Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 09:23 PM EDT

PDB ID	:	4MJO
Title	:	Human liver fructose-1,6-bisphosphatase(d-fructose-1,6-bisphosphate, 1-phosphohydrolase) (e.c.3.1.3.11) complexed with the allosteric inhibitor 3
Authors	:	Ruf, A.; Joseph, C.; Tetaz, T.; Benz, J.
Deposited on	:	2013-09-04
Resolution	:	2.40 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:

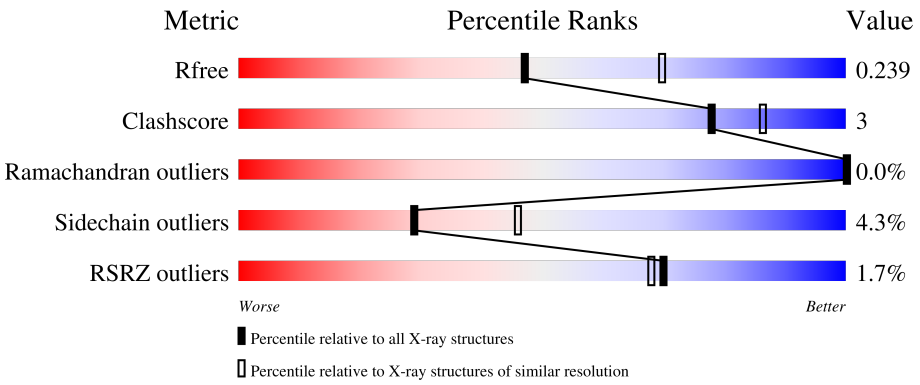
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	338	2% 86% 7% • 6%
1	B	338	2% 85% 8% • 6%
1	C	338	% 86% 7% • 6%
1	D	338	% 87% 6% • 6%
1	E	338	2% 86% 8% • 6%

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Mol	Chain	Length	Quality of chain
1	F	338	3% 83% 9% • 6%
1	G	338	% 86% 7% • 6%
1	H	338	2% 86% 7% 6%

2 Entry composition (i)

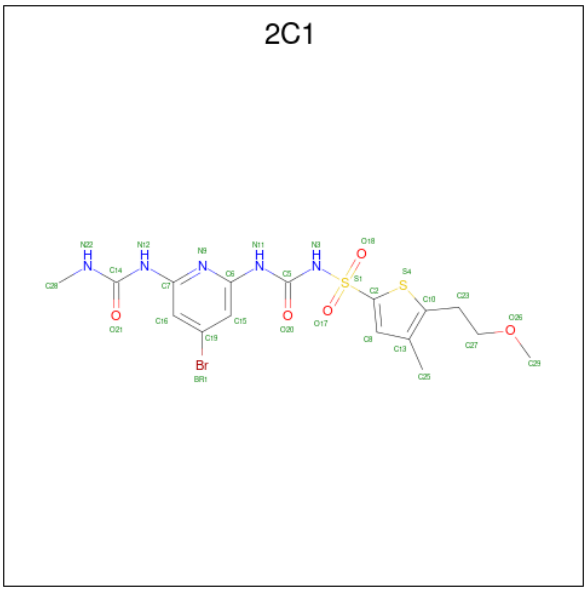
There are 3 unique types of molecules in this entry. The entry contains 20383 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fructose-1,6-bisphosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	2448	1558	414	459	17	0	1	0
1	B	317	2433	1548	411	457	17	0	1	0
1	C	317	2427	1545	408	457	17	0	0	0
1	D	318	2442	1554	413	458	17	0	1	0
1	E	319	2449	1559	414	459	17	0	1	0
1	F	317	2432	1547	411	457	17	0	1	0
1	G	317	2432	1547	411	457	17	0	1	0
1	H	317	2427	1545	408	457	17	0	0	0

- Molecule 2 is N-({4-bromo-6-[(methylcarbamoyl)amino]pyridin-2-yl}carbamoyl)-5-(2-methoxyethyl)-4-methylthiophene-2-sulfonamide (three-letter code: 2C1) (formula: $C_{16}H_{20}BrN_5O_5S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	S		
2	A	1	29	1	16	5	5	2	0	0
2	B	1	29	1	16	5	5	2	0	0
2	C	1	29	1	16	5	5	2	0	0
2	D	1	29	1	16	5	5	2	0	0
2	E	1	29	1	16	5	5	2	0	0
2	F	1	29	1	16	5	5	2	0	0
2	G	1	29	1	16	5	5	2	0	0
2	H	1	29	1	16	5	5	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	78	78	78	0	0
3	B	75	75	75	0	0
3	C	108	108	108	0	0
3	D	110	110	110	0	0

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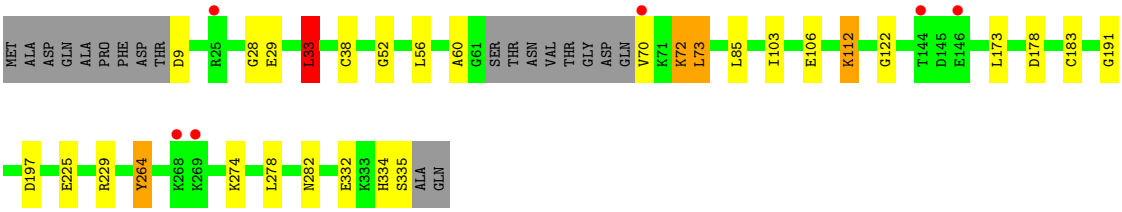
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	E	53	53	53	0	0
			Total	O		
3	F	56	56	56	0	0
			Total	O		
3	G	97	97	97	0	0
			Total	O		
3	H	84	84	84	0	0

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.

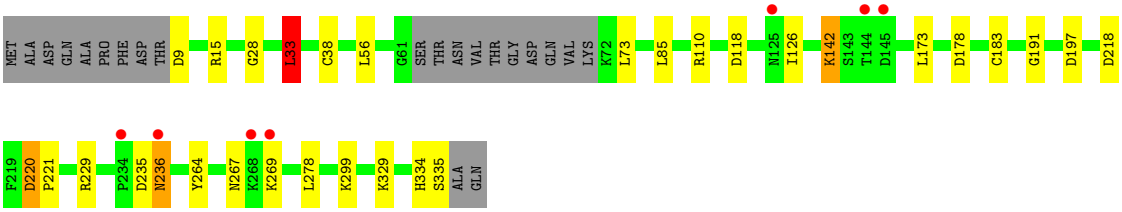
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain A:



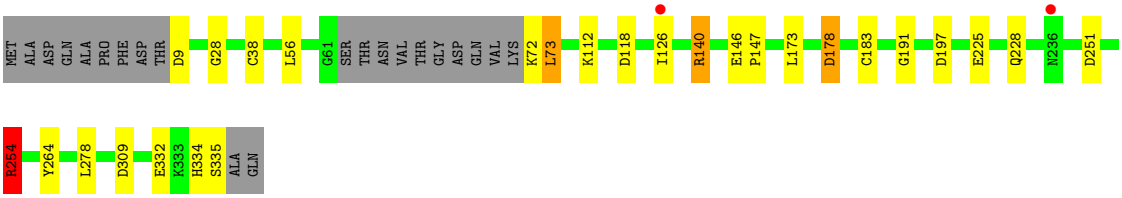
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain B:



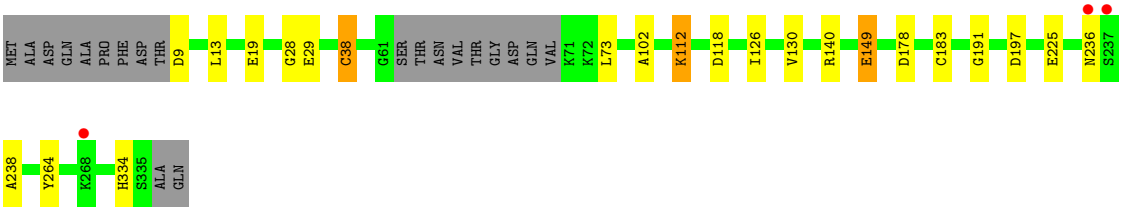
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain C:



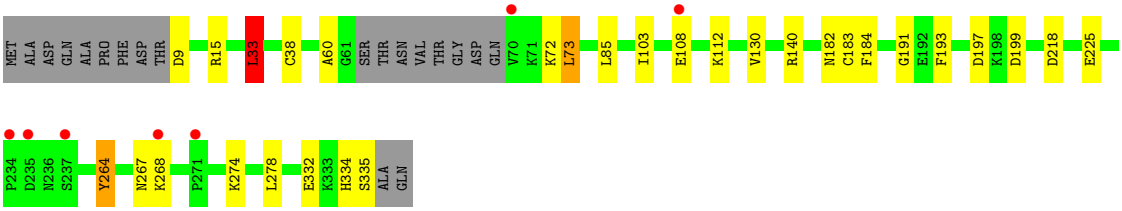
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain D:



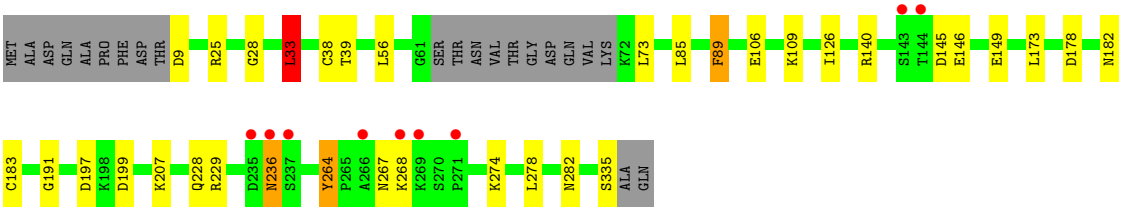
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain E:



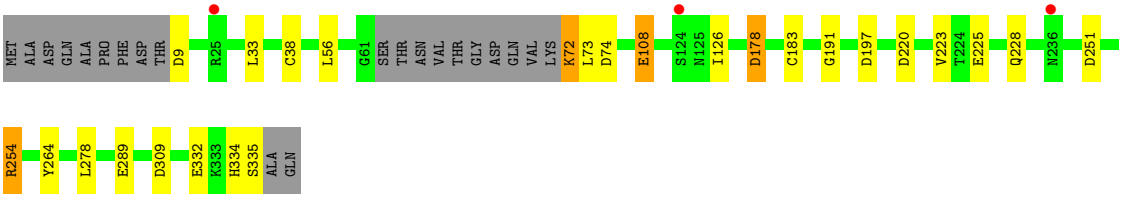
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain F:



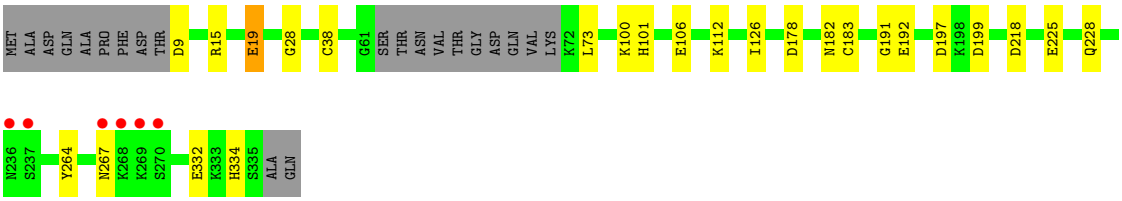
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain G:



• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.97Å 286.31Å 83.69Å 90.00° 97.79° 90.00°	Depositor
Resolution (Å)	29.74 – 2.40 29.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.74-2.40) 96.6 (29.73-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.236 0.210 , 0.239	Depositor DCC
R_{free} test set	5784 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20383	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2C1

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	0.56	0/2497	0.72	3/3371 (0.1%)
1	B	0.54	0/2481	0.73	5/3350 (0.1%)
1	C	0.57	0/2470	0.76	5/3336 (0.1%)
1	D	0.63	2/2490 (0.1%)	0.73	0/3361
1	E	0.54	0/2497	0.73	3/3371 (0.1%)
1	F	0.56	0/2481	0.74	3/3350 (0.1%)
1	G	0.58	0/2481	0.76	5/3350 (0.1%)
1	H	0.57	0/2470	0.72	1/3336 (0.0%)
All	All	0.57	2/19867 (0.0%)	0.74	25/26825 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	149	GLU	CD-OE2	-5.67	1.19	1.25
1	D	19	GLU	CD-OE1	5.41	1.31	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	220	ASP	CB-CG-OD2	-8.02	111.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	ASP	CB-CG-OD1	7.72	125.25	118.30
1	G	178	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	A	103	ILE	CG1-CB-CG2	-7.32	95.29	111.40
1	E	103	ILE	CG1-CB-CG2	-7.30	95.35	111.40
1	C	309	ASP	CB-CG-OD2	7.02	124.62	118.30
1	A	33	LEU	CA-CB-CG	6.47	130.17	115.30
1	E	33	LEU	CA-CB-CG	6.42	130.06	115.30
1	C	254	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	33	LEU	CA-CB-CG	6.35	129.91	115.30
1	H	106	GLU	CA-CB-CG	6.12	126.86	113.40
1	G	178	ASP	CB-CG-OD1	6.06	123.75	118.30
1	G	309	ASP	CB-CG-OD2	6.04	123.73	118.30
1	F	33	LEU	CA-CB-CG	5.95	128.98	115.30
1	C	178	ASP	CB-CG-OD1	5.85	123.56	118.30
1	C	178	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	E	73	LEU	CB-CG-CD1	5.80	120.86	111.00
1	A	73	LEU	CB-CG-CD1	5.67	120.65	111.00
1	G	309	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	C	309	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	F	89	PHE	CB-CG-CD1	5.18	124.43	120.80
1	B	142	LYS	CA-CB-CG	5.15	124.73	113.40
1	F	229	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	G	33	LEU	CB-CG-CD1	5.07	119.62	111.00
1	B	229	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ALA	Peptide
1	E	60	ALA	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	2448	0	2496	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2433	0	2478	14	0
1	C	2427	0	2469	13	0
1	D	2442	0	2491	18	0
1	E	2449	0	2500	15	0
1	F	2432	0	2474	18	1
1	G	2432	0	2474	9	0
1	H	2427	0	2469	13	1
2	A	29	0	20	1	0
2	B	29	0	20	2	0
2	C	29	0	20	2	0
2	D	29	0	20	1	0
2	E	29	0	20	2	0
2	F	29	0	20	2	0
2	G	29	0	20	1	0
2	H	29	0	20	2	0
3	A	78	0	0	5	0
3	B	75	0	0	2	0
3	C	108	0	0	5	0
3	D	110	0	0	9	0
3	E	53	0	0	3	0
3	F	56	0	0	2	0
3	G	97	0	0	2	0
3	H	84	0	0	2	0
All	All	20383	0	20011	114	1

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 3.

All (114) 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:D:38:CYS:HB2	3:D:580:HOH:O	1.60	0.99
1:E:108:GLU:HG3	3:E:526:HOH:O	1.71	0.89
1:A:72:LYS:HG3	3:A:531:HOH:O	1.78	0.82
1:D:140[A]:ARG:NH2	3:D:541:HOH:O	2.06	0.77
1:C:118:ASP:OD1	3:C:549:HOH:O	2.04	0.74
1:H:126:ILE:HG13	3:H:559:HOH:O	1.87	0.74
1:C:118:ASP:OD2	3:C:604:HOH:O	2.09	0.70
1:F:89:PHE:HE1	1:F:109:LYS:HG2	1.56	0.69
1:C:251:ASP:OD1	1:C:254:ARG:NH2	2.26	0.69
1:D:102:ALA:CB	1:D:149:GLU:HG2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ALA:HB3	1:D:149:GLU:HG2	1.73	0.69
1:G:251:ASP:OD1	1:G:254:ARG:NH2	2.26	0.68
1:F:106:GLU:OE2	3:F:529:HOH:O	2.12	0.67
1:A:122:GLY:O	3:A:572:HOH:O	2.15	0.62
1:C:146:GLU:CG	3:C:602:HOH:O	2.46	0.61
1:A:106:GLU:HG2	3:A:558:HOH:O	2.00	0.61
1:G:72:LYS:HG2	1:G:74:ASP:OD1	2.01	0.61
1:B:118:ASP:OD2	3:B:575:HOH:O	2.16	0.61
1:C:146:GLU:HG3	1:C:147:PRO:HD2	1.83	0.60
1:E:191:GLY:HA3	1:G:191:GLY:HA3	1.83	0.60
1:D:118:ASP:OD1	3:D:566:HOH:O	2.17	0.59
1:E:33:LEU:HD13	1:E:85:LEU:HD22	1.85	0.59
1:B:334:HIS:O	1:F:207:LYS:HE3	2.04	0.57
1:A:33:LEU:HD13	1:A:85:LEU:HD22	1.86	0.57
1:C:146:GLU:HG2	3:C:602:HOH:O	2.04	0.57
1:D:126:ILE:HA	3:D:570:HOH:O	2.05	0.56
1:G:220:ASP:OD1	1:G:223:VAL:HG23	2.05	0.56
1:F:264:TYR:CZ	1:F:274:LYS:HD3	2.40	0.56
1:A:191:GLY:HA3	1:C:191:GLY:HA3	1.86	0.56
1:F:33:LEU:HD13	1:F:85:LEU:HD22	1.87	0.56
1:B:33:LEU:HD13	1:B:85:LEU:HD22	1.88	0.55
1:G:108:GLU:HG2	3:G:549:HOH:O	2.06	0.54
1:B:220:ASP:OD1	1:B:221:PRO:HD2	2.08	0.53
1:F:89:PHE:CE1	1:F:109:LYS:HG2	2.41	0.53
1:H:126:ILE:HA	3:H:559:HOH:O	2.09	0.53
1:H:28:GLY:HA2	2:H:401:2C1:C5	2.38	0.53
1:B:218:ASP:OD2	1:B:269:LYS:HD2	2.09	0.52
1:D:126:ILE:HG13	3:D:570:HOH:O	2.08	0.52
1:D:112:LYS:HB2	1:D:140[B]:ARG:CZ	2.40	0.52
1:E:15:ARG:HG3	3:E:553:HOH:O	2.08	0.52
1:H:225:GLU:OE1	1:H:334:HIS:HE1	1.93	0.52
1:A:225:GLU:OE1	1:A:334:HIS:HE1	1.92	0.52
1:D:225:GLU:OE1	1:D:334:HIS:HE1	1.93	0.51
1:C:72:LYS:N	3:C:606:HOH:O	2.42	0.51
1:B:191:GLY:HA3	1:D:191:GLY:HA3	1.93	0.51
1:A:229:ARG:HD2	3:A:576:HOH:O	2.09	0.51
1:E:140[B]:ARG:HH11	1:E:140[B]:ARG:HG3	1.76	0.51
1:C:225:GLU:OE1	1:C:334:HIS:HE1	1.94	0.51
1:E:33:LEU:CD1	1:E:85:LEU:HD22	2.41	0.50
1:G:225:GLU:OE1	1:G:334:HIS:HE1	1.94	0.50
1:A:33:LEU:CD1	1:A:85:LEU:HD22	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:CYS:HB2	1:C:197:ASP:HB2	1.94	0.50
1:E:225:GLU:OE1	1:E:334:HIS:HE1	1.94	0.50
1:F:191:GLY:HA3	1:H:191:GLY:HA3	1.93	0.50
1:E:264:TYR:OH	1:E:274:LYS:HD2	2.11	0.49
1:G:183:CYS:HB2	1:G:197:ASP:HB2	1.95	0.49
1:F:33:LEU:CD1	1:F:85:LEU:HD22	2.42	0.49
1:F:146:GLU:HG3	3:F:548:HOH:O	2.12	0.49
1:A:264:TYR:OH	1:A:274:LYS:HD2	2.13	0.49
1:E:183:CYS:HB2	1:E:197:ASP:HB2	1.95	0.49
1:F:28:GLY:HA3	2:H:401:2C1:H9	1.95	0.48
1:D:130:VAL:O	3:D:570:HOH:O	2.20	0.48
1:B:28:GLY:HA3	2:D:401:2C1:H9	1.96	0.48
1:A:183:CYS:HB2	1:A:197:ASP:HB2	1.96	0.48
1:H:183:CYS:HB2	1:H:197:ASP:HB2	1.96	0.48
1:E:130:VAL:HG11	3:E:543:HOH:O	2.14	0.47
1:B:33:LEU:CD1	1:B:85:LEU:HD22	2.44	0.47
1:A:29:GLU:OE1	1:A:112:LYS:HG2	2.14	0.47
1:C:112:LYS:HB2	1:C:140:ARG:NH1	2.29	0.46
1:F:28:GLY:HA2	2:F:401:2C1:C5	2.44	0.46
1:A:28:GLY:HA3	2:C:401:2C1:H9	1.97	0.46
1:B:28:GLY:HA2	2:B:401:2C1:C5	2.46	0.46
1:A:28:GLY:HA2	2:A:401:2C1:C5	2.46	0.46
1:D:102:ALA:HB2	1:D:149:GLU:HG2	1.98	0.46
2:F:401:2C1:H9	1:H:28:GLY:HA3	1.97	0.46
1:D:13:LEU:HD21	3:D:580:HOH:O	2.16	0.45
1:B:218:ASP:O	1:B:267:ASN:HB2	2.15	0.45
1:D:29:GLU:OE1	1:D:112:LYS:HG2	2.15	0.45
1:F:182:ASN:ND2	1:F:199:ASP:H	2.15	0.45
1:D:183:CYS:HB2	1:D:197:ASP:HB2	1.98	0.45
1:E:218:ASP:O	1:E:267:ASN:HB2	2.17	0.45
1:F:183:CYS:HB2	1:F:197:ASP:HB2	1.98	0.45
1:B:235:ASP:O	1:B:236:ASN:CB	2.65	0.44
1:B:183:CYS:HB2	1:B:197:ASP:HB2	2.00	0.43
2:E:401:2C1:O20	2:E:401:2C1:H4	2.17	0.43
2:G:401:2C1:H11	2:G:401:2C1:H13	1.86	0.43
1:B:15:ARG:HD3	3:D:597:HOH:O	2.19	0.43
1:E:182:ASN:ND2	1:E:199:ASP:H	2.16	0.43
1:E:73:LEU:HA	1:E:73:LEU:HD23	1.79	0.43
1:H:100:LYS:HA	1:H:100:LYS:HD2	1.91	0.43
1:F:267:ASN:OD1	1:F:267:ASN:N	2.52	0.42
1:H:182:ASN:ND2	1:H:199:ASP:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:LEU:HD23	1:E:278:LEU:HA	1.88	0.42
1:A:52:GLY:HA2	3:B:515:HOH:O	2.19	0.42
1:H:218:ASP:O	1:H:267:ASN:HB2	2.20	0.42
1:F:73:LEU:HD23	1:F:126:ILE:HD13	2.02	0.42
1:F:282:ASN:HD22	1:F:282:ASN:HA	1.73	0.42
2:B:401:2C1:H9	1:D:28:GLY:HA3	2.01	0.41
1:D:73:LEU:HD23	1:D:126:ILE:HD13	2.02	0.41
1:A:72:LYS:HG2	3:A:574:HOH:O	2.19	0.41
2:E:401:2C1:H11	2:E:401:2C1:H13	1.95	0.41
1:A:282:ASN:HD22	1:A:282:ASN:HA	1.76	0.41
1:F:89:PHE:CD1	1:F:109:LYS:HA	2.56	0.41
1:G:73:LEU:HD23	1:G:126:ILE:HD13	2.02	0.41
1:G:289:GLU:OE2	3:G:512:HOH:O	2.22	0.41
1:H:73:LEU:HD23	1:H:126:ILE:HD13	2.02	0.41
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.76	0.41
1:C:73:LEU:HD23	1:C:126:ILE:HD13	2.02	0.41
1:H:15:ARG:O	1:H:19:GLU:HB2	2.21	0.41
1:E:184:PHE:HB3	1:E:193:PHE:HB3	2.03	0.40
1:C:28:GLY:HA2	2:C:401:2C1:C5	2.51	0.40
1:D:238:ALA:O	3:D:607:HOH:O	2.21	0.40
1:B:73:LEU:HD23	1:B:126:ILE:HD13	2.02	0.40
1:F:39:THR:HG23	1:H:192:GLU:HG3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:149:GLU:OE1	1:H:100:LYS:CB[1_455]	1.97	0.23

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	316/338 (94%)	312 (99%)	4 (1%)	0	100	100
1	B	314/338 (93%)	308 (98%)	6 (2%)	0	100	100
1	C	313/338 (93%)	309 (99%)	4 (1%)	0	100	100
1	D	315/338 (93%)	308 (98%)	7 (2%)	0	100	100
1	E	316/338 (94%)	311 (98%)	5 (2%)	0	100	100
1	F	314/338 (93%)	307 (98%)	6 (2%)	1 (0%)	41	55
1	G	314/338 (93%)	310 (99%)	4 (1%)	0	100	100
1	H	313/338 (93%)	307 (98%)	6 (2%)	0	100	100
All	All	2515/2704 (93%)	2472 (98%)	42 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	236	ASN

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	267/281 (95%)	254 (95%)	13 (5%)	25	40
1	B	265/281 (94%)	251 (95%)	14 (5%)	22	37
1	C	264/281 (94%)	251 (95%)	13 (5%)	25	40
1	D	266/281 (95%)	260 (98%)	6 (2%)	50	70
1	E	267/281 (95%)	258 (97%)	9 (3%)	37	56
1	F	265/281 (94%)	249 (94%)	16 (6%)	19	31
1	G	265/281 (94%)	253 (96%)	12 (4%)	27	44
1	H	264/281 (94%)	255 (97%)	9 (3%)	37	56
All	All	2123/2248 (94%)	2031 (96%)	92 (4%)	29	46

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	33	LEU
1	A	38	CYS
1	A	56	LEU
1	A	70	VAL
1	A	72	LYS
1	A	112	LYS
1	A	173	LEU
1	A	178	ASP
1	A	264	TYR
1	A	278	LEU
1	A	332	GLU
1	A	335	SER
1	B	9	ASP
1	B	33	LEU
1	B	38	CYS
1	B	56	LEU
1	B	110	ARG
1	B	142	LYS
1	B	173	LEU
1	B	178	ASP
1	B	236	ASN
1	B	264	TYR
1	B	278	LEU
1	B	299	LYS
1	B	329	LYS
1	B	335	SER
1	C	9	ASP
1	C	38	CYS
1	C	56	LEU
1	C	73	LEU
1	C	140	ARG
1	C	173	LEU
1	C	178	ASP
1	C	228	GLN
1	C	254	ARG
1	C	264	TYR
1	C	278	LEU
1	C	332	GLU
1	C	335	SER
1	D	9	ASP
1	D	38	CYS
1	D	112	LYS

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Mol	Chain	Res	Type
1	D	178	ASP
1	D	236	ASN
1	D	264	TYR
1	E	9	ASP
1	E	33	LEU
1	E	38	CYS
1	E	72	LYS
1	E	112	LYS
1	E	264	TYR
1	E	268	LYS
1	E	332	GLU
1	E	335	SER
1	F	9	ASP
1	F	25	ARG
1	F	33	LEU
1	F	38	CYS
1	F	56	LEU
1	F	140[A]	ARG
1	F	140[B]	ARG
1	F	145	ASP
1	F	173	LEU
1	F	178	ASP
1	F	228	GLN
1	F	236	ASN
1	F	264	TYR
1	F	268	LYS
1	F	278	LEU
1	F	335	SER
1	G	9	ASP
1	G	38	CYS
1	G	56	LEU
1	G	72	LYS
1	G	108	GLU
1	G	178	ASP
1	G	228	GLN
1	G	254	ARG
1	G	264	TYR
1	G	278	LEU
1	G	332	GLU
1	G	335	SER
1	H	9	ASP
1	H	19	GLU

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Mol	Chain	Res	Type
1	H	38	CYS
1	H	101	HIS
1	H	112	LYS
1	H	178	ASP
1	H	228	GLN
1	H	264	TYR
1	H	332	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	182	ASN
1	A	282	ASN
1	A	334	HIS
1	B	182	ASN
1	B	282	ASN
1	C	125	ASN
1	C	182	ASN
1	C	282	ASN
1	C	334	HIS
1	D	35	ASN
1	D	182	ASN
1	D	272	ASN
1	D	282	ASN
1	D	334	HIS
1	E	125	ASN
1	E	182	ASN
1	E	282	ASN
1	E	334	HIS
1	F	35	ASN
1	F	125	ASN
1	F	182	ASN
1	F	236	ASN
1	F	282	ASN
1	G	182	ASN
1	G	282	ASN
1	G	334	HIS
1	H	182	ASN
1	H	228	GLN
1	H	282	ASN
1	H	334	HIS

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)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	2C1	D	401	-	28,30,30	2.86	11 (39%)	28,42,42	2.95	9 (32%)
2	2C1	A	401	-	28,30,30	3.28	12 (42%)	28,42,42	3.80	10 (35%)
2	2C1	E	401	-	28,30,30	2.95	10 (35%)	28,42,42	3.54	13 (46%)
2	2C1	C	401	-	28,30,30	2.90	9 (32%)	28,42,42	4.00	10 (35%)
2	2C1	F	401	-	28,30,30	2.94	6 (21%)	28,42,42	3.05	12 (42%)
2	2C1	H	401	-	28,30,30	3.18	8 (28%)	28,42,42	3.10	12 (42%)
2	2C1	G	401	-	28,30,30	3.20	9 (32%)	28,42,42	2.99	11 (39%)
2	2C1	B	401	-	28,30,30	2.92	10 (35%)	28,42,42	3.37	10 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2C1	D	401	-	-	1/18/25/25	0/2/2/2
2	2C1	A	401	-	-	0/18/25/25	0/2/2/2
2	2C1	E	401	-	-	2/18/25/25	0/2/2/2
2	2C1	C	401	-	-	3/18/25/25	0/2/2/2
2	2C1	F	401	-	-	1/18/25/25	0/2/2/2
2	2C1	H	401	-	-	1/18/25/25	0/2/2/2
2	2C1	G	401	-	-	2/18/25/25	0/2/2/2
2	2C1	B	401	-	-	2/18/25/25	0/2/2/2

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	2C1	C2-S1	-12.00	1.57	1.76
2	A	401	2C1	C2-S1	-11.67	1.58	1.76
2	F	401	2C1	C2-S1	-11.10	1.59	1.76
2	E	401	2C1	C2-S1	-10.94	1.59	1.76
2	H	401	2C1	C2-S1	-10.86	1.59	1.76
2	B	401	2C1	C2-S1	-10.48	1.60	1.76
2	C	401	2C1	C2-S1	-10.26	1.60	1.76
2	D	401	2C1	C2-S1	-10.03	1.61	1.76
2	A	401	2C1	S1-N3	-7.05	1.49	1.64
2	G	401	2C1	C10-S4	-6.39	1.62	1.74
2	H	401	2C1	S1-N3	-6.23	1.51	1.64
2	H	401	2C1	C10-S4	-6.14	1.62	1.74
2	F	401	2C1	C10-S4	-6.10	1.62	1.74
2	A	401	2C1	C10-S4	-6.09	1.62	1.74
2	G	401	2C1	S1-N3	-5.87	1.52	1.64
2	C	401	2C1	C10-S4	-5.76	1.63	1.74
2	E	401	2C1	C10-S4	-5.75	1.63	1.74
2	C	401	2C1	S1-N3	-5.72	1.52	1.64
2	D	401	2C1	C10-S4	-5.62	1.63	1.74
2	F	401	2C1	S1-N3	-5.53	1.52	1.64
2	E	401	2C1	S1-N3	-5.50	1.52	1.64
2	B	401	2C1	S1-N3	-5.47	1.52	1.64
2	B	401	2C1	C10-S4	-5.03	1.64	1.74
2	H	401	2C1	C8-C13	-4.73	1.26	1.38
2	D	401	2C1	S1-N3	-4.68	1.54	1.64
2	D	401	2C1	C8-C13	-4.52	1.26	1.38
2	C	401	2C1	C8-C13	-4.37	1.27	1.38
2	G	401	2C1	C8-C13	-4.36	1.27	1.38
2	H	401	2C1	C5-N3	-3.97	1.30	1.39
2	H	401	2C1	C2-S4	-3.94	1.65	1.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	2C1	C8-C13	-3.85	1.28	1.38
2	A	401	2C1	C8-C13	-3.63	1.29	1.38
2	A	401	2C1	O17-S1	-3.42	1.39	1.43
2	B	401	2C1	C8-C13	-3.37	1.29	1.38
2	A	401	2C1	C5-N3	-3.18	1.32	1.39
2	D	401	2C1	C5-N3	-3.17	1.32	1.39
2	B	401	2C1	C5-N3	-3.07	1.32	1.39
2	E	401	2C1	C8-C13	-3.03	1.30	1.38
2	D	401	2C1	BR1-C19	3.02	1.96	1.90
2	G	401	2C1	C5-N3	-2.99	1.32	1.39
2	G	401	2C1	C2-S4	-2.98	1.67	1.72
2	B	401	2C1	C5-N11	-2.97	1.31	1.37
2	C	401	2C1	C5-N3	-2.93	1.32	1.39
2	E	401	2C1	BR1-C19	2.91	1.96	1.90
2	F	401	2C1	C5-N3	-2.85	1.33	1.39
2	A	401	2C1	C6-N11	-2.82	1.34	1.40
2	E	401	2C1	C2-S4	-2.80	1.67	1.72
2	B	401	2C1	C2-S4	-2.80	1.67	1.72
2	B	401	2C1	C23-C10	-2.75	1.49	1.50
2	H	401	2C1	BR1-C19	2.71	1.95	1.90
2	E	401	2C1	C5-N3	-2.69	1.33	1.39
2	E	401	2C1	C5-N11	-2.69	1.31	1.37
2	A	401	2C1	C23-C10	-2.66	1.49	1.50
2	C	401	2C1	BR1-C19	2.62	1.95	1.90
2	B	401	2C1	C6-N11	-2.61	1.34	1.40
2	A	401	2C1	C5-N11	-2.51	1.32	1.37
2	E	401	2C1	C23-C10	2.45	1.52	1.50
2	H	401	2C1	O18-S1	2.44	1.46	1.43
2	B	401	2C1	BR1-C19	2.37	1.95	1.90
2	A	401	2C1	C2-S4	-2.36	1.68	1.72
2	C	401	2C1	O18-S1	2.35	1.46	1.43
2	D	401	2C1	C5-N11	-2.32	1.32	1.37
2	G	401	2C1	C6-N11	-2.27	1.35	1.40
2	D	401	2C1	C23-C10	2.19	1.51	1.50
2	A	401	2C1	BR1-C19	2.18	1.94	1.90
2	A	401	2C1	C7-N12	-2.18	1.35	1.40
2	F	401	2C1	O18-S1	2.13	1.45	1.43
2	G	401	2C1	C14-N12	-2.10	1.33	1.37
2	C	401	2C1	C2-S4	-2.08	1.68	1.72
2	E	401	2C1	C6-N11	-2.08	1.35	1.40
2	C	401	2C1	C15-C19	2.06	1.42	1.38
2	D	401	2C1	C6-N11	-2.04	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	2C1	C15-C19	2.04	1.42	1.38
2	G	401	2C1	BR1-C19	2.03	1.94	1.90
2	D	401	2C1	C2-S4	-2.01	1.68	1.72

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	2C1	O18-S1-O17	-16.59	99.16	119.55
2	A	401	2C1	O18-S1-O17	-15.24	100.81	119.55
2	E	401	2C1	O18-S1-O17	-11.56	105.34	119.55
2	B	401	2C1	O18-S1-O17	-11.47	105.45	119.55
2	D	401	2C1	O18-S1-O17	-11.17	105.82	119.55
2	E	401	2C1	C2-S1-N3	11.11	120.25	107.27
2	H	401	2C1	O18-S1-O17	-10.44	106.71	119.55
2	F	401	2C1	O18-S1-O17	-10.07	107.17	119.55
2	G	401	2C1	O18-S1-O17	-9.60	107.74	119.55
2	B	401	2C1	C2-S1-N3	9.50	118.37	107.27
2	A	401	2C1	C2-S1-N3	7.89	116.49	107.27
2	G	401	2C1	C2-S1-N3	7.86	116.45	107.27
2	F	401	2C1	C2-S1-N3	7.67	116.23	107.27
2	C	401	2C1	C2-S1-N3	7.47	116.00	107.27
2	H	401	2C1	C2-S1-N3	7.46	115.98	107.27
2	C	401	2C1	O18-S1-C2	4.85	115.64	107.66
2	H	401	2C1	C16-C19-C15	-4.52	114.83	121.51
2	F	401	2C1	O18-S1-C2	4.47	115.02	107.66
2	D	401	2C1	C16-C19-C15	-4.47	114.92	121.51
2	B	401	2C1	C16-C19-C15	-4.40	115.02	121.51
2	E	401	2C1	C16-C19-C15	-4.22	115.28	121.51
2	D	401	2C1	O17-S1-C2	4.21	114.59	107.66
2	A	401	2C1	C16-C19-C15	-4.20	115.32	121.51
2	D	401	2C1	BR1-C19-C15	4.10	124.97	119.27
2	C	401	2C1	C16-C19-C15	-3.93	115.71	121.51
2	B	401	2C1	N12-C7-N9	3.85	122.39	113.24
2	D	401	2C1	N12-C7-N9	3.75	122.16	113.24
2	A	401	2C1	O18-S1-C2	3.69	113.74	107.66
2	A	401	2C1	O21-C14-N12	-3.67	117.41	123.62
2	G	401	2C1	C7-N12-C14	-3.65	125.28	130.41
2	F	401	2C1	C16-C19-C15	-3.59	116.21	121.51
2	A	401	2C1	C28-N22-C14	3.59	128.10	121.61
2	G	401	2C1	N12-C7-N9	3.55	121.67	113.24
2	C	401	2C1	C28-N22-C14	3.38	127.72	121.61
2	F	401	2C1	C28-N22-C14	3.36	127.68	121.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	2C1	C28-N22-C14	3.34	127.65	121.61
2	G	401	2C1	C16-C19-C15	-3.33	116.59	121.51
2	D	401	2C1	C2-S1-N3	3.25	111.07	107.27
2	B	401	2C1	O21-C14-N12	-3.25	118.13	123.62
2	E	401	2C1	N12-C7-N9	3.23	120.92	113.24
2	A	401	2C1	N12-C7-N9	3.23	120.92	113.24
2	F	401	2C1	N12-C7-N9	3.20	120.85	113.24
2	H	401	2C1	C28-N22-C14	3.19	127.37	121.61
2	C	401	2C1	BR1-C19-C15	3.05	123.51	119.27
2	G	401	2C1	C28-N22-C14	3.04	127.11	121.61
2	H	401	2C1	N12-C7-N9	2.99	120.34	113.24
2	C	401	2C1	C7-N9-C6	2.97	122.59	117.91
2	C	401	2C1	N12-C7-N9	2.95	120.26	113.24
2	H	401	2C1	BR1-C19-C15	2.92	123.32	119.27
2	E	401	2C1	C7-N9-C6	2.87	122.43	117.91
2	D	401	2C1	C7-N12-C14	-2.86	126.39	130.41
2	H	401	2C1	O21-C14-N12	-2.81	118.86	123.62
2	F	401	2C1	BR1-C19-C16	2.78	123.12	119.27
2	C	401	2C1	C7-N12-C14	-2.73	126.57	130.41
2	E	401	2C1	C28-N22-C14	2.71	126.50	121.61
2	H	401	2C1	C7-N12-C14	-2.68	126.64	130.41
2	A	401	2C1	BR1-C19-C15	2.64	122.93	119.27
2	H	401	2C1	O20-C5-N11	2.62	128.05	123.62
2	F	401	2C1	C7-N9-C6	2.59	121.99	117.91
2	A	401	2C1	C7-N12-C14	-2.59	126.77	130.41
2	G	401	2C1	C7-N9-C6	2.55	121.93	117.91
2	B	401	2C1	BR1-C19-C15	2.46	122.68	119.27
2	H	401	2C1	C7-N9-C6	2.45	121.77	117.91
2	H	401	2C1	N3-C5-N11	-2.44	111.69	114.93
2	B	401	2C1	N3-C5-N11	-2.43	111.71	114.93
2	G	401	2C1	O18-S1-C2	2.40	111.60	107.66
2	D	401	2C1	C7-N9-C6	2.36	121.62	117.91
2	G	401	2C1	BR1-C19-C16	2.32	122.48	119.27
2	E	401	2C1	BR1-C19-C15	2.26	122.41	119.27
2	G	401	2C1	O17-S1-C2	2.25	111.36	107.66
2	F	401	2C1	O21-C14-N12	-2.24	119.84	123.62
2	F	401	2C1	N3-C5-N11	-2.19	112.02	114.93
2	G	401	2C1	O21-C14-N12	-2.19	119.93	123.62
2	E	401	2C1	BR1-C19-C16	2.19	122.30	119.27
2	B	401	2C1	BR1-C19-C16	2.18	122.29	119.27
2	B	401	2C1	O17-S1-C2	2.16	111.21	107.66
2	E	401	2C1	C6-N11-C5	-2.15	127.39	130.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	401	2C1	C7-N12-C14	-2.13	127.42	130.41
2	A	401	2C1	N3-C5-N11	-2.12	112.11	114.93
2	E	401	2C1	C7-N12-C14	-2.11	127.44	130.41
2	E	401	2C1	O17-S1-C2	2.11	111.13	107.66
2	E	401	2C1	C16-C7-N9	-2.09	118.98	123.41
2	H	401	2C1	C16-C7-N9	-2.08	119.00	123.41
2	C	401	2C1	C15-C6-N9	-2.08	119.01	123.41
2	D	401	2C1	C16-C7-N9	-2.05	119.07	123.41
2	F	401	2C1	C16-C7-N9	-2.01	119.15	123.41
2	E	401	2C1	O21-C14-N12	-2.01	120.23	123.62

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	2C1	C10-C23-C27-O26
2	C	401	2C1	C10-C23-C27-O26
2	G	401	2C1	C13-C10-C23-C27
2	H	401	2C1	C10-C23-C27-O26
2	E	401	2C1	C23-C27-O26-C29
2	F	401	2C1	C23-C27-O26-C29
2	D	401	2C1	C5-N3-S1-O17
2	C	401	2C1	C5-N3-S1-O17
2	C	401	2C1	C23-C27-O26-C29
2	E	401	2C1	C13-C10-C23-C27
2	B	401	2C1	C23-C27-O26-C29
2	G	401	2C1	C23-C27-O26-C29

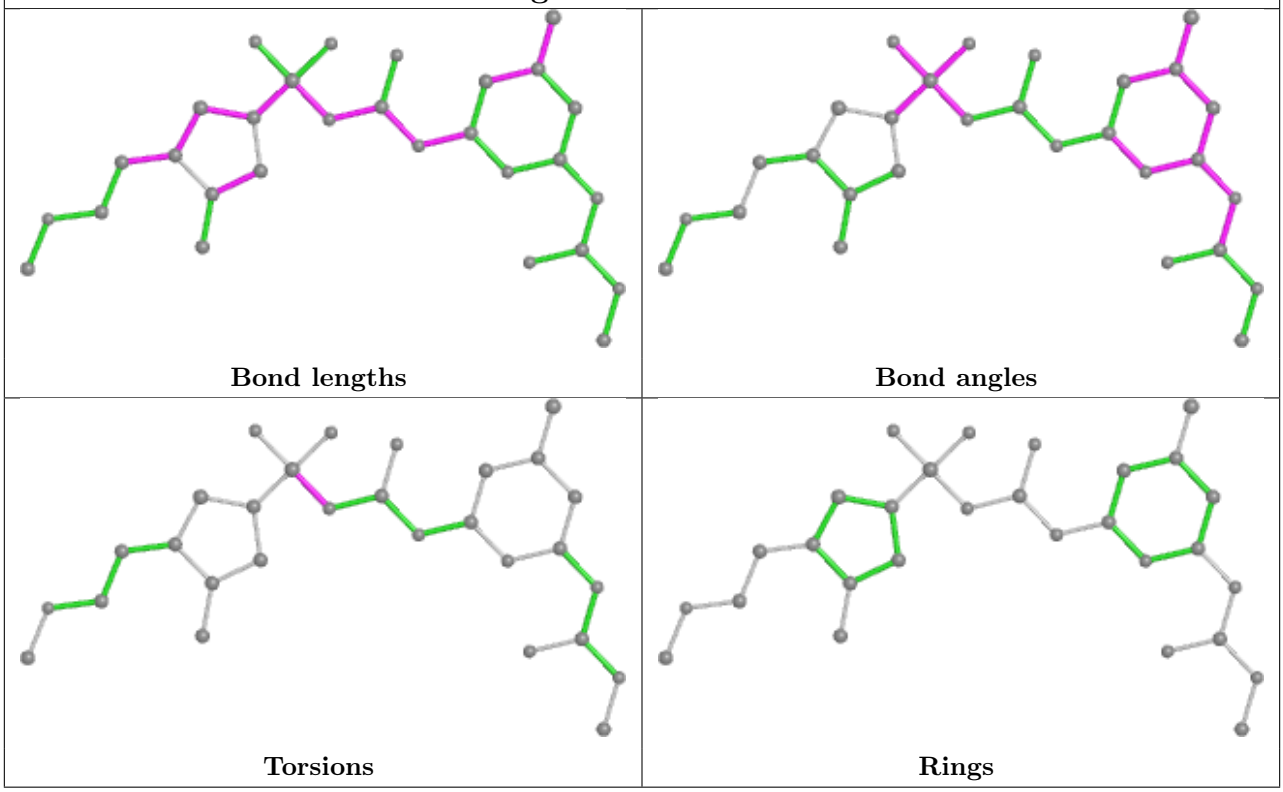
There are no ring outliers.

8 monomers are involved in 13 short contacts:

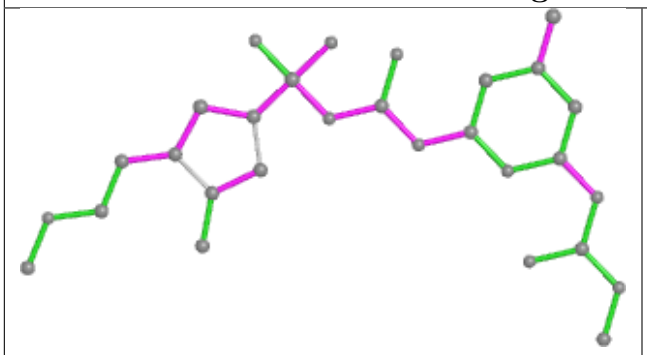
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	2C1	1	0
2	A	401	2C1	1	0
2	E	401	2C1	2	0
2	C	401	2C1	2	0
2	F	401	2C1	2	0
2	H	401	2C1	2	0
2	G	401	2C1	1	0
2	B	401	2C1	2	0

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.

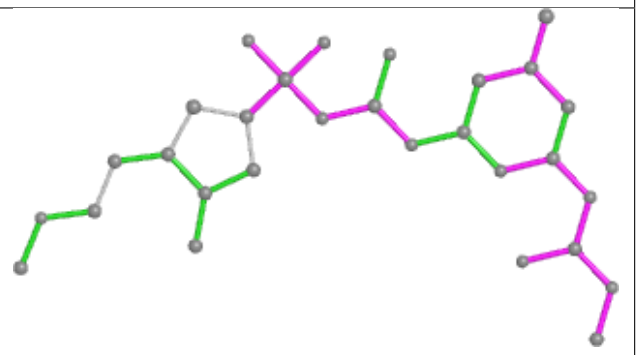
Ligand 2C1 D 401



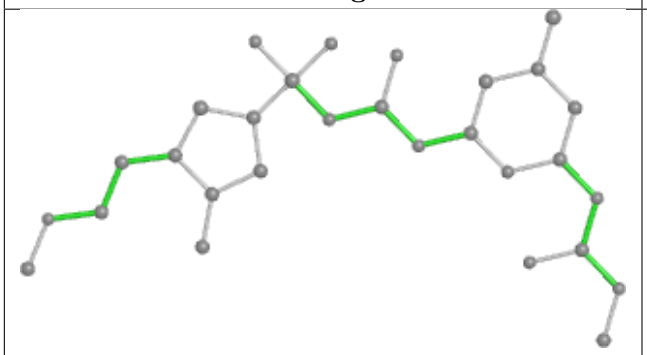
Ligand 2C1 A 401



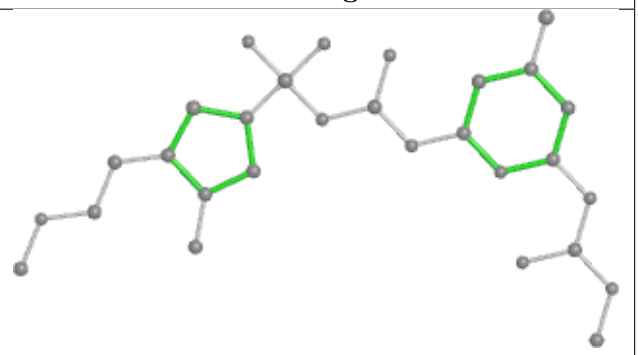
Bond lengths



Bond angles

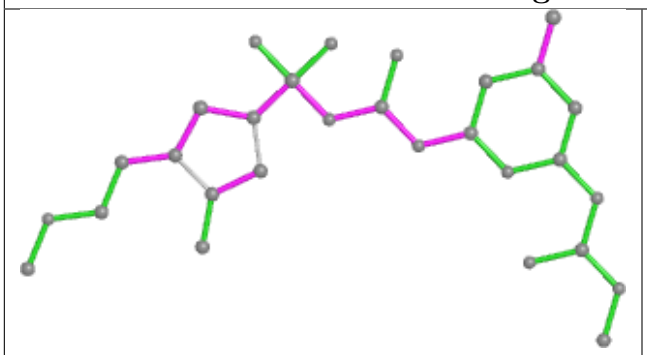


Torsions

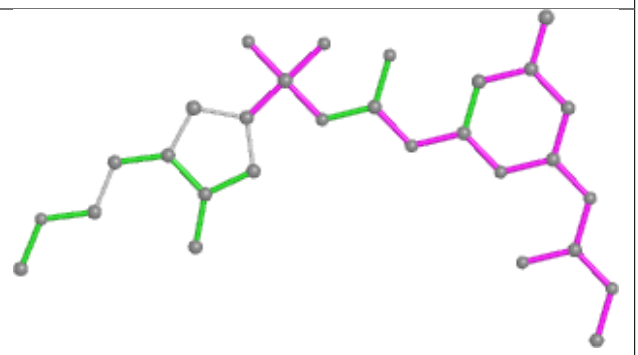


Rings

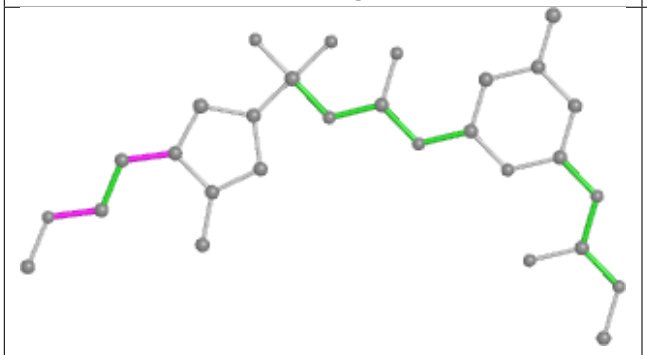
Ligand 2C1 E 401



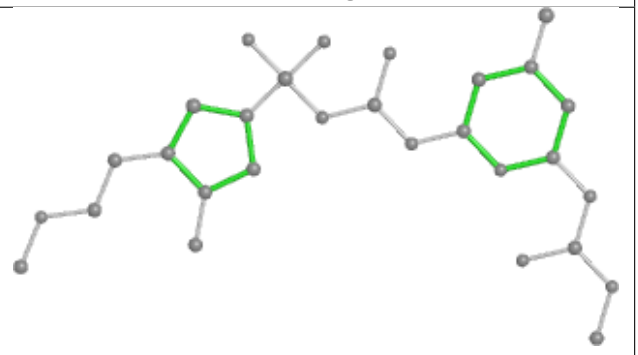
Bond lengths



Bond angles

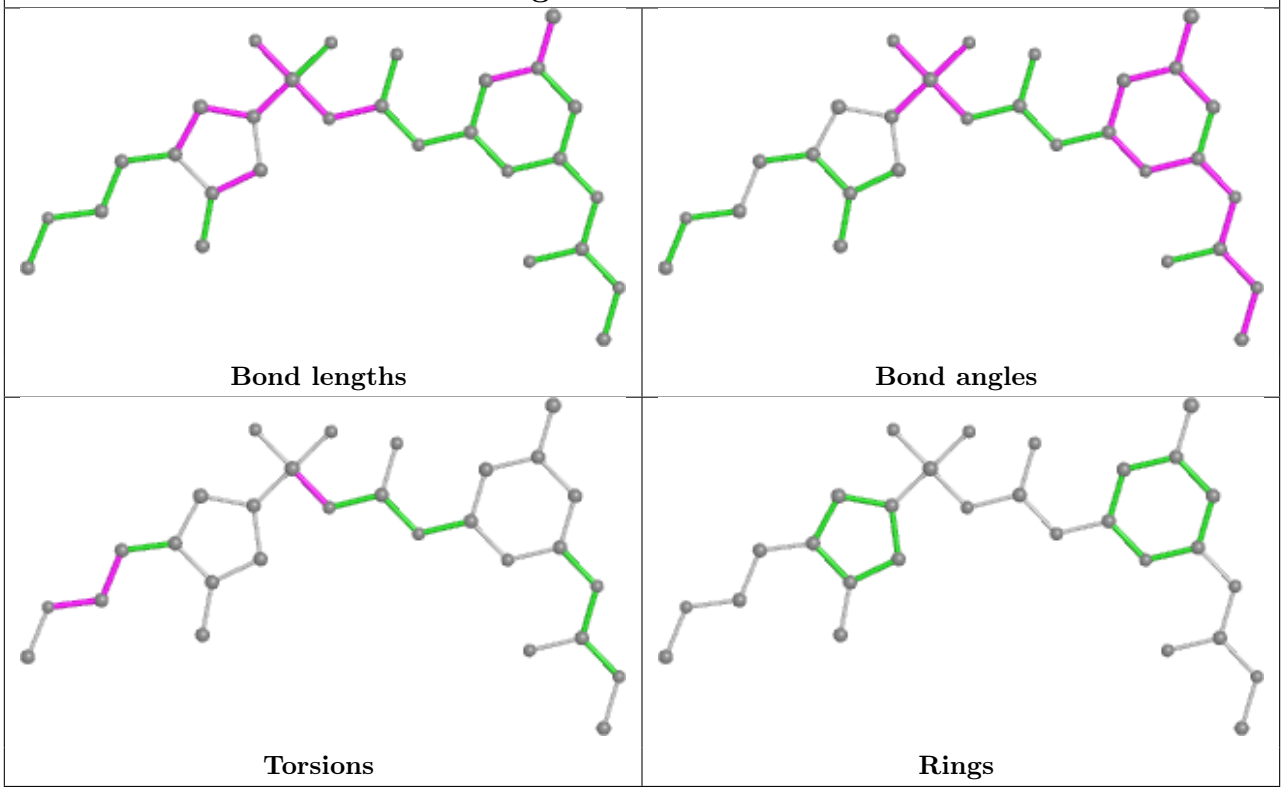


Torsions

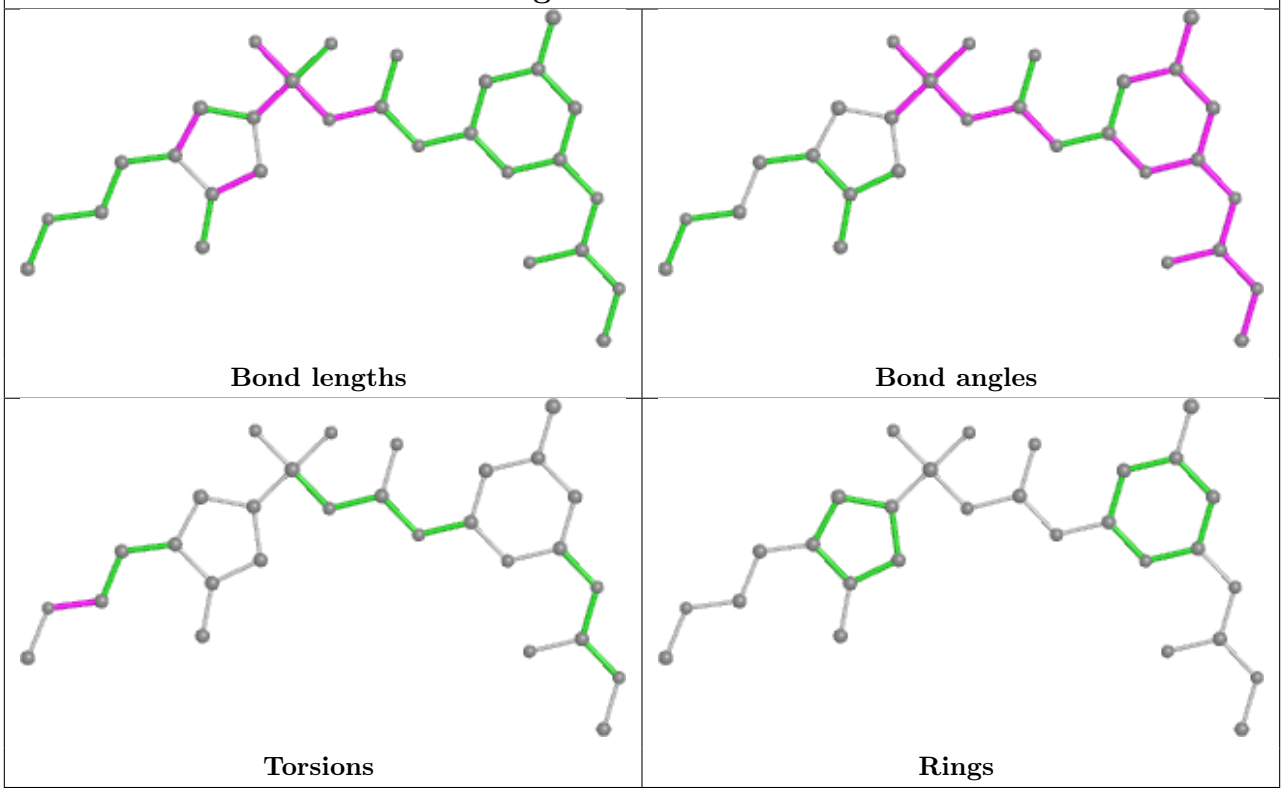


Rings

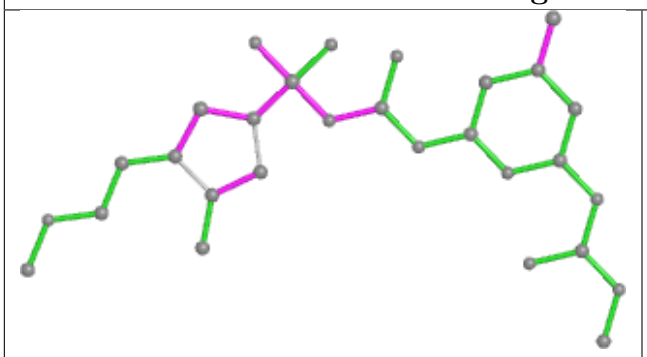
Ligand 2C1 C 401



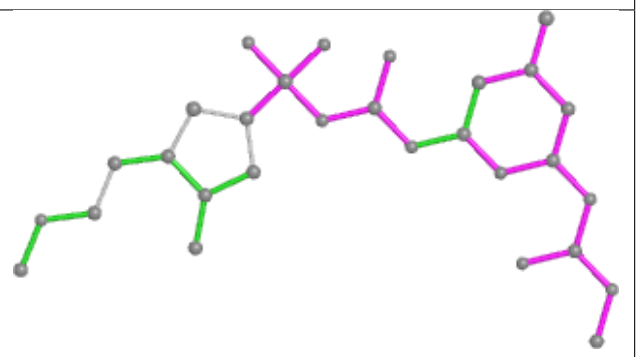
Ligand 2C1 F 401



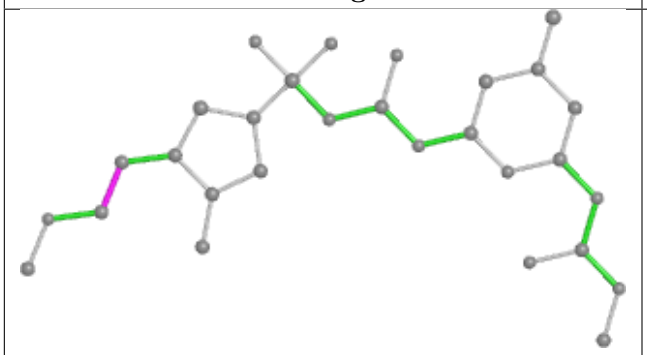
Ligand 2C1 H 401



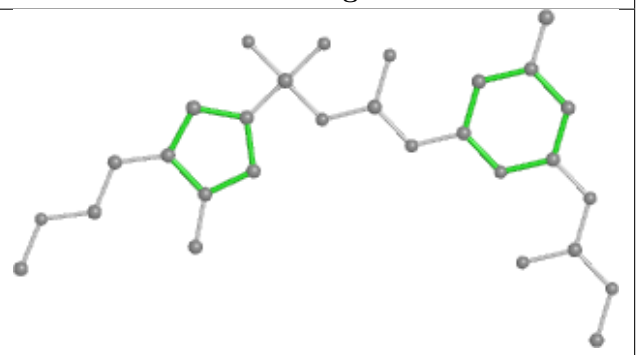
Bond lengths



Bond angles

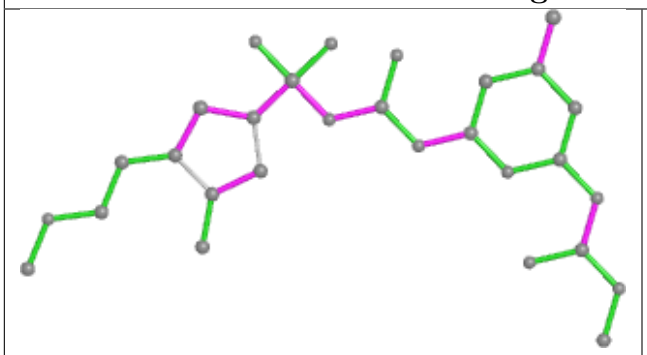


Torsions

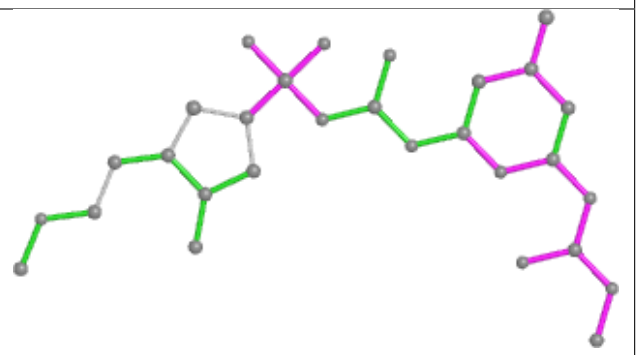


Rings

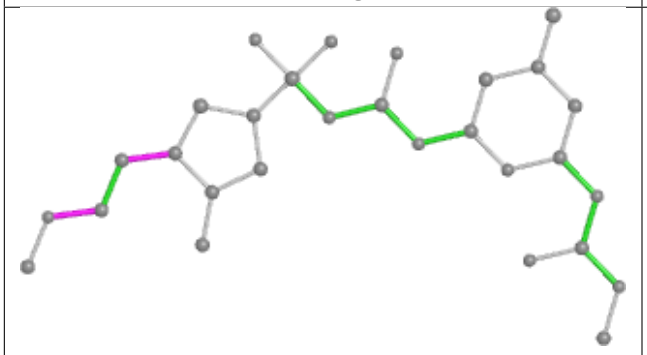
Ligand 2C1 G 401



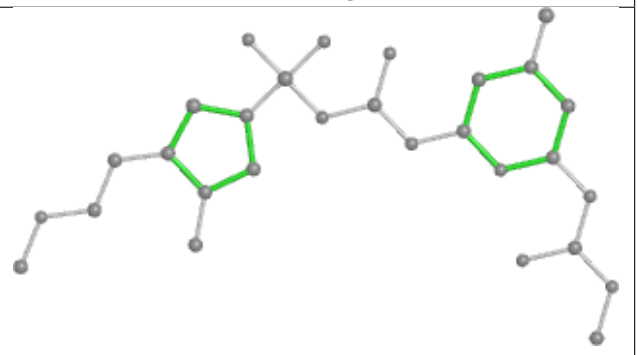
Bond lengths



Bond angles

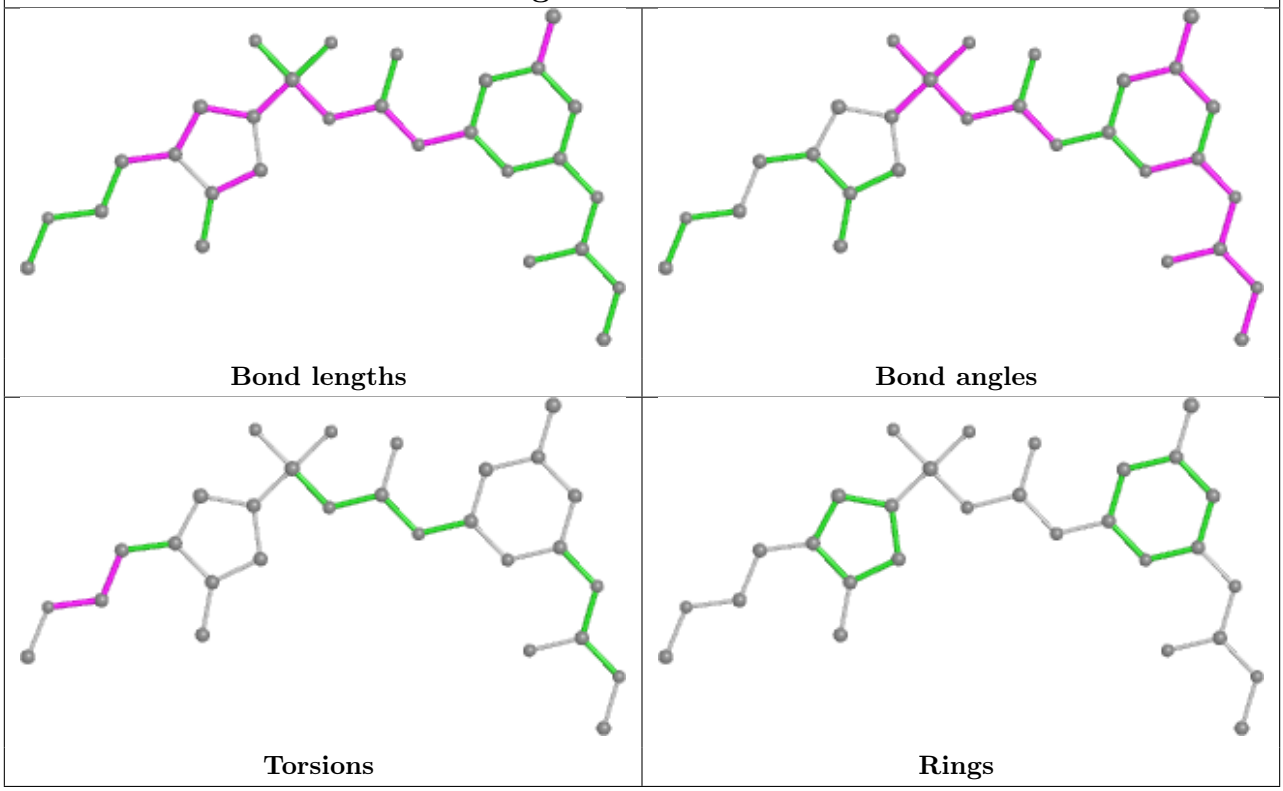


Torsions



Rings

Ligand 2C1 B 401



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	319/338 (94%)	-0.17	6 (1%)	66	64	18, 32, 60, 73	0
1	B	317/338 (93%)	-0.04	7 (2%)	62	60	20, 34, 60, 98	0
1	C	317/338 (93%)	-0.28	2 (0%)	89	88	18, 30, 53, 66	0
1	D	318/338 (94%)	-0.29	3 (0%)	84	82	16, 28, 49, 64	0
1	E	319/338 (94%)	-0.04	7 (2%)	62	60	20, 39, 65, 88	0
1	F	317/338 (93%)	-0.05	9 (2%)	53	51	22, 36, 64, 91	0
1	G	317/338 (93%)	-0.28	3 (0%)	84	82	18, 30, 50, 67	0
1	H	317/338 (93%)	-0.23	6 (1%)	66	64	18, 31, 55, 79	0
All	All	2541/2704 (93%)	-0.17	43 (1%)	70	68	16, 32, 58, 98	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	VAL	4.4
1	B	145	ASP	4.3
1	C	236	ASN	4.3
1	F	268	LYS	3.9
1	E	235	ASP	3.8
1	A	268	LYS	3.8
1	E	70	VAL	3.7
1	B	269	LYS	3.7
1	F	143	SER	3.6
1	H	236	ASN	3.5
1	F	269	LYS	3.4
1	D	236	ASN	3.3
1	E	268	LYS	3.3
1	B	236	ASN	3.2
1	A	144	THR	3.2
1	F	144	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	236	ASN	2.9
1	H	268	LYS	2.9
1	E	237	SER	2.8
1	H	237	SER	2.8
1	D	268	LYS	2.8
1	G	124	SER	2.7
1	F	237	SER	2.7
1	B	144	THR	2.6
1	F	266	ALA	2.6
1	E	234	PRO	2.6
1	B	268	LYS	2.6
1	H	267	ASN	2.6
1	H	270	SER	2.5
1	H	269	LYS	2.4
1	B	234	PRO	2.4
1	G	236	ASN	2.3
1	F	271	PRO	2.3
1	D	237	SER	2.3
1	E	108	GLU	2.2
1	A	146	GLU	2.2
1	F	235	ASP	2.2
1	A	269	LYS	2.1
1	C	126	ILE	2.1
1	A	25	ARG	2.1
1	G	25	ARG	2.1
1	E	271	PRO	2.0
1	B	125	ASN	2.0

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

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,

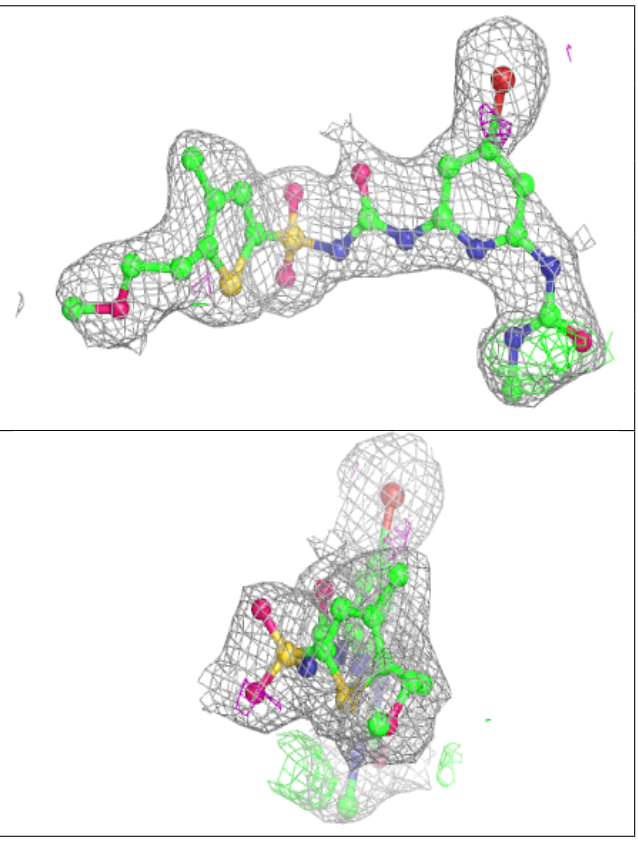
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	2C1	D	401	29/29	0.94	0.12	29,41,68,94	0
2	2C1	B	401	29/29	0.95	0.14	30,42,67,94	0
2	2C1	C	401	29/29	0.95	0.14	27,39,72,118	0
2	2C1	A	401	29/29	0.95	0.12	28,37,71,90	0
2	2C1	F	401	29/29	0.95	0.13	29,42,84,112	0
2	2C1	E	401	29/29	0.97	0.13	30,35,55,91	0
2	2C1	G	401	29/29	0.97	0.10	29,40,71,97	0
2	2C1	H	401	29/29	0.97	0.13	29,37,75,92	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.

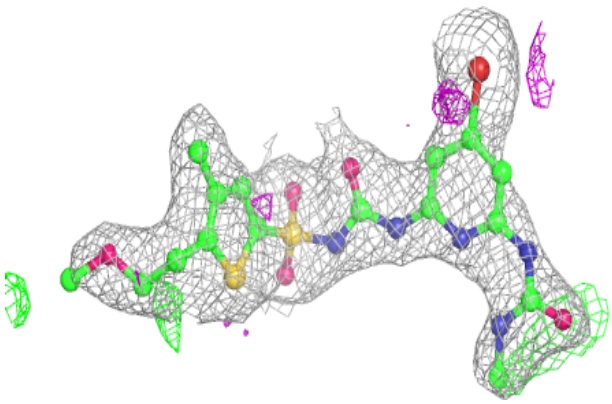
Electron density around 2C1 D 401:

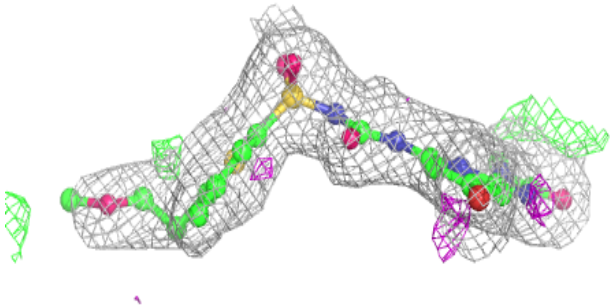
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

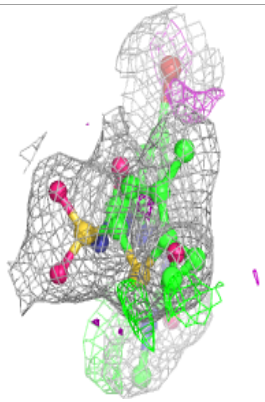


Electron density around 2C1 B 401:

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

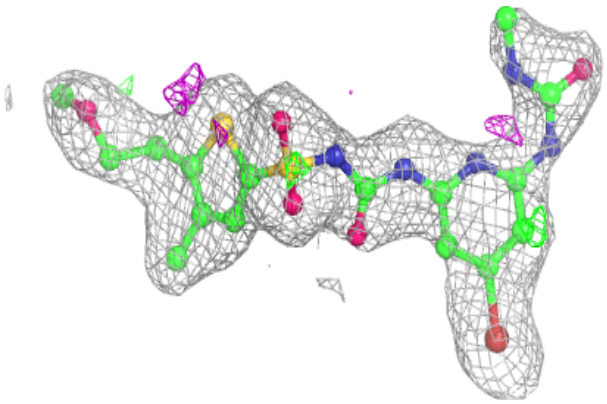


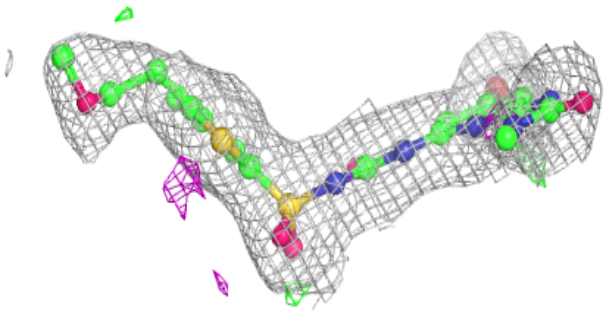


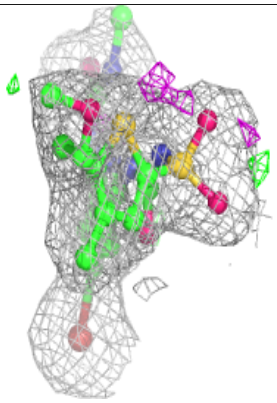


Electron density around 2C1 C 401:

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

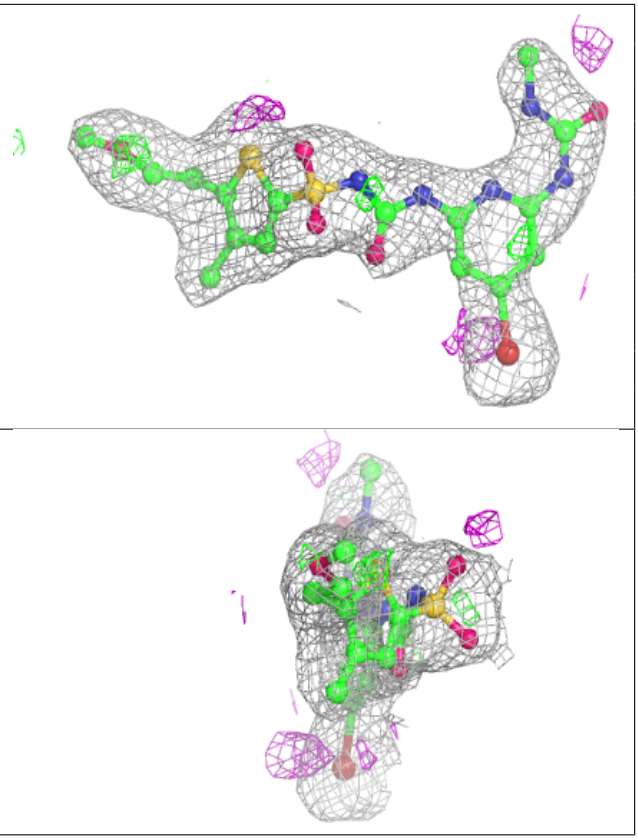






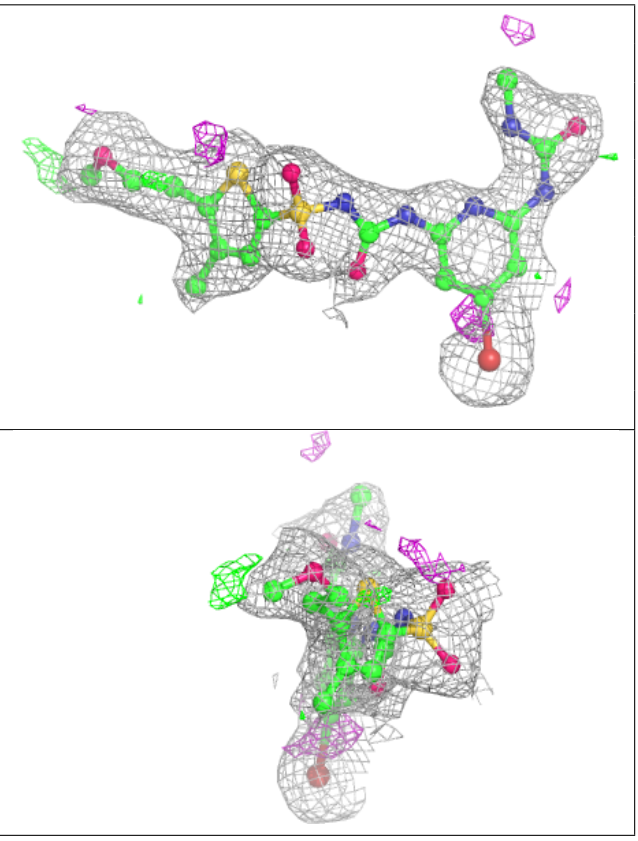
Electron density around 2C1 A 401:

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



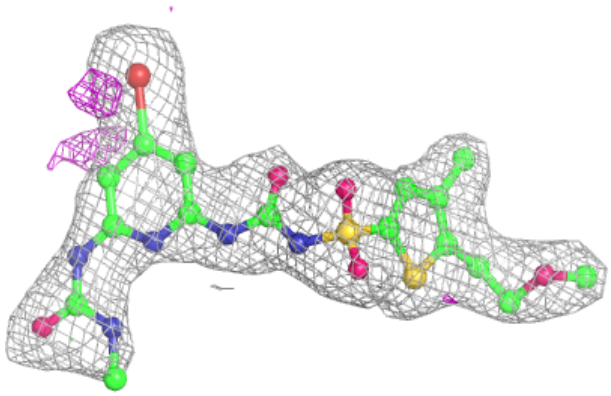
Electron density around 2C1 F 401:

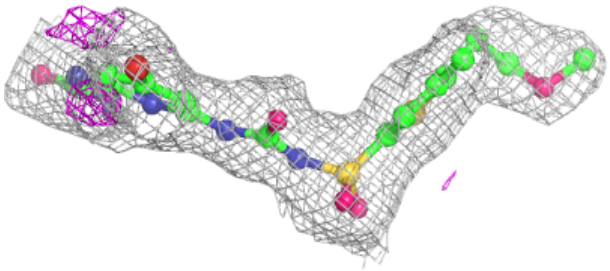
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

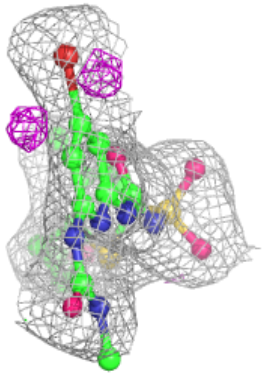


Electron density around 2C1 E 401:

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

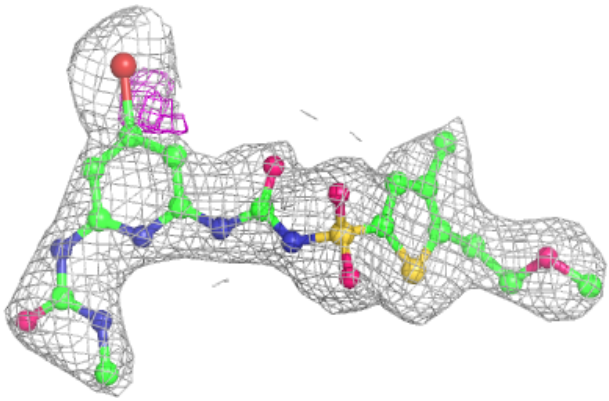


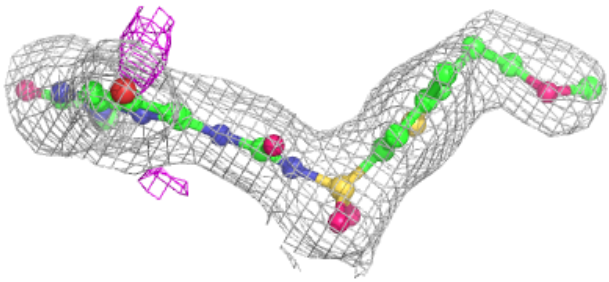


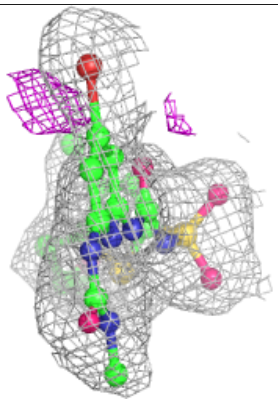


Electron density around 2C1 G 401:

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

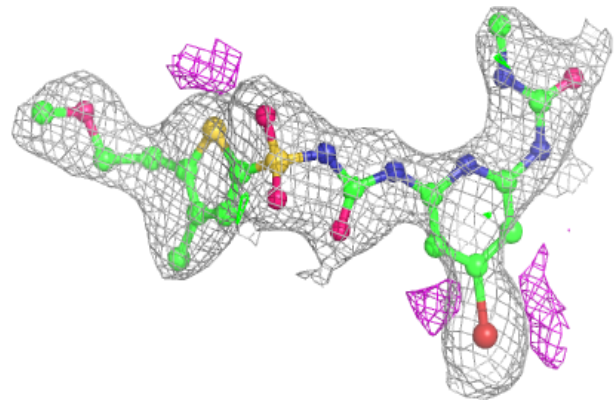


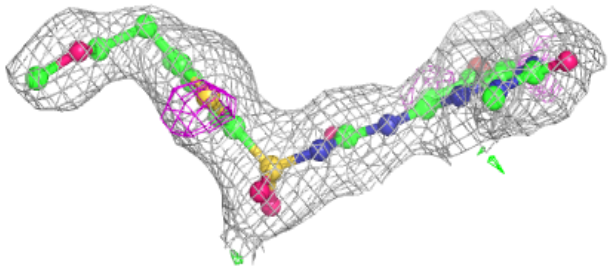


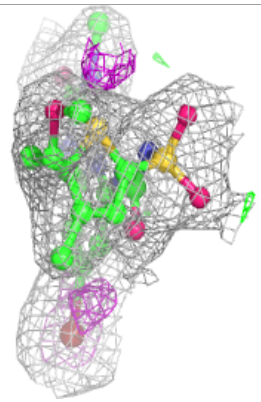


Electron density around 2C1 H 401:

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







6.5 Other polymers (i)

There are no such residues in this entry.