	0.41
1:F:240:ALA:HB2	1:F:249:LYS:NZ	2.35	0.41
2:L:11:ILE:N	2:L:11:ILE:HD13	2.36	0.41
1:F:265:LEU:HD13	1:F:296:TRP:CZ2	2.56	0.41
1:E:23:LYS:HA	1:E:160:LEU:HD21	2.03	0.41
1:E:41:ASP:OD1	1:E:41:ASP:N	2.44	0.41
1:C:126:GLY:HA2	1:C:327:PHE:CZ	2.56	0.40
3:C:351:G96:N1	3:C:351:G96:H21	2.36	0.40
1:D:76:LYS:O	1:D:80:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:HIS:ND1	1:D:217:LYS:HD2	2.36	0.40
1:F:54:PHE:CD2	1:F:79:VAL:HG22	2.56	0.40
1:B:76:LYS:O	1:B:80:VAL:HG23	2.21	0.40
1:F:315:ILE:N	1:F:315:ILE:HD12	2.37	0.40
1:A:115:ASN:HB2	1:A:117:TYR:CE1	2.57	0.40
1:B:104:VAL:HG21	4:B:752:HOH:O	2.21	0.40
1:C:208:GLU:OE1	1:C:277:LEU:HD13	2.22	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	339/350 (97%)	330 (97%)	9 (3%)	0	100	100
1	B	342/350 (98%)	330 (96%)	10 (3%)	2 (1%)	25	26
1	C	340/350 (97%)	331 (97%)	9 (3%)	0	100	100
1	D	342/350 (98%)	330 (96%)	11 (3%)	1 (0%)	41	46
1	E	334/350 (95%)	324 (97%)	9 (3%)	1 (0%)	41	46
1	F	339/350 (97%)	331 (98%)	8 (2%)	0	100	100
2	G	16/20 (80%)	15 (94%)	1 (6%)	0	100	100
2	H	18/20 (90%)	16 (89%)	2 (11%)	0	100	100
2	I	18/20 (90%)	15 (83%)	3 (17%)	0	100	100
2	J	17/20 (85%)	16 (94%)	1 (6%)	0	100	100
2	K	18/20 (90%)	16 (89%)	2 (11%)	0	100	100
2	L	16/20 (80%)	14 (88%)	2 (12%)	0	100	100
All	All	2139/2220 (96%)	2068 (97%)	67 (3%)	4 (0%)	47	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	14	SER
1	B	15	VAL
1	D	6	ALA
1	B	14	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/302 (100%)	296 (98%)	5 (2%)	60	74
1	B	301/302 (100%)	291 (97%)	10 (3%)	38	49
1	C	300/302 (99%)	289 (96%)	11 (4%)	34	43
1	D	296/302 (98%)	290 (98%)	6 (2%)	55	69
1	E	294/302 (97%)	287 (98%)	7 (2%)	49	62
1	F	301/302 (100%)	292 (97%)	9 (3%)	41	53
2	G	13/15 (87%)	13 (100%)	0	100	100
2	H	15/15 (100%)	15 (100%)	0	100	100
2	I	15/15 (100%)	14 (93%)	1 (7%)	16	18
2	J	14/15 (93%)	12 (86%)	2 (14%)	3	2
2	K	15/15 (100%)	14 (93%)	1 (7%)	16	18
2	L	13/15 (87%)	12 (92%)	1 (8%)	13	13
All	All	1878/1902 (99%)	1825 (97%)	53 (3%)	43	56

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	36	ASN
1	A	163	ILE
1	A	242	GLN
1	A	277	LEU
1	B	36	ASN
1	B	39	HIS

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Mol	Chain	Res	Type
1	B	45	ARG
1	B	92	LYS
1	B	120	MET
1	B	183	THR
1	B	285	LYS
1	B	295	LYS
1	B	331	GLU
1	B	345	LYS
1	C	28	LYS
1	C	31	GLU
1	C	41	ASP
1	C	53	SER
1	C	60	VAL
1	C	92	LYS
1	C	114	SER
1	C	160	LEU
1	C	195	THR
1	C	285	LYS
1	C	336	ARG
1	D	21	LYS
1	D	36	ASN
1	D	45	ARG
1	D	92	LYS
1	D	163	ILE
1	D	342	LYS
1	E	31	GLU
1	E	41	ASP
1	E	45	ARG
1	E	60	VAL
1	E	81	LYS
1	E	92	LYS
1	E	137	ARG
1	F	13	GLU
1	F	31	GLU
1	F	51	THR
1	F	81	LYS
1	F	92	LYS
1	F	241	ASP
1	F	242	GLN
1	F	285	LYS
1	F	345	LYS
2	I	15	ARG

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Mol	Chain	Res	Type
2	J	5	THR
2	J	15	ARG
2	K	15	ARG
2	L	24	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	HIS
1	B	293	ASN
1	C	286	ASN
1	E	32	ASN
1	E	62	HIS
1	E	271	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

17 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	SEP	D	338	1	8,9,10	1.61	1 (12%)	7,12,14	1.70	1 (14%)
1	TPO	F	197	1	8,10,11	0.75	0	10,14,16	1.13	1 (10%)
1	SEP	F	338	1	8,9,10	1.62	1 (12%)	7,12,14	2.04	2 (28%)
1	SEP	B	338	1	8,9,10	1.65	1 (12%)	7,12,14	1.61	1 (14%)
1	TPO	B	197	1	8,10,11	0.65	0	10,14,16	1.08	0
1	SEP	A	338	1	8,9,10	1.53	1 (12%)	7,12,14	1.87	2 (28%)
1	SEP	D	10	1	8,9,10	1.64	1 (12%)	7,12,14	1.55	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SEP	F	10	1	8,9,10	1.65	1 (12%)	7,12,14	1.39	1 (14%)
1	TPO	A	197	1	8,10,11	0.74	0	10,14,16	1.11	0
1	SEP	C	10	1	8,9,10	1.68	1 (12%)	7,12,14	1.88	1 (14%)
1	SEP	A	10	1	8,9,10	1.67	1 (12%)	7,12,14	1.69	1 (14%)
1	SEP	E	338	1	8,9,10	1.60	1 (12%)	7,12,14	1.74	1 (14%)
1	TPO	E	197	1	8,10,11	0.80	0	10,14,16	1.05	1 (10%)
1	TPO	D	197	1	8,10,11	0.71	0	10,14,16	1.16	0
1	SEP	C	338	1	8,9,10	1.56	1 (12%)	7,12,14	1.52	2 (28%)
1	TPO	C	197	1	8,10,11	0.76	0	10,14,16	1.06	0
1	SEP	B	10	1	8,9,10	1.66	1 (12%)	7,12,14	1.45	1 (14%)

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
1	SEP	D	338	1	-	3/6/8/10	-
1	TPO	F	197	1	-	0/9/11/13	-
1	SEP	F	338	1	-	3/6/8/10	-
1	SEP	B	338	1	-	3/6/8/10	-
1	TPO	B	197	1	-	1/9/11/13	-
1	SEP	A	338	1	-	3/6/8/10	-
1	SEP	D	10	1	-	1/6/8/10	-
1	SEP	F	10	1	-	2/6/8/10	-
1	TPO	A	197	1	-	0/9/11/13	-
1	SEP	C	10	1	-	2/6/8/10	-
1	SEP	A	10	1	-	2/6/8/10	-
1	SEP	E	338	1	-	3/6/8/10	-
1	TPO	E	197	1	-	0/9/11/13	-
1	TPO	D	197	1	-	1/9/11/13	-
1	SEP	C	338	1	-	3/6/8/10	-
1	TPO	C	197	1	-	0/9/11/13	-
1	SEP	B	10	1	-	2/6/8/10	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	10	SEP	P-O1P	3.68	1.61	1.50
1	B	10	SEP	P-O1P	3.66	1.61	1.50
1	B	338	SEP	P-O1P	3.64	1.61	1.50
1	A	10	SEP	P-O1P	3.61	1.61	1.50
1	F	10	SEP	P-O1P	3.61	1.61	1.50
1	F	338	SEP	P-O1P	3.60	1.61	1.50
1	D	10	SEP	P-O1P	3.54	1.61	1.50
1	D	338	SEP	P-O1P	3.53	1.61	1.50
1	E	338	SEP	P-O1P	3.51	1.61	1.50
1	C	338	SEP	P-O1P	3.36	1.60	1.50
1	A	338	SEP	P-O1P	3.29	1.60	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	338	SEP	OG-CB-CA	4.72	112.73	108.14
1	C	10	SEP	OG-CB-CA	4.48	112.50	108.14
1	E	338	SEP	OG-CB-CA	4.04	112.07	108.14
1	D	338	SEP	OG-CB-CA	3.89	111.93	108.14
1	A	10	SEP	OG-CB-CA	3.84	111.88	108.14
1	A	338	SEP	OG-CB-CA	3.76	111.81	108.14
1	B	338	SEP	OG-CB-CA	3.70	111.75	108.14
1	B	10	SEP	OG-CB-CA	3.14	111.20	108.14
1	F	10	SEP	OG-CB-CA	3.08	111.15	108.14
1	D	10	SEP	OG-CB-CA	3.00	111.06	108.14
1	C	338	SEP	OG-CB-CA	2.90	110.97	108.14
1	A	338	SEP	OG-P-O1P	2.78	113.96	106.44
1	C	338	SEP	OG-P-O1P	2.31	112.70	106.44
1	F	197	TPO	O3P-P-O2P	2.23	116.17	107.80
1	F	338	SEP	OG-P-O1P	2.11	112.14	106.44
1	E	197	TPO	O3P-P-O2P	2.07	115.56	107.80

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	10	SEP	CB-OG-P-O2P
1	A	10	SEP	CB-OG-P-O3P
1	A	338	SEP	N-CA-CB-OG
1	A	338	SEP	CA-CB-OG-P
1	A	338	SEP	CB-OG-P-O2P
1	B	10	SEP	N-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	B	10	SEP	C-CA-CB-OG
1	B	338	SEP	C-CA-CB-OG
1	B	338	SEP	CA-CB-OG-P
1	C	10	SEP	CB-OG-P-O3P
1	C	338	SEP	N-CA-CB-OG
1	C	338	SEP	CA-CB-OG-P
1	D	338	SEP	C-CA-CB-OG
1	D	338	SEP	CA-CB-OG-P
1	E	338	SEP	C-CA-CB-OG
1	E	338	SEP	CA-CB-OG-P
1	F	10	SEP	C-CA-CB-OG
1	F	338	SEP	N-CA-CB-OG
1	F	338	SEP	CA-CB-OG-P
1	F	338	SEP	CB-OG-P-O2P
1	C	10	SEP	CA-CB-OG-P
1	D	10	SEP	CA-CB-OG-P
1	B	338	SEP	N-CA-CB-OG
1	D	338	SEP	N-CA-CB-OG
1	E	338	SEP	N-CA-CB-OG
1	F	10	SEP	N-CA-CB-OG
1	C	338	SEP	CB-OG-P-O2P
1	B	197	TPO	CB-OG1-P-O3P
1	D	197	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	10	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	G96	C	351	-	31,37,37	2.33	1 (3%)	31,53,53	1.19	2 (6%)
3	G96	B	351	-	31,37,37	2.47	1 (3%)	31,53,53	1.31	4 (12%)
3	G96	E	351	-	31,37,37	2.49	1 (3%)	31,53,53	1.33	5 (16%)
3	G96	F	351	-	31,37,37	2.27	1 (3%)	31,53,53	1.23	4 (12%)
3	G96	A	351	-	31,37,37	2.30	1 (3%)	31,53,53	1.23	3 (9%)
3	G96	D	351	-	31,37,37	2.42	2 (6%)	31,53,53	1.26	3 (9%)

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	G96	C	351	-	-	2/15/21/21	0/4/4/4
3	G96	B	351	-	-	3/15/21/21	0/4/4/4
3	G96	E	351	-	-	0/15/21/21	0/4/4/4
3	G96	F	351	-	-	1/15/21/21	0/4/4/4
3	G96	A	351	-	-	1/15/21/21	0/4/4/4
3	G96	D	351	-	-	2/15/21/21	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	351	G96	C12-C13	-13.07	1.28	1.43
3	B	351	G96	C12-C13	-13.00	1.28	1.43
3	D	351	G96	C12-C13	-12.68	1.28	1.43
3	C	351	G96	C12-C13	-12.27	1.29	1.43
3	A	351	G96	C12-C13	-12.12	1.29	1.43
3	F	351	G96	C12-C13	-11.90	1.29	1.43
3	D	351	G96	C16-N6	2.29	1.35	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	351	G96	C7-O1-C10	4.00	122.91	117.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	351	G96	C12-N4-C10	3.71	121.78	115.10
3	A	351	G96	C12-N4-C10	3.67	121.70	115.10
3	D	351	G96	C11-C10-N4	-3.47	120.13	124.17
3	D	351	G96	C12-N4-C10	3.44	121.28	115.10
3	C	351	G96	C12-N4-C10	3.43	121.28	115.10
3	F	351	G96	C11-C10-N4	-3.43	120.17	124.17
3	B	351	G96	C11-C10-N4	-3.40	120.20	124.17
3	B	351	G96	C7-O1-C10	3.30	121.99	117.69
3	E	351	G96	C11-C10-N4	-3.26	120.37	124.17
3	B	351	G96	C12-N4-C10	3.24	120.93	115.10
3	D	351	G96	C7-O1-C10	3.21	121.87	117.69
3	C	351	G96	C11-C10-N4	-3.15	120.50	124.17
3	E	351	G96	C12-N4-C10	3.15	120.76	115.10
3	A	351	G96	C11-C10-N4	-3.09	120.56	124.17
3	E	351	G96	C1-C24-C23	-2.52	108.39	113.23
3	F	351	G96	C7-O1-C10	2.42	120.85	117.69
3	B	351	G96	C1-C24-C23	-2.28	108.84	113.23
3	A	351	G96	C1-C24-C23	-2.27	108.86	113.23
3	E	351	G96	C11-C15-C14	-2.12	118.55	120.55
3	F	351	G96	C1-C24-C23	-2.07	109.25	113.23

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	351	G96	N4-C12-C13-C17
3	D	351	G96	C13-C17-C18-C20
3	F	351	G96	C12-C13-C17-C18
3	A	351	G96	C12-C13-C17-C18
3	C	351	G96	C12-C13-C17-C18
3	B	351	G96	C22-C21-N5-C16
3	B	351	G96	C13-C17-C18-C20
3	C	351	G96	C13-C17-C18-C20
3	D	351	G96	C13-C17-C18-C19

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	351	G96	2	0
3	B	351	G96	4	0

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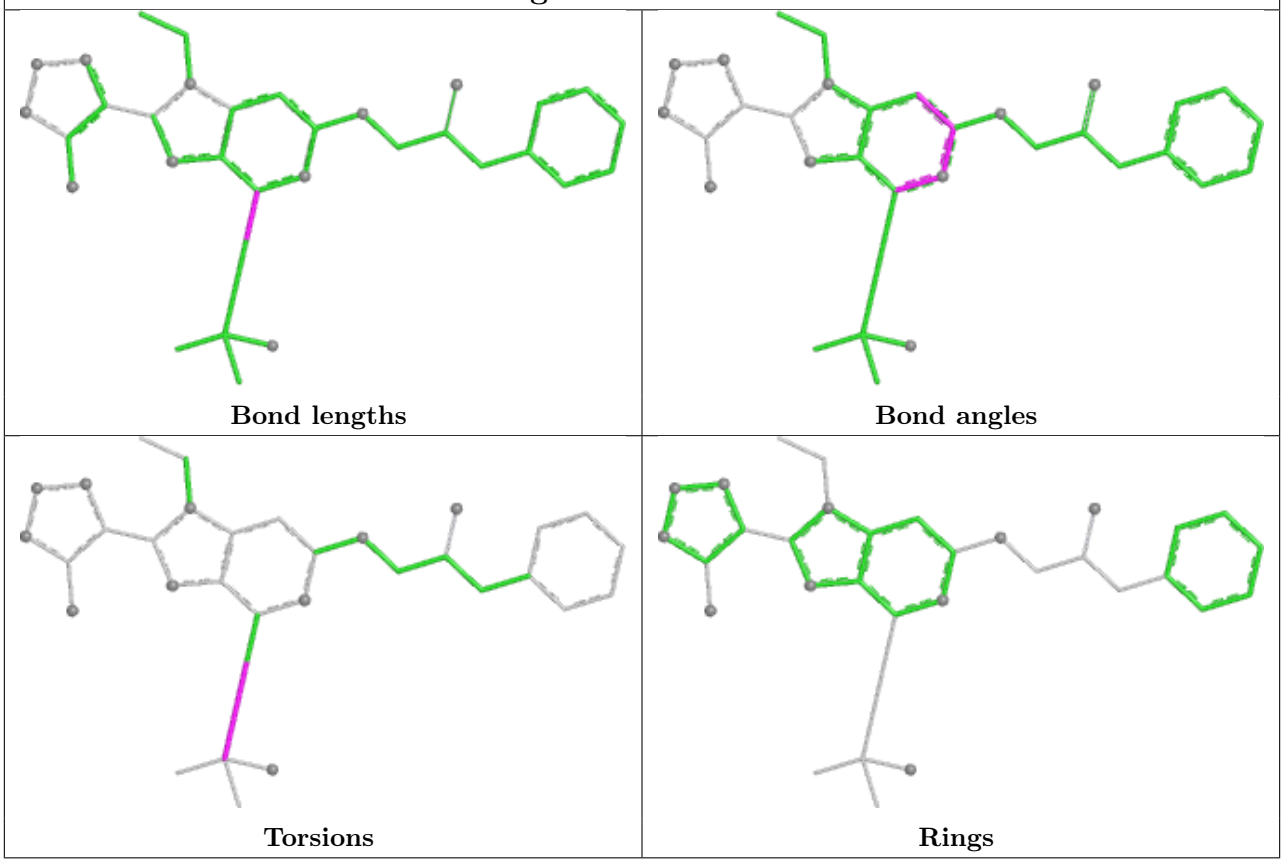
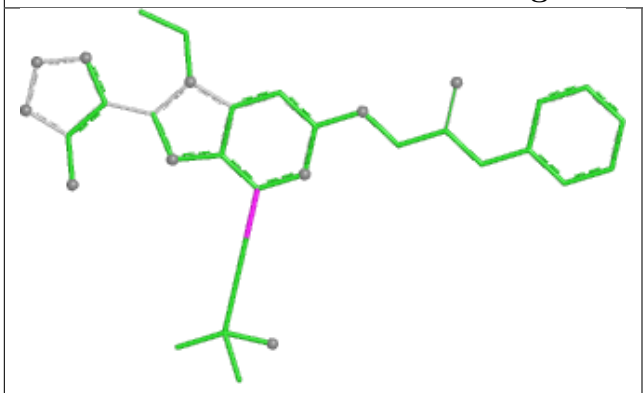
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	351	G96	2	0
3	D	351	G96	2	0

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.

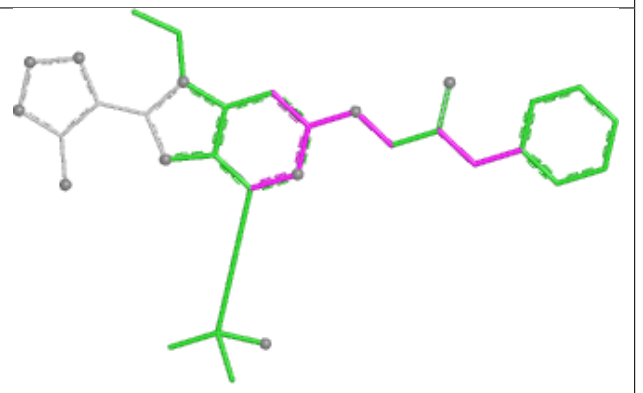
Ligand G96 C 351



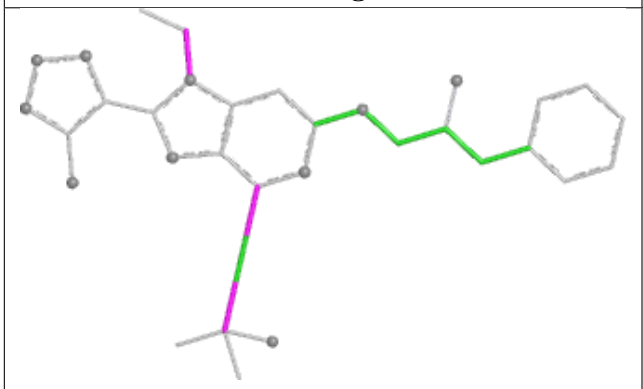
Ligand G96 B 351



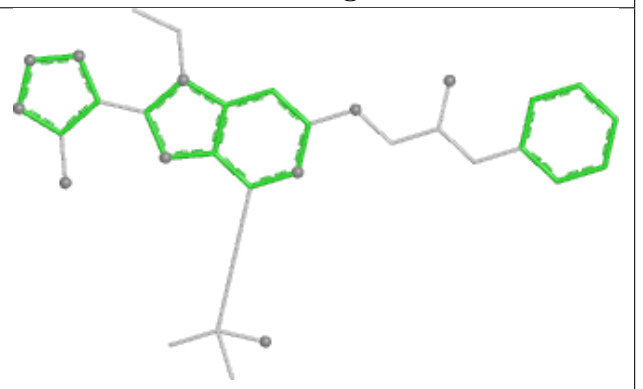
Bond lengths



Bond angles

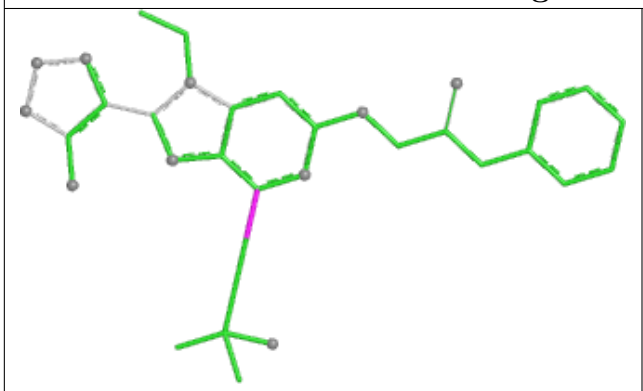


Torsions

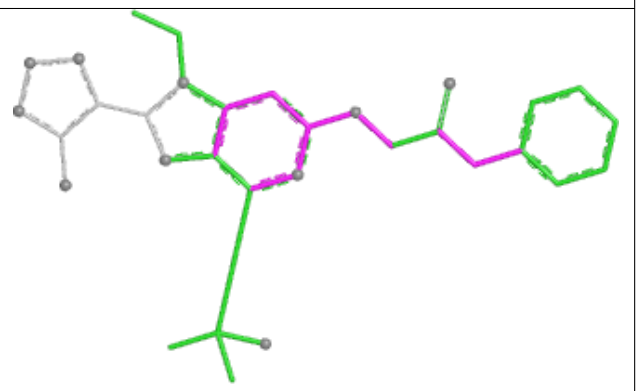


Rings

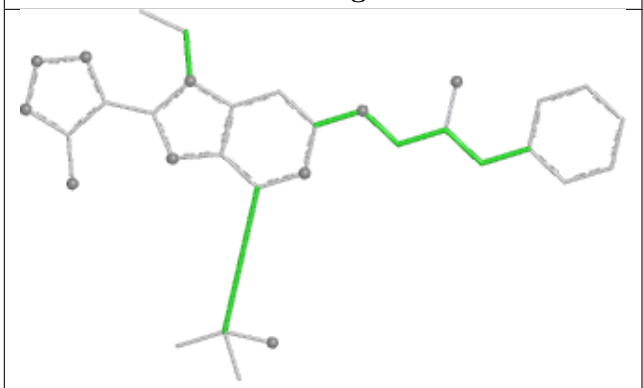
Ligand G96 E 351



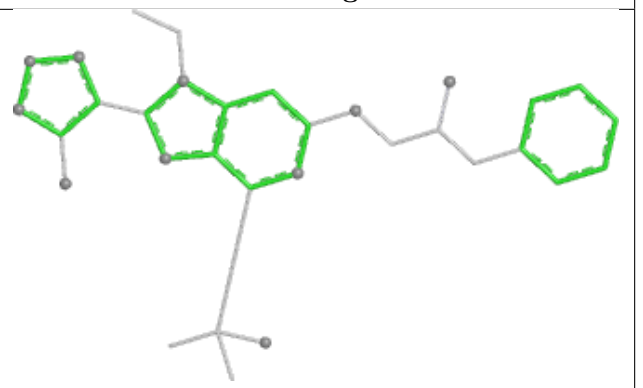
Bond lengths



Bond angles

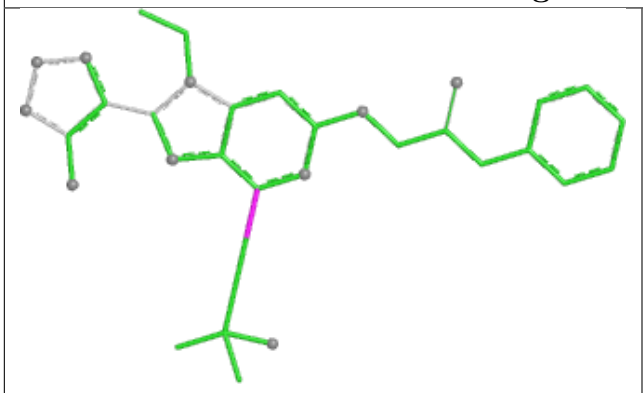


Torsions

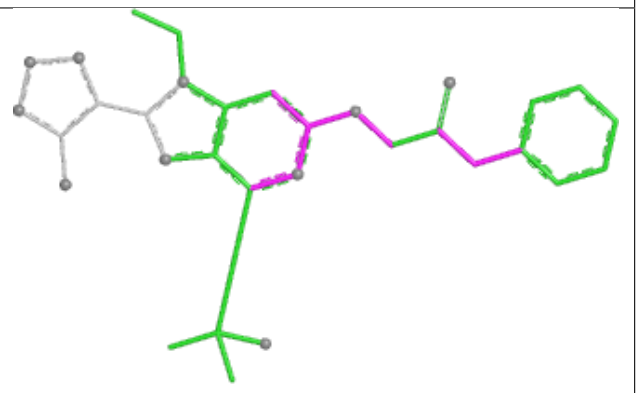


Rings

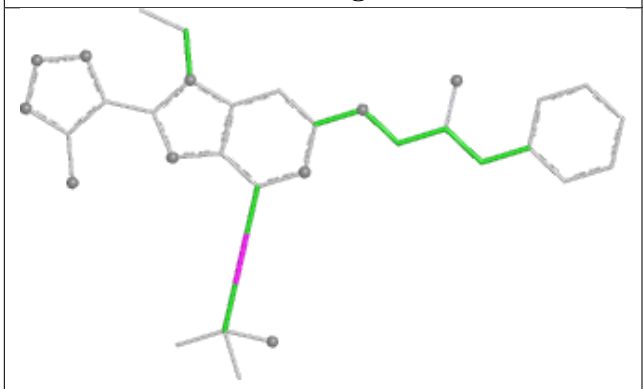
Ligand G96 F 351



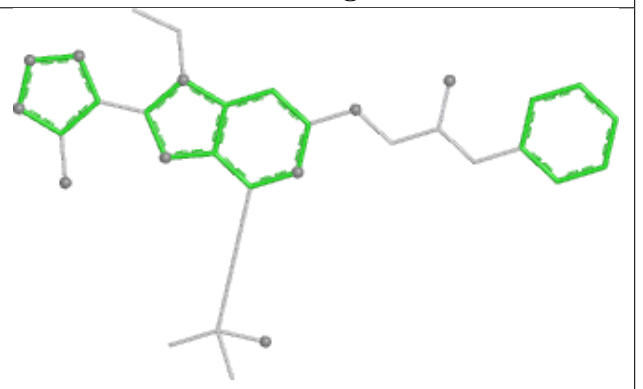
Bond lengths



Bond angles

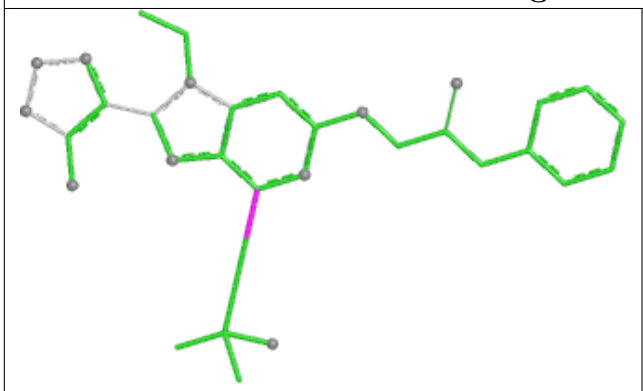


Torsions

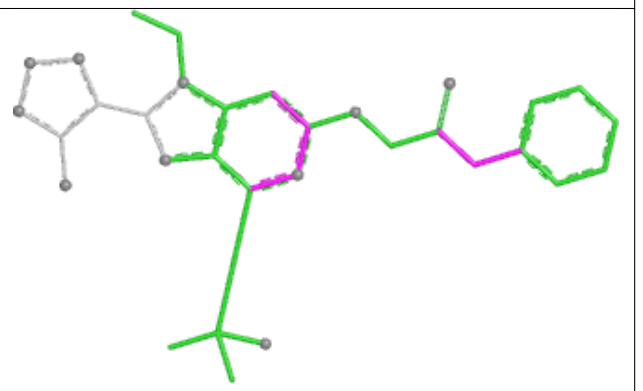


Rings

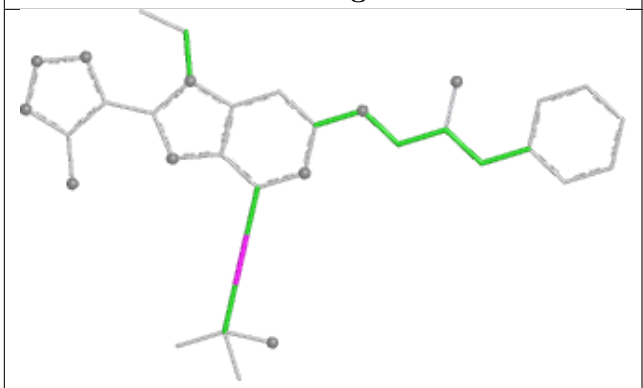
Ligand G96 A 351



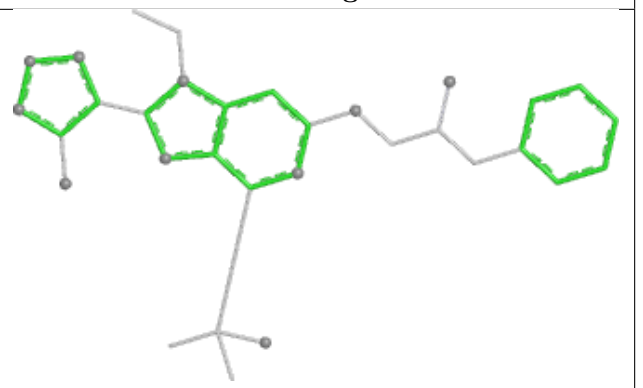
Bond lengths



Bond angles

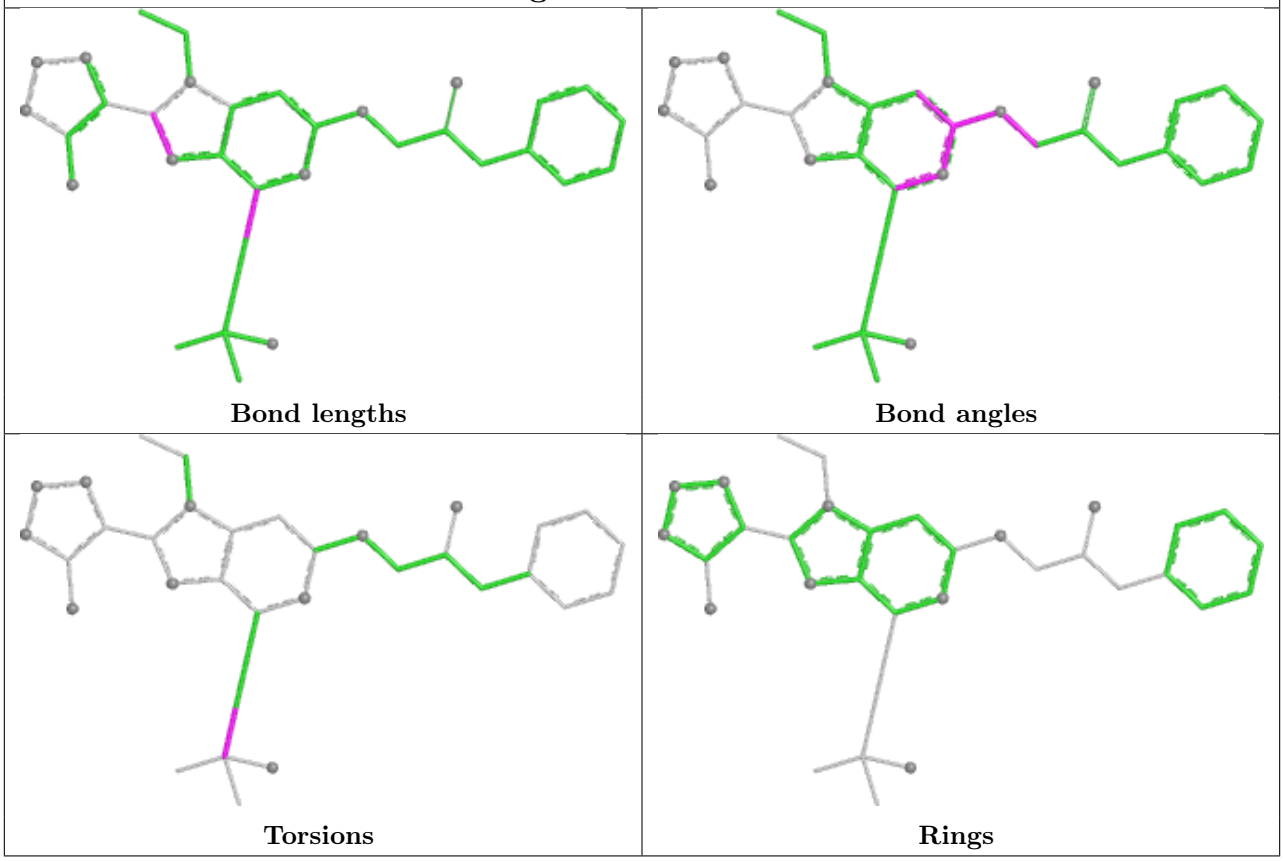


Torsions



Rings

Ligand G96 D 351



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	341/350 (97%)	0.61	21 (6%)	20	19	14, 16, 25, 48	0
1	B	344/350 (98%)	0.46	15 (4%)	34	32	14, 16, 26, 35	0
1	C	341/350 (97%)	0.71	26 (7%)	13	12	14, 16, 25, 53	0
1	D	344/350 (98%)	0.59	16 (4%)	31	30	14, 16, 23, 31	0
1	E	336/350 (96%)	0.72	27 (8%)	12	11	14, 16, 22, 31	0
1	F	341/350 (97%)	0.93	51 (14%)	2	2	14, 16, 25, 39	0
2	G	18/20 (90%)	0.82	2 (11%)	5	4	20, 21, 29, 32	0
2	H	20/20 (100%)	0.98	2 (10%)	7	6	20, 22, 37, 38	0
2	I	20/20 (100%)	1.68	4 (20%)	1	1	20, 22, 37, 38	0
2	J	19/20 (95%)	1.02	2 (10%)	6	5	20, 22, 32, 35	0
2	K	20/20 (100%)	1.32	3 (15%)	2	2	20, 22, 35, 36	0
2	L	19/20 (95%)	3.30	11 (57%)	0	0	20, 22, 35, 36	0
All	All	2163/2220 (97%)	0.71	180 (8%)	11	10	14, 16, 26, 53	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	24	ASP	10.6
1	F	9	GLY	9.9
2	I	24	ASP	9.4
1	C	9	GLY	9.0
2	I	23	HIS	8.3
2	L	7	TYR	6.8
2	H	24	ASP	6.7
2	K	24	ASP	6.7
1	F	13	GLU	6.7
2	L	23	HIS	6.7
2	K	23	HIS	6.4

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Mol	Chain	Res	Type	RSRZ
2	L	22	ILE	5.9
1	F	11	GLU	5.7
1	C	7	LYS	5.4
2	I	22	ILE	5.4
2	G	14	GLY	5.0
1	E	339	ILE	5.0
2	L	13	SER	4.8
1	E	16	LYS	4.8
2	L	6	THR	4.7
1	E	15	VAL	4.6
2	H	23	HIS	4.6
1	B	339	ILE	4.5
1	E	335	ILE	4.5
1	D	8	LYS	4.4
1	A	9	GLY	4.4
1	E	336	ARG	4.4
2	L	12	ALA	4.3
1	C	33	PRO	4.3
1	C	11	GLU	4.2
1	F	34	ALA	4.2
1	E	18	PHE	4.2
1	F	321	PRO	4.1
2	J	23	HIS	4.0
1	F	246	ILE	4.0
1	E	19	LEU	4.0
1	C	336	ARG	4.0
1	C	8	LYS	4.0
1	F	253	GLY	3.7
1	A	34	ALA	3.7
1	C	34	ALA	3.7
2	J	5	THR	3.7
1	F	132	LEU	3.7
1	A	336	ARG	3.6
1	A	321	PRO	3.6
1	F	336	ARG	3.5
1	B	14	SER	3.4
2	L	21	ALA	3.4
1	E	41	ASP	3.4
2	L	10	PHE	3.4
1	F	241	ASP	3.3
1	F	17	GLU	3.3
1	E	340	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	G	12	ALA	3.3
1	F	277	LEU	3.3
1	E	113	ASN	3.2
1	F	14	SER	3.2
1	C	35	GLN	3.2
1	F	7	LYS	3.1
1	F	63	MET	3.1
1	E	334	GLU	3.1
1	A	318	PHE	3.1
1	B	7	LYS	3.1
1	C	13	GLU	3.1
1	F	318	PHE	3.1
1	F	12	GLN	3.0
1	A	13	GLU	3.0
1	D	213	LYS	3.0
1	C	167	LEU	3.0
1	B	336	ARG	3.0
1	F	263	SER	3.0
2	K	17	GLY	3.0
1	B	340	ASN	2.9
1	F	213	LYS	2.9
1	F	285	LYS	2.9
1	F	295	LYS	2.9
1	A	227	LEU	2.9
1	C	331	GLU	2.8
1	F	255	VAL	2.8
1	D	331	GLU	2.8
1	C	64	GLU	2.8
1	F	299	THR	2.8
1	F	256	ARG	2.8
1	B	132	LEU	2.8
1	B	172	LEU	2.8
1	E	329	ASP	2.7
1	F	33	PRO	2.7
2	L	14	GLY	2.7
1	F	273	LEU	2.7
1	F	317	LYS	2.7
1	B	244	ILE	2.7
1	E	233	ALA	2.7
1	C	334	GLU	2.7
1	D	333	GLU	2.7
1	F	21	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	172	LEU	2.7
1	D	241	ASP	2.7
1	E	36	ASN	2.7
1	C	12	GLN	2.7
1	B	39	HIS	2.7
1	C	132	LEU	2.7
1	A	64	GLU	2.6
1	A	172	LEU	2.6
1	F	15	VAL	2.6
1	F	227	LEU	2.6
1	F	172	LEU	2.6
1	A	232	ALA	2.6
1	E	20	ALA	2.6
1	D	295	LYS	2.6
1	F	243	PRO	2.6
1	F	252	SER	2.5
1	F	276	ASP	2.5
1	E	132	LEU	2.5
1	F	248	GLU	2.5
1	E	295	LYS	2.5
1	C	320	GLY	2.5
1	E	244	ILE	2.5
1	C	17	GLU	2.5
1	F	286	ASN	2.5
1	A	132	LEU	2.5
1	F	254	LYS	2.5
1	D	329	ASP	2.5
1	E	278	THR	2.4
1	C	339	ILE	2.4
1	E	333	GLU	2.4
1	C	36	ASN	2.4
1	B	5	ALA	2.4
1	E	62	HIS	2.4
1	F	320	GLY	2.4
1	E	14	SER	2.4
1	C	228	ILE	2.4
1	F	245	GLN	2.4
1	A	322	GLY	2.4
1	D	335	ILE	2.4
1	F	298	ALA	2.4
1	B	12	GLN	2.4
1	A	333	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	231	MET	2.3
1	E	285	LYS	2.3
1	A	138	PHE	2.3
2	L	20	ASN	2.3
1	C	232	ALA	2.3
1	F	244	ILE	2.3
1	F	16	LYS	2.3
1	A	244	ILE	2.3
1	A	143	ALA	2.3
1	B	232	ALA	2.3
1	C	344	GLY	2.3
1	E	286	ASN	2.3
1	A	36	ASN	2.2
2	I	20	ASN	2.2
1	C	227	LEU	2.2
1	C	231	MET	2.2
1	C	333	GLU	2.2
1	E	21	LYS	2.2
1	B	135	ILE	2.2
1	F	8	LYS	2.2
1	F	89	LEU	2.2
1	D	164	TYR	2.2
1	F	191	VAL	2.1
1	F	250	ILE	2.1
1	A	276	ASP	2.1
1	C	128	MET	2.1
1	D	242	GLN	2.1
1	B	334	GLU	2.1
1	F	25	ASP	2.1
1	B	227	LEU	2.1
1	E	330	TYR	2.1
1	A	139	SER	2.1
1	F	35	GLN	2.1
1	E	51	THR	2.1
1	A	182	VAL	2.1
1	D	39	HIS	2.1
1	F	278	THR	2.1
1	F	271	ASN	2.1
1	D	182	VAL	2.1
1	D	339	ILE	2.1
1	F	293	ASN	2.1
1	D	337	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	34	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	C	10	10/11	0.58	0.45	49,50,52,52	0
1	SEP	A	10	10/11	0.69	0.26	45,46,46,46	0
1	SEP	F	10	10/11	0.70	0.39	37,38,38,38	0
1	SEP	D	10	10/11	0.85	0.19	22,23,23,24	0
1	SEP	E	338	10/11	0.87	0.17	26,26,27,27	0
1	SEP	C	338	10/11	0.88	0.17	25,27,27,27	0
1	SEP	B	10	10/11	0.89	0.16	30,31,32,32	0
1	SEP	D	338	10/11	0.90	0.17	26,26,27,27	0
1	SEP	A	338	10/11	0.92	0.14	25,26,27,27	0
1	SEP	B	338	10/11	0.92	0.17	26,27,27,27	0
1	SEP	F	338	10/11	0.94	0.11	25,26,27,27	0
1	TPO	E	197	11/12	0.95	0.12	11,13,15,15	0
1	TPO	F	197	11/12	0.96	0.16	12,14,15,15	0
1	TPO	B	197	11/12	0.97	0.12	10,13,14,15	0
1	TPO	C	197	11/12	0.97	0.14	11,13,15,15	0
1	TPO	D	197	11/12	0.97	0.14	11,13,14,15	0
1	TPO	A	197	11/12	0.98	0.14	11,13,15,15	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

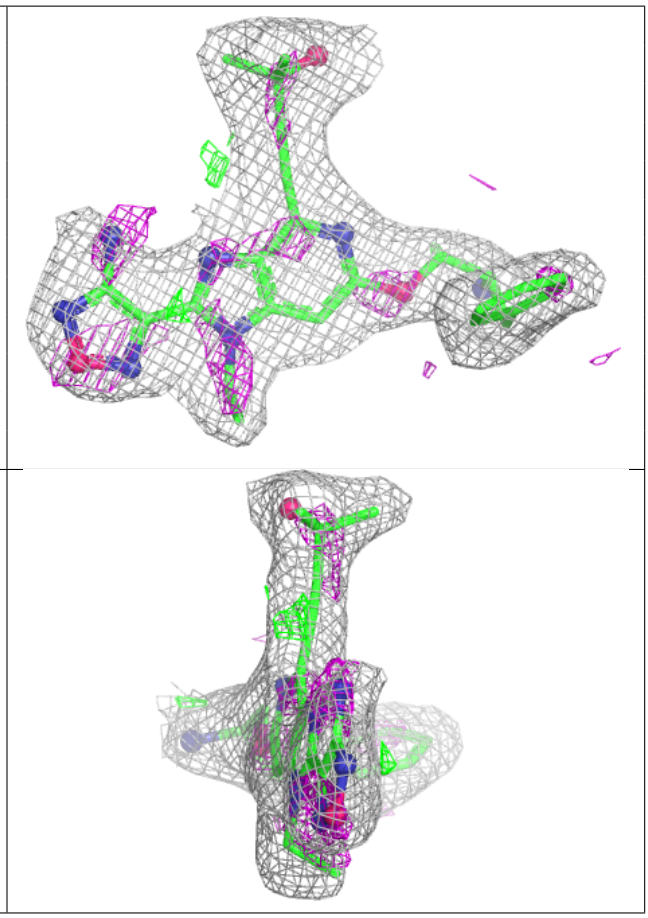
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	G96	C	351	34/34	0.92	0.14	10,11,12,13	0
3	G96	E	351	34/34	0.92	0.13	13,14,19,20	0
3	G96	F	351	34/34	0.93	0.13	13,14,17,17	0
3	G96	D	351	34/34	0.94	0.12	8,10,15,15	0
3	G96	B	351	34/34	0.94	0.11	5,6,12,12	0
3	G96	A	351	34/34	0.94	0.10	4,5,7,7	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.

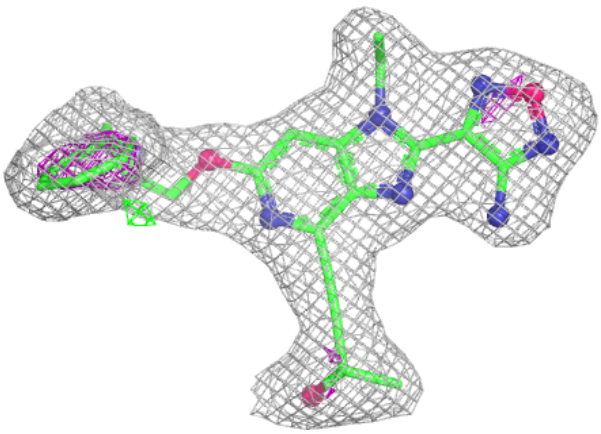
Electron density around G96 C 351:

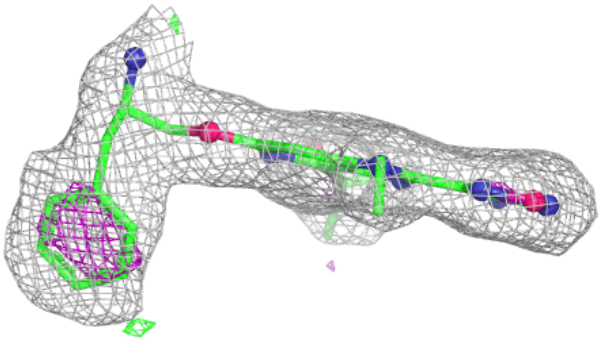
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

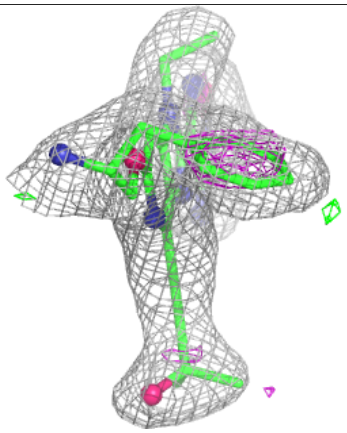


Electron density around G96 E 351:

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

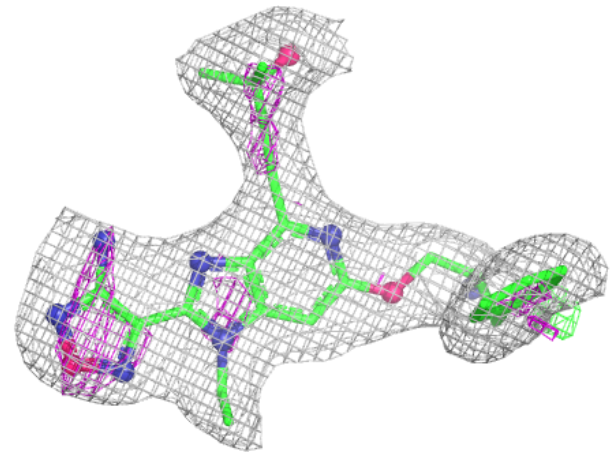


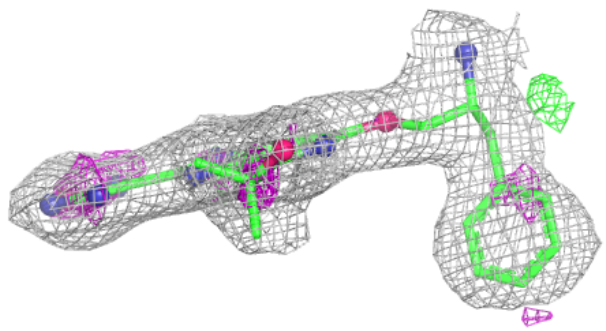


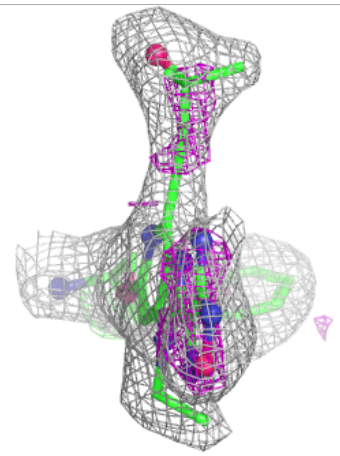


Electron density around G96 F 351:

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

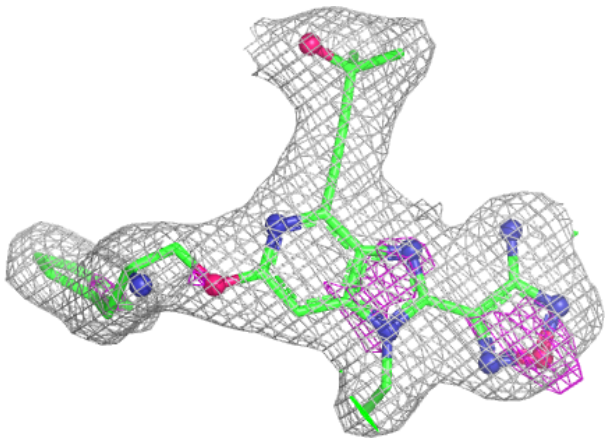


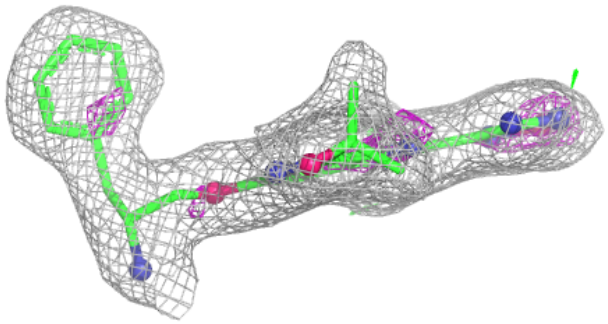


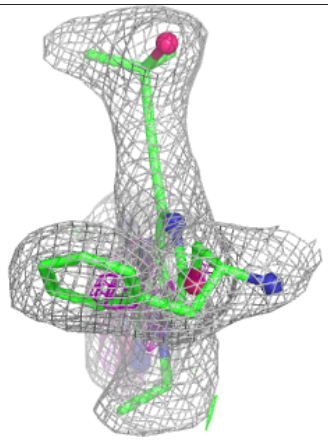


Electron density around G96 D 351:

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

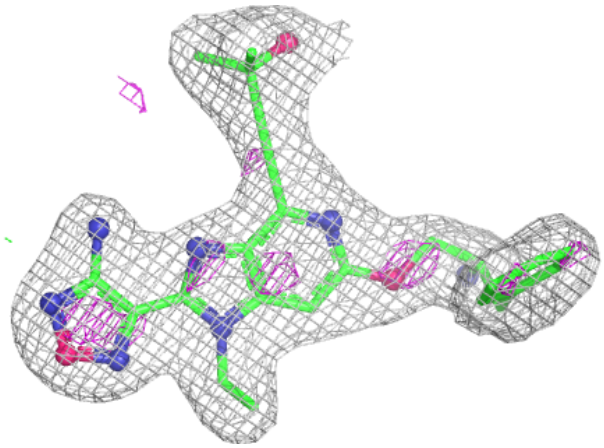


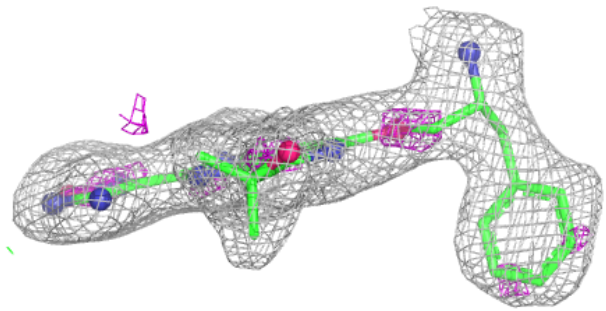


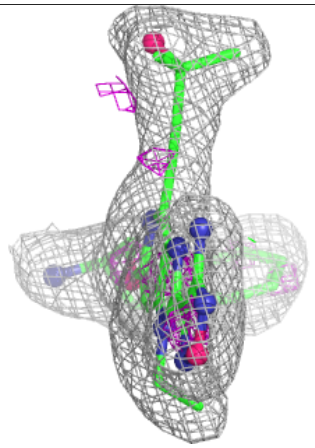


Electron density around G96 B 351:

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

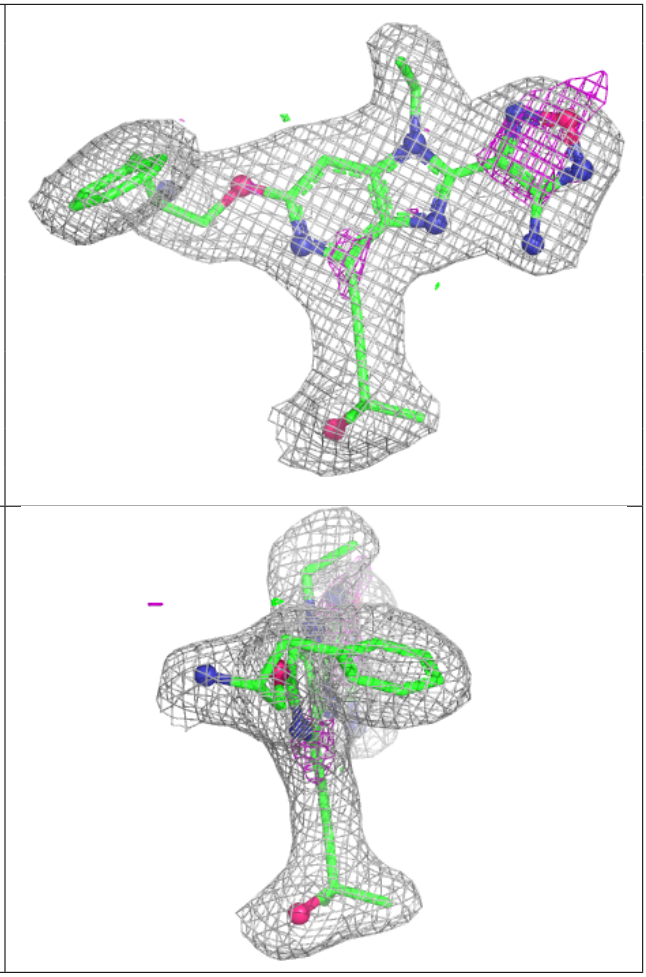






Electron density around G96 A 351:

$2mF_o$-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.