Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 09:52 pm GMT

PDB ID	:	5FAJ
Title	:	Alanine Racemase from Streptomyces coelicolor A3(2) in complex with D-Cycloserine
Authors	:	Tassoni, R.; Pannu, N.S.
Deposited on	:	2015-12-11
Resolution	:	1.64 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:

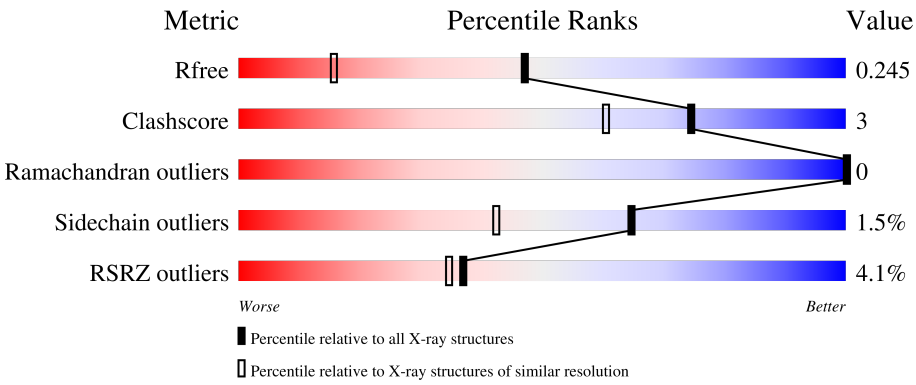
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	410	% 90% • • 6%
1	B	410	87% 5% 7%
1	C	410	5% 87% 6% 7%
1	D	410	9% 87% 6% • 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12321 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 Alanine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	2922	1830	550	530	12	0	7	0
1	B	382	2851	1789	526	523	13	0	3	0
1	C	382	2846	1785	526	523	12	0	1	0
1	D	382	2843	1784	523	523	13	0	2	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP O86786
A	-17	GLY	-	expression tag	UNP O86786
A	-16	SER	-	expression tag	UNP O86786
A	-15	HIS	-	expression tag	UNP O86786
A	-14	HIS	-	expression tag	UNP O86786
A	-13	HIS	-	expression tag	UNP O86786
A	-12	HIS	-	expression tag	UNP O86786
A	-11	HIS	-	expression tag	UNP O86786
A	-10	HIS	-	expression tag	UNP O86786
A	-9	SER	-	expression tag	UNP O86786
A	-8	SER	-	expression tag	UNP O86786
A	-7	GLY	-	expression tag	UNP O86786
A	-6	LEU	-	expression tag	UNP O86786
A	-5	VAL	-	expression tag	UNP O86786
A	-4	PRO	-	expression tag	UNP O86786
A	-3	ARG	-	expression tag	UNP O86786
A	-2	GLY	-	expression tag	UNP O86786
A	-1	SER	-	expression tag	UNP O86786
A	0	HIS	-	expression tag	UNP O86786
B	-18	MET	-	initiating methionine	UNP O86786
B	-17	GLY	-	expression tag	UNP O86786

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP O86786
B	-15	HIS	-	expression tag	UNP O86786
B	-14	HIS	-	expression tag	UNP O86786
B	-13	HIS	-	expression tag	UNP O86786
B	-12	HIS	-	expression tag	UNP O86786
B	-11	HIS	-	expression tag	UNP O86786
B	-10	HIS	-	expression tag	UNP O86786
B	-9	SER	-	expression tag	UNP O86786
B	-8	SER	-	expression tag	UNP O86786
B	-7	GLY	-	expression tag	UNP O86786
B	-6	LEU	-	expression tag	UNP O86786
B	-5	VAL	-	expression tag	UNP O86786
B	-4	PRO	-	expression tag	UNP O86786
B	-3	ARG	-	expression tag	UNP O86786
B	-2	GLY	-	expression tag	UNP O86786
B	-1	SER	-	expression tag	UNP O86786
B	0	HIS	-	expression tag	UNP O86786
C	-18	MET	-	initiating methionine	UNP O86786
C	-17	GLY	-	expression tag	UNP O86786
C	-16	SER	-	expression tag	UNP O86786
C	-15	HIS	-	expression tag	UNP O86786
C	-14	HIS	-	expression tag	UNP O86786
C	-13	HIS	-	expression tag	UNP O86786
C	-12	HIS	-	expression tag	UNP O86786
C	-11	HIS	-	expression tag	UNP O86786
C	-10	HIS	-	expression tag	UNP O86786
C	-9	SER	-	expression tag	UNP O86786
C	-8	SER	-	expression tag	UNP O86786
C	-7	GLY	-	expression tag	UNP O86786
C	-6	LEU	-	expression tag	UNP O86786
C	-5	VAL	-	expression tag	UNP O86786
C	-4	PRO	-	expression tag	UNP O86786
C	-3	ARG	-	expression tag	UNP O86786
C	-2	GLY	-	expression tag	UNP O86786
C	-1	SER	-	expression tag	UNP O86786
C	0	HIS	-	expression tag	UNP O86786
D	-18	MET	-	initiating methionine	UNP O86786
D	-17	GLY	-	expression tag	UNP O86786
D	-16	SER	-	expression tag	UNP O86786
D	-15	HIS	-	expression tag	UNP O86786
D	-14	HIS	-	expression tag	UNP O86786
D	-13	HIS	-	expression tag	UNP O86786

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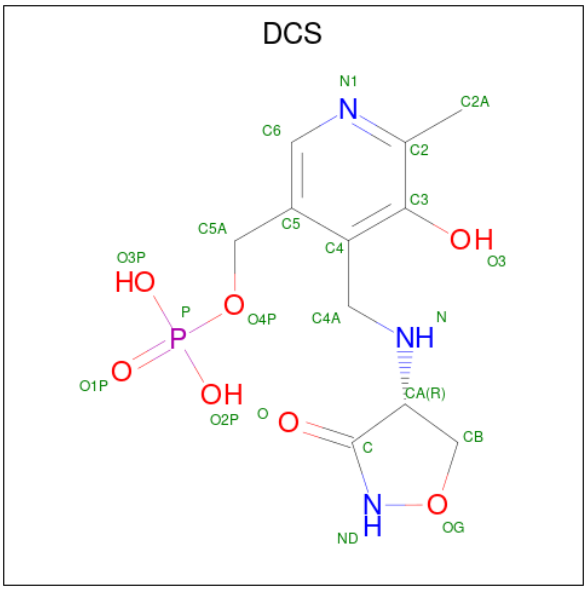
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP O86786
D	-11	HIS	-	expression tag	UNP O86786
D	-10	HIS	-	expression tag	UNP O86786
D	-9	SER	-	expression tag	UNP O86786
D	-8	SER	-	expression tag	UNP O86786
D	-7	GLY	-	expression tag	UNP O86786
D	-6	LEU	-	expression tag	UNP O86786
D	-5	VAL	-	expression tag	UNP O86786
D	-4	PRO	-	expression tag	UNP O86786
D	-3	ARG	-	expression tag	UNP O86786
D	-2	GLY	-	expression tag	UNP O86786
D	-1	SER	-	expression tag	UNP O86786
D	0	HIS	-	expression tag	UNP O86786

- Molecule 2 is D-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL]-N,O-CYCLOSERYLAMIDE (three-letter code: DCS) (formula: $C_{11}H_{16}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
2	C	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
2	D	1	Total	C	N	O	P	0	0
			22	11	3	7	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	3	Total Na 3 3	0	0
3	D	1	Total Na 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	2	Total Cl 2 2	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is water.

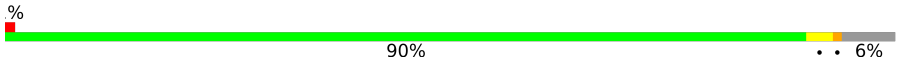
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	221	Total O 221 221	0	0
5	B	231	Total O 231 231	0	0
5	C	165	Total O 165 165	0	0
5	D	143	Total O 143 143	0	0

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.

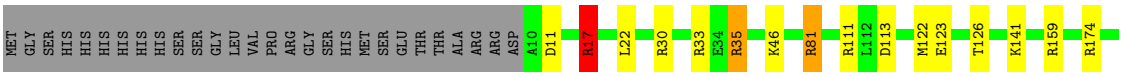
- Molecule 1: Alanine racemase

Chain A:



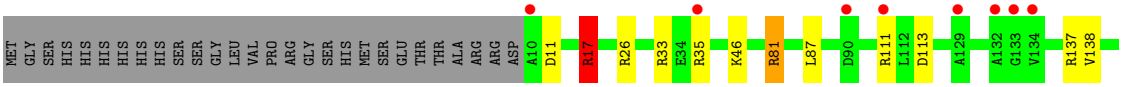
- Molecule 1: Alanine racemase

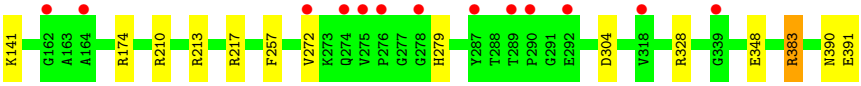
Chain B:



- Molecule 1: Alanine racemase

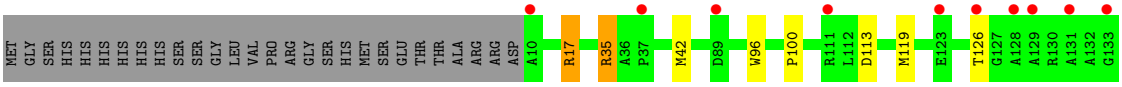
Chain C:

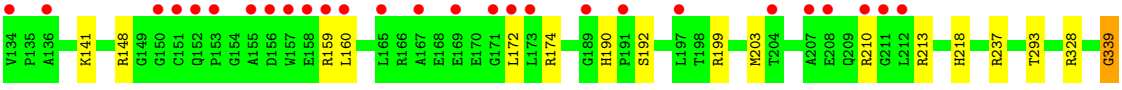




- Molecule 1: Alanine racemase

Chain D:





R357
R383
E391

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.74Å 88.71Å 109.14Å 90.00° 102.25° 90.00°	Depositor
Resolution (Å)	106.60 – 1.64 49.14 – 1.64	Depositor EDS
% Data completeness (in resolution range)	77.3 (106.60-1.64) 77.3 (49.14-1.64)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.208 , 0.241 0.216 , 0.245	Depositor DCC
R_{free} test set	6996 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12321	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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 37.75 % 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 4.0910e-04. 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: CL, KCX, DCS, NA

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	0.93	1/3002 (0.0%)	0.97	10/4091 (0.2%)
1	B	0.94	0/2916	0.99	15/3980 (0.4%)
1	C	0.83	0/2908	0.93	13/3970 (0.3%)
1	D	0.82	0/2905	0.96	9/3966 (0.2%)
All	All	0.88	1/11731 (0.0%)	0.96	47/16007 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ASP	CB-CG	-5.22	1.40	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	383	ARG	NE-CZ-NH2	9.87	125.24	120.30
1	A	148[A]	ARG	NE-CZ-NH1	-9.85	115.37	120.30
1	A	148[B]	ARG	NE-CZ-NH1	-9.85	115.37	120.30
1	D	383	ARG	NE-CZ-NH1	-8.52	116.04	120.30
1	B	328	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	D	328	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	D	35[A]	ARG	CG-CD-NE	-7.99	95.02	111.80
1	D	35[B]	ARG	CG-CD-NE	-7.99	95.02	111.80
1	C	328	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	D	357	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	A	111	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	217[A]	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	217[B]	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	B	210	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	B	35	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	B	111	ARG	NE-CZ-NH2	6.88	123.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	B	159[A]	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	159[B]	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	17	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	11	ASP	CB-CG-OD1	6.39	124.05	118.30
1	D	339	GLY	N-CA-C	-6.13	97.78	113.10
1	B	81	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	33	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	C	111	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	137	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	17	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	D	210	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	33	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	D	17	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	C	81	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	17	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	C	210	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	33	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	87	LEU	N-CA-C	-5.44	96.31	111.00
1	A	81	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	33	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	217	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	33	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	217	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	17	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	C	33	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	111	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	30[A]	ARG	CA-C-O	5.11	130.84	120.10
1	B	30[B]	ARG	CA-C-O	5.11	130.84	120.10
1	C	137	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	357	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2922	0	2916	17	1
1	B	2851	0	2824	10	1
1	C	2846	0	2816	12	0
1	D	2843	0	2811	28	0
2	A	22	0	13	4	0
2	B	22	0	13	2	0
2	C	22	0	14	4	0
2	D	22	0	14	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	221	0	0	5	0
5	B	231	0	0	3	0
5	C	165	0	0	6	0
5	D	143	0	0	10	0
All	All	12321	0	11421	73	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 (73) 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:199:ARG:HG2	5:D:543:HOH:O	1.22	1.30
1:A:148[B]:ARG:HH21	1:A:148[B]:ARG:CG	1.60	1.12
1:D:203:MET:SD	5:D:543:HOH:O	2.08	1.11
1:D:199:ARG:CG	5:D:543:HOH:O	1.79	1.08
1:A:148[B]:ARG:HH21	1:A:148[B]:ARG:HG2	0.90	1.05
1:D:218:HIS:HE1	5:D:583:HOH:O	1.48	0.96
1:A:148[B]:ARG:HG2	1:A:148[B]:ARG:NH2	1.73	0.95
1:A:141:KCX:OQ2	1:A:148[B]:ARG:NH2	2.01	0.94
1:A:217[A]:ARG:NH2	5:A:503:HOH:O	2.02	0.91
1:A:166[C]:ARG:NH2	5:A:501:HOH:O	1.71	0.89
1:D:218:HIS:CE1	5:D:583:HOH:O	2.24	0.88
1:B:174:ARG:HH22	1:B:213:ARG:HB2	1.38	0.85
1:C:17:ARG:NH2	1:C:348:GLU:OE2	2.08	0.85
1:B:174:ARG:NH2	1:B:213:ARG:HB2	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ARG:NH2	1:B:348:GLU:OE2	2.09	0.83
1:B:11:ASP:HA	5:B:579:HOH:O	1.88	0.74
1:D:293:THR:OG1	1:D:339:GLY:O	2.05	0.72
1:C:35[A]:ARG:NH1	5:C:502:HOH:O	2.22	0.72
1:A:148[B]:ARG:NH1	5:A:502:HOH:O	1.95	0.66
2:B:401:DCS:OG	5:B:502:HOH:O	2.12	0.66
1:C:272:VAL:O	5:C:501:HOH:O	2.13	0.66
1:D:119:MET:HE3	1:D:159:ARG:HG2	1.76	0.66
2:D:401:DCS:ND	5:D:501:HOH:O	2.29	0.63
2:A:401:DCS:H4A2	2:A:401:DCS:O4P	1.97	0.62
1:D:119:MET:HE1	1:D:159:ARG:HG3	1.82	0.61
1:D:199:ARG:HG3	5:D:543:HOH:O	1.70	0.61
1:D:119:MET:HE3	1:D:159:ARG:CG	2.32	0.60
1:D:190:HIS:HD2	1:D:192:SER:OG	1.85	0.59
1:A:148[B]:ARG:CG	1:A:148[B]:ARG:NH2	2.36	0.59
1:D:35[B]:ARG:HH21	1:D:35[B]:ARG:HB3	1.68	0.59
1:D:119:MET:CE	1:D:159:ARG:HG3	2.34	0.58
1:D:35[B]:ARG:HB3	1:D:35[B]:ARG:NH2	2.18	0.57
1:D:148:ARG:HD3	5:D:524:HOH:O	2.03	0.57
1:C:304:ASP:OD1	1:C:383:ARG:HD2	2.05	0.57
1:D:203:MET:HG3	5:D:543:HOH:O	2.04	0.56
1:C:46:LYS:HZ1	2:C:401:DCS:HA	1.71	0.56
1:D:174:ARG:HH22	1:D:213:ARG:HB2	1.71	0.55
1:C:35[A]:ARG:NH1	1:C:257:PHE:O	2.39	0.54
1:C:174:ARG:HH22	1:C:213:ARG:HB2	1.72	0.54
2:C:401:DCS:O4P	2:C:401:DCS:C4A	2.55	0.54
1:D:119:MET:HE2	1:D:160:LEU:HA	1.88	0.54
1:A:46:LYS:HZ3	2:A:401:DCS:HA	1.73	0.54
1:D:42[B]:MET:CE	1:D:237:ARG:HD2	2.39	0.52
1:D:119:MET:CE	1:D:159:ARG:CG	2.87	0.52
1:D:126:THR:HG23	1:D:172:LEU:HD13	1.92	0.52
1:D:126:THR:CG2	1:D:172:LEU:HD13	2.39	0.51
2:C:401:DCS:O4P	2:C:401:DCS:H4A1	2.11	0.51
1:A:148[B]:ARG:HH21	1:A:148[B]:ARG:CB	2.24	0.48
1:D:203:MET:CG	5:D:543:HOH:O	2.46	0.48
1:B:46:LYS:HZ3	2:B:401:DCS:H4A1	1.80	0.47
1:B:174:ARG:HH22	1:B:213:ARG:CB	2.20	0.47
1:A:217[A]:ARG:HG3	1:A:217[A]:ARG:HH21	1.82	0.45
1:A:328[B]:ARG:NH1	5:A:510:HOH:O	2.50	0.45
2:D:401:DCS:H4A2	2:D:401:DCS:O4P	2.16	0.45
1:C:174:ARG:NH1	5:C:511:HOH:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LYS:NZ	2:C:401:DCS:HA	2.31	0.44
1:A:46:LYS:NZ	2:A:401:DCS:HA	2.32	0.44
1:B:174:ARG:NH2	5:B:511:HOH:O	2.50	0.44
1:C:279:HIS:CE1	5:C:505:HOH:O	2.71	0.44
1:D:42[B]:MET:HE3	1:D:237:ARG:HD2	1.99	0.43
1:C:390:ASN:HA	5:C:631:HOH:O	2.19	0.43
1:D:119:MET:CE	1:D:160:LEU:HA	2.49	0.43
1:C:26:ARG:NH1	5:C:516:HOH:O	2.52	0.43
1:B:280:GLY:HA3	1:B:285:HIS:CD2	2.54	0.42
1:D:119:MET:HE1	1:D:159:ARG:O	2.19	0.42
1:A:17:ARG:HD2	5:A:684:HOH:O	2.19	0.42
1:A:46:LYS:CE	2:A:401:DCS:H4A1	2.50	0.42
1:A:148[B]:ARG:NH2	1:A:148[B]:ARG:CB	2.83	0.42
1:D:42[B]:MET:CE	1:D:237:ARG:CD	2.97	0.41
1:A:217[A]:ARG:HH21	1:A:217[A]:ARG:CG	2.34	0.41
1:B:22:LEU:CD1	1:B:391:GLU:HG3	2.51	0.41
1:B:122:MET:O	1:B:126:THR:HG23	2.21	0.40
1:D:96:TRP:CE2	2:D:401:DCS:H2A3	2.56	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:A:166[B]:ARG:NE	1:B:123:GLU:OE1[1_455]	2.14	0.06

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	390/410 (95%)	376 (96%)	14 (4%)	0	100	100
1	B	382/410 (93%)	371 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	381/410 (93%)	368 (97%)	13 (3%)	0	100	100
1	D	381/410 (93%)	370 (97%)	11 (3%)	0	100	100
All	All	1534/1640 (94%)	1485 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	284/297 (96%)	281 (99%)	3 (1%)	73	55
1	B	276/297 (93%)	272 (99%)	4 (1%)	67	45
1	C	275/297 (93%)	269 (98%)	6 (2%)	52	25
1	D	275/297 (93%)	272 (99%)	3 (1%)	73	55
All	All	1110/1188 (93%)	1094 (99%)	16 (1%)	65	45

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	35	ARG
1	A	250	GLU
1	B	17	ARG
1	B	35	ARG
1	B	81	ARG
1	B	113	ASP
1	C	17	ARG
1	C	81	ARG
1	C	113	ASP
1	C	138	VAL
1	C	383	ARG
1	C	391	GLU
1	D	17	ARG

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Mol	Chain	Res	Type
1	D	100	PRO
1	D	113	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	HIS
1	A	333	GLN
1	B	333	GLN
1	D	190	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)

4 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	KCX	A	141	1	9,11,12	0.81	0	5,12,14	0.96	0
1	KCX	B	141	1	9,11,12	1.92	1 (11%)	5,12,14	1.63	1 (20%)
1	KCX	D	141	1	9,11,12	2.55	2 (22%)	5,12,14	2.63	1 (20%)
1	KCX	C	141	1	9,11,12	2.06	2 (22%)	5,12,14	1.53	1 (20%)

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	KCX	A	141	1	-	1/9/10/12	-
1	KCX	B	141	1	-	1/9/10/12	-
1	KCX	D	141	1	-	1/9/10/12	-
1	KCX	C	141	1	-	1/9/10/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	141	KCX	OQ1-CX	6.27	1.33	1.21
1	B	141	KCX	OQ1-CX	5.35	1.31	1.21
1	C	141	KCX	OQ1-CX	5.24	1.31	1.21
1	D	141	KCX	CX-NZ	-3.29	1.29	1.35
1	C	141	KCX	CB-CA	2.11	1.56	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	141	KCX	CE-NZ-CX	5.22	130.26	121.89
1	B	141	KCX	OQ1-CX-NZ	-3.38	119.72	124.96
1	C	141	KCX	OQ1-CX-NZ	-3.24	119.94	124.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	141	KCX	CG-CD-CE-NZ
1	A	141	KCX	CG-CD-CE-NZ
1	C	141	KCX	CG-CD-CE-NZ
1	B	141	KCX	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	141	KCX	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

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	DCS	A	401	-	22,23,23	3.04	8 (36%)	25,33,33	2.70	10 (40%)
2	DCS	D	401	-	22,23,23	3.06	4 (18%)	25,33,33	3.39	11 (44%)
2	DCS	B	401	-	22,23,23	2.82	7 (31%)	25,33,33	2.65	14 (56%)
2	DCS	C	401	-	22,23,23	2.87	8 (36%)	25,33,33	2.58	15 (60%)

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	DCS	A	401	-	-	4/10/21/21	0/2/2/2
2	DCS	D	401	-	-	4/10/21/21	0/2/2/2
2	DCS	B	401	-	-	2/10/21/21	0/2/2/2
2	DCS	C	401	-	-	5/10/21/21	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	DCS	C3-C2	8.75	1.49	1.40
2	C	401	DCS	C3-C2	7.37	1.48	1.40
2	A	401	DCS	C5-C4	7.30	1.50	1.40
2	A	401	DCS	C3-C2	7.07	1.48	1.40
2	D	401	DCS	C3-C4	6.55	1.50	1.40
2	C	401	DCS	C3-C4	6.33	1.49	1.40
2	D	401	DCS	C5-C4	6.29	1.49	1.40
2	B	401	DCS	C5-C4	6.27	1.49	1.40
2	A	401	DCS	C3-C4	6.03	1.49	1.40
2	A	401	DCS	CA-C	-5.94	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	DCS	C3-C2	5.93	1.46	1.40
2	D	401	DCS	CA-C	-5.66	1.48	1.52
2	C	401	DCS	C5-C4	5.10	1.47	1.40
2	B	401	DCS	C3-C4	5.10	1.47	1.40
2	C	401	DCS	CA-C	-4.92	1.48	1.52
2	B	401	DCS	P-O2P	-4.71	1.36	1.54
2	C	401	DCS	C-ND	-3.61	1.30	1.34
2	B	401	DCS	P-O1P	3.30	1.61	1.50
2	B	401	DCS	C2-N1	3.29	1.40	1.33
2	B	401	DCS	C-ND	-3.03	1.30	1.34
2	C	401	DCS	P-O3P	-2.71	1.44	1.54
2	A	401	DCS	CA-N	-2.24	1.41	1.46
2	A	401	DCS	P-O1P	-2.17	1.43	1.50
2	A	401	DCS	C-ND	-2.13	1.31	1.34
2	C	401	DCS	CA-N	-2.12	1.41	1.46
2	A	401	DCS	C4A-N	-2.04	1.40	1.46
2	C	401	DCS	C4A-N	-2.00	1.40	1.46

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	DCS	O-C-CA	-11.39	117.94	126.18
2	D	401	DCS	C4A-C4-C3	6.19	126.67	120.04
2	A	401	DCS	O-C-CA	-6.14	121.74	126.18
2	B	401	DCS	C4-C4A-N	5.14	125.93	111.78
2	A	401	DCS	O-C-ND	5.00	132.15	125.73
2	A	401	DCS	C4A-C4-C3	5.00	125.40	120.04
2	D	401	DCS	O-C-ND	4.84	131.94	125.73
2	C	401	DCS	O-C-ND	4.52	131.53	125.73
2	B	401	DCS	C2A-C2-C3	-4.47	115.37	120.89
2	A	401	DCS	CB-OG-ND	4.33	112.32	105.72
2	C	401	DCS	CB-OG-ND	4.15	112.06	105.72
2	D	401	DCS	O2P-P-O4P	-4.15	95.68	106.73
2	C	401	DCS	O2P-P-O4P	-3.95	96.21	106.73
2	B	401	DCS	O3P-P-O2P	3.95	122.73	107.64
2	C	401	DCS	C4A-N-CA	3.92	121.35	113.92
2	B	401	DCS	O4P-P-O1P	-3.91	95.49	106.47
2	A	401	DCS	O3P-P-O1P	3.87	125.85	110.68
2	D	401	DCS	C4A-C4-C5	-3.85	115.42	119.71
2	B	401	DCS	C2A-C2-N1	3.75	125.00	117.67
2	B	401	DCS	C6-N1-C2	3.73	126.07	119.17
2	C	401	DCS	C2A-C2-C3	-3.53	116.53	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	DCS	C4-C3-C2	-3.27	115.06	120.06
2	B	401	DCS	O3P-P-O4P	-3.24	98.12	106.73
2	A	401	DCS	C4-C3-C2	-3.21	115.14	120.06
2	D	401	DCS	CB-OG-ND	3.15	110.52	105.72
2	B	401	DCS	C4-C3-C2	-3.13	115.26	120.06
2	C	401	DCS	C6-C5-C4	3.01	120.25	118.12
2	B	401	DCS	CB-OG-ND	2.93	110.19	105.72
2	A	401	DCS	C4A-C4-C5	-2.91	116.48	119.71
2	C	401	DCS	C4A-C4-C3	2.87	123.11	120.04
2	C	401	DCS	O3P-P-O2P	2.86	118.58	107.64
2	B	401	DCS	O-C-CA	2.84	128.23	126.18
2	A	401	DCS	C6-N1-C2	2.80	124.36	119.17
2	C	401	DCS	O-C-CA	-2.76	124.18	126.18
2	D	401	DCS	C6-N1-C2	2.71	124.19	119.17
2	D	401	DCS	C4-C3-C2	-2.61	116.05	120.06
2	B	401	DCS	C4A-N-CA	-2.59	109.00	113.92
2	A	401	DCS	O3P-P-O4P	-2.54	99.97	106.73
2	D	401	DCS	C4A-N-CA	2.52	118.69	113.92
2	C	401	DCS	O4P-P-O1P	-2.51	99.44	106.47
2	D	401	DCS	O4P-C5A-C5	2.44	114.01	109.35
2	D	401	DCS	O3P-P-O2P	2.44	116.95	107.64
2	C	401	DCS	C6-N1-C2	2.40	123.62	119.17
2	C	401	DCS	O3-C3-C2	2.38	122.67	117.49
2	C	401	DCS	O3P-P-O1P	2.37	119.95	110.68
2	B	401	DCS	C5-C6-N1	-2.33	119.93	123.82
2	A	401	DCS	O3-C3-C4	2.26	124.76	118.13
2	B	401	DCS	O3-C3-C2	2.14	122.16	117.49
2	C	401	DCS	C2A-C2-N1	2.14	121.85	117.67
2	B	401	DCS	C3-C4-C5	2.12	120.75	118.72

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	DCS	CB-CA-N-C4A
2	C	401	DCS	C4-C5-C5A-O4P
2	C	401	DCS	C6-C5-C5A-O4P
2	C	401	DCS	CB-CA-N-C4A
2	D	401	DCS	C5-C4-C4A-N
2	D	401	DCS	CB-CA-N-C4A
2	A	401	DCS	C5-C4-C4A-N
2	C	401	DCS	C5-C4-C4A-N

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Mol	Chain	Res	Type	Atoms
2	C	401	DCS	C3-C4-C4A-N
2	B	401	DCS	C5A-O4P-P-O1P
2	A	401	DCS	C4-C4A-N-CA
2	B	401	DCS	CB-CA-N-C4A
2	A	401	DCS	C3-C4-C4A-N
2	D	401	DCS	C3-C4-C4A-N
2	D	401	DCS	C4-C5-C5A-O4P

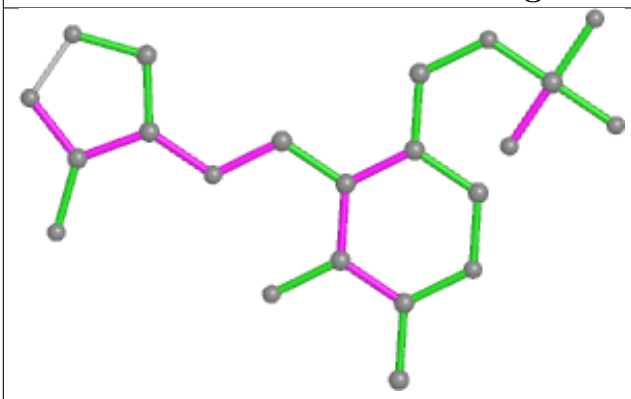
There are no ring outliers.

4 monomers are involved in 13 short contacts:

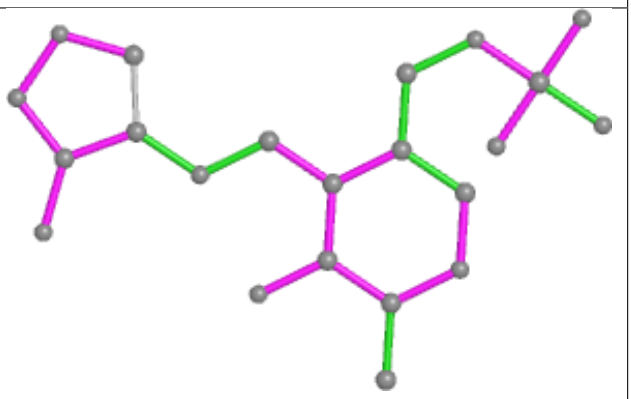
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	DCS	4	0
2	D	401	DCS	3	0
2	B	401	DCS	2	0
2	C	401	DCS	4	0

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.

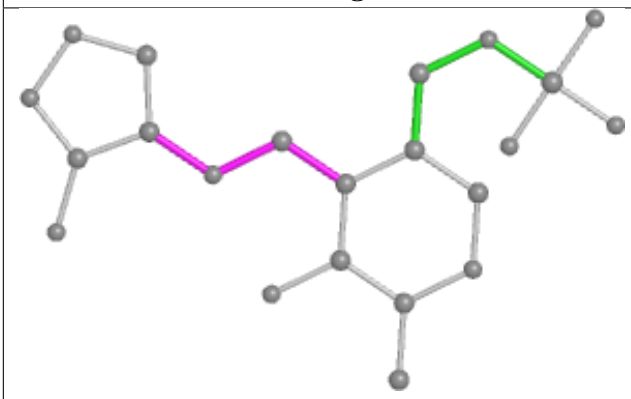
Ligand DCS A 401



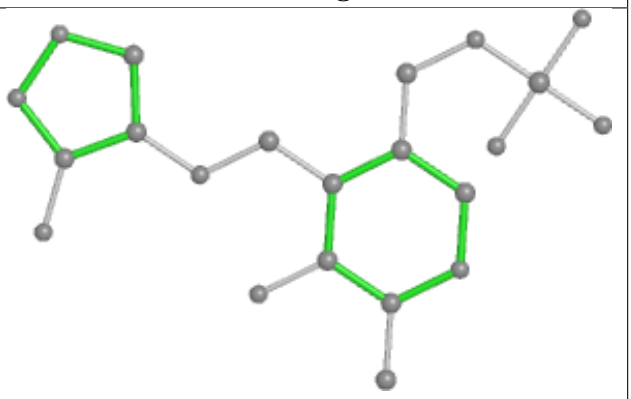
Bond lengths



Bond angles

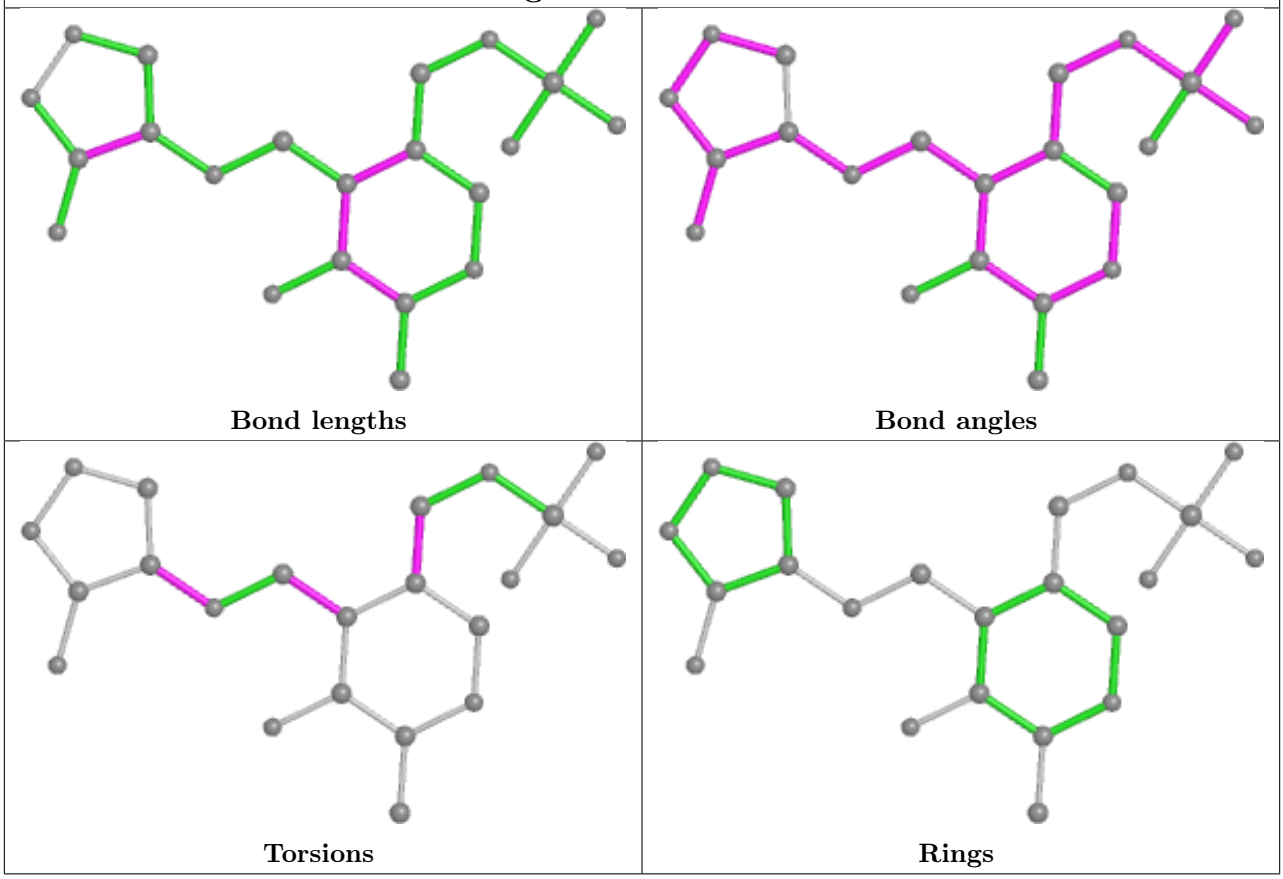


Torsions

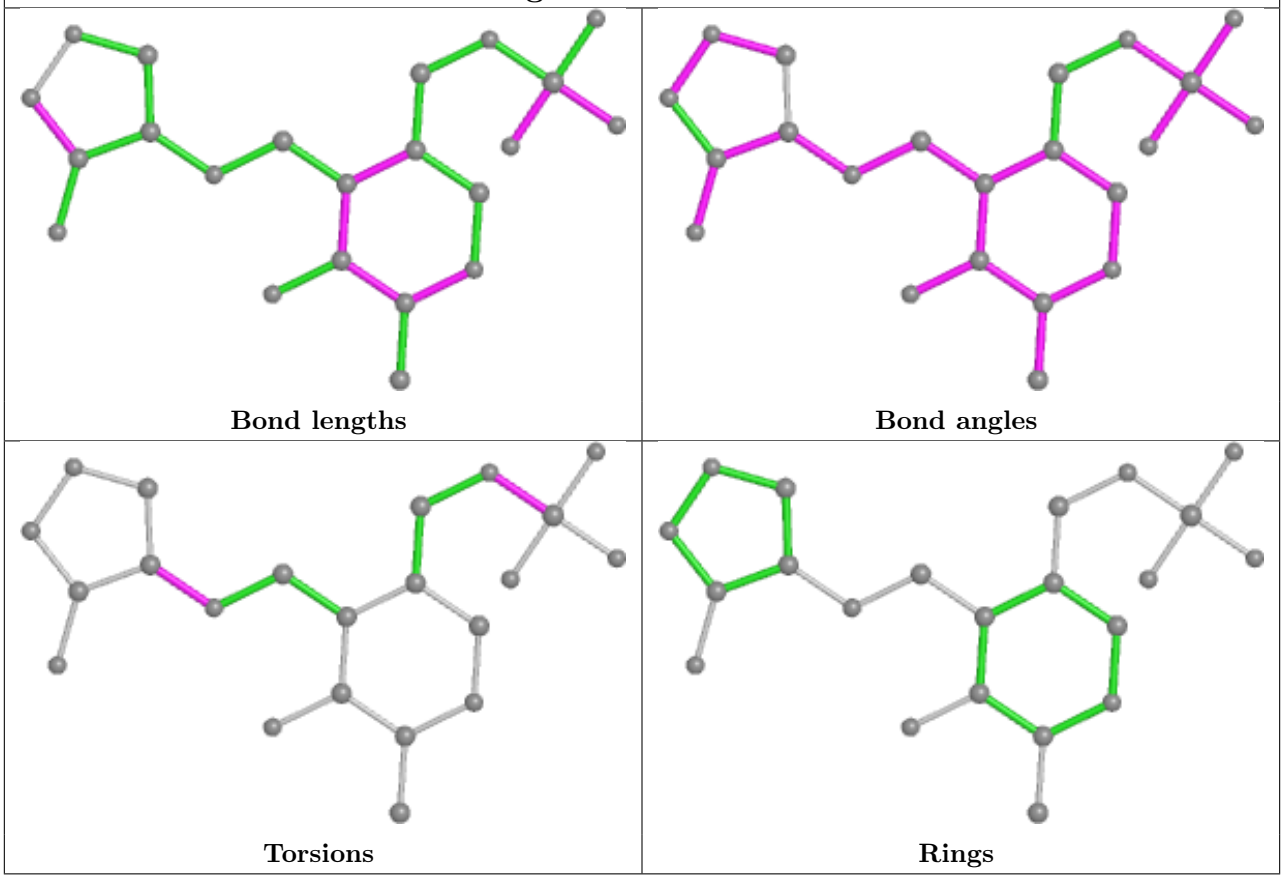


Rings

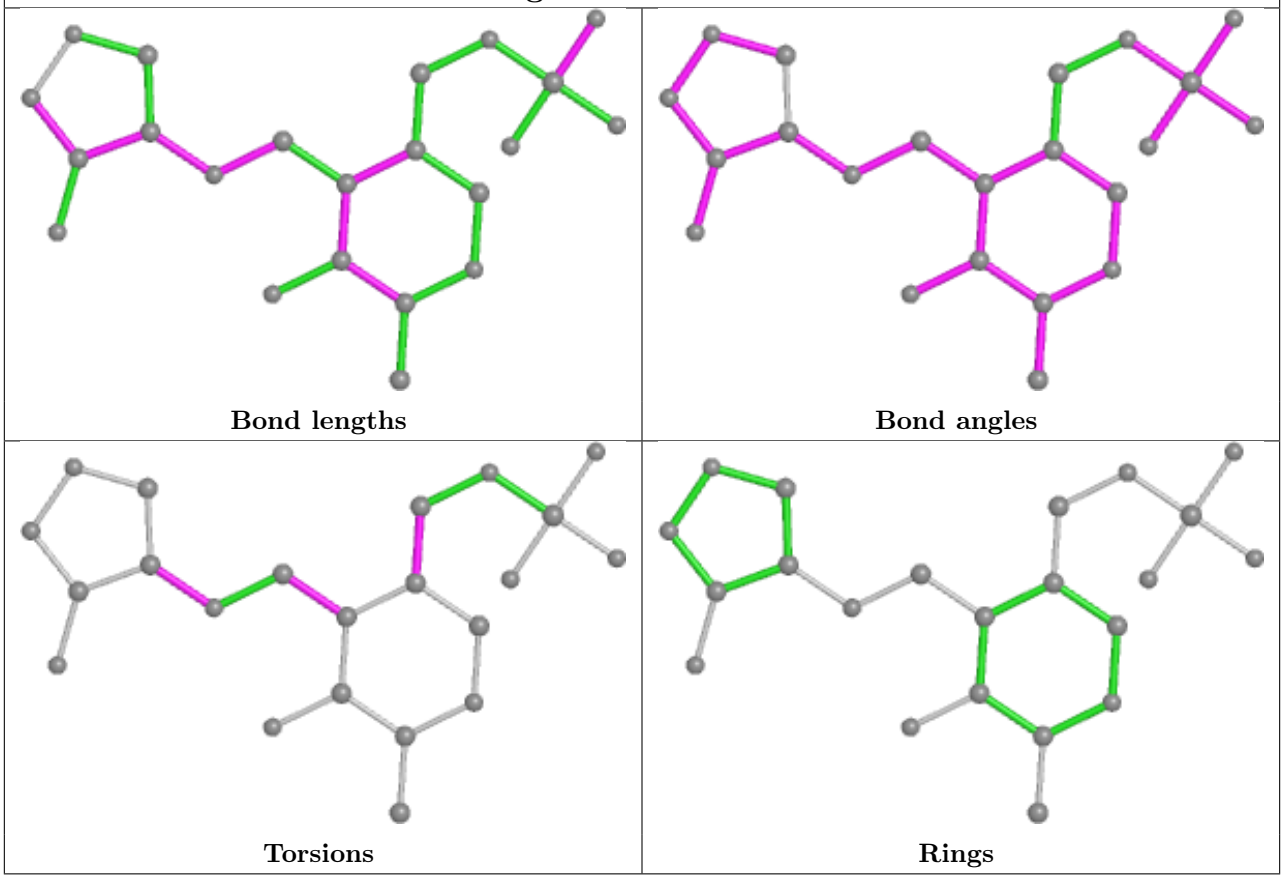
Ligand DCS D 401



Ligand DCS B 401



Ligand DCS C 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	384/410 (93%)	-0.05	5 (1%) 77 78	13, 26, 47, 73	0
1	B	381/410 (92%)	-0.10	0 100 100	13, 25, 43, 70	0
1	C	381/410 (92%)	0.28	21 (5%) 25 23	15, 33, 61, 81	0
1	D	381/410 (92%)	0.48	37 (9%) 7 6	15, 34, 70, 93	0
All	All	1527/1640 (93%)	0.15	63 (4%) 37 35	13, 29, 61, 93	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	160	LEU	5.6
1	C	290	PRO	5.6
1	D	211	GLY	5.2
1	D	133	GLY	5.2
1	D	212	LEU	4.9
1	D	157	TRP	4.4
1	D	172	LEU	4.4
1	D	189	GLY	4.3
1	D	167	ALA	4.2
1	D	10	ALA	4.0
1	D	151	CYS	3.9
1	D	153	PRO	3.9
1	D	208	GLU	3.6
1	D	171	GLY	3.6
1	D	155	ALA	3.6
1	C	133	GLY	3.5
1	C	276	PRO	3.5
1	A	7	ARG	3.3
1	C	10	ALA	3.3
1	C	275	VAL	3.2
1	D	134	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	274	GLN	3.1
1	C	339	GLY	3.1
1	D	89	ASP	3.0
1	D	207	ALA	2.9
1	C	292	GLU	2.9
1	D	158	GLU	2.9
1	D	169	GLU	2.9
1	D	126	THR	2.9
1	D	173	LEU	2.8
1	D	159	ARG	2.8
1	D	136	ALA	2.8
1	D	156	ASP	2.8
1	C	129	ALA	2.7
1	A	89	ASP	2.6
1	A	111	ARG	2.6
1	C	287	TYR	2.6
1	D	128	ALA	2.6
1	D	131	ALA	2.5
1	C	90	ASP	2.5
1	C	134	VAL	2.5
1	D	152	GLN	2.5
1	D	204	THR	2.5
1	D	111	ARG	2.4
1	C	35[A]	ARG	2.4
1	D	123	GLU	2.4
1	C	289	THR	2.4
1	C	318	VAL	2.4
1	A	90	ASP	2.4
1	D	165	LEU	2.4
1	C	164	ALA	2.3
1	D	191	PRO	2.2
1	C	132	ALA	2.2
1	C	272	VAL	2.2
1	D	129	ALA	2.2
1	D	37	PRO	2.2
1	C	278	GLY	2.2
1	D	150	GLY	2.2
1	A	8	ARG	2.1
1	C	162	GLY	2.1
1	C	111	ARG	2.1
1	D	210	ARG	2.0
1	D	197	LEU	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	KCX	D	141	12/13	0.81	0.13	41,44,82,84	0
1	KCX	C	141	12/13	0.93	0.07	24,28,51,64	0
1	KCX	A	141	12/13	0.95	0.08	21,26,56,63	0
1	KCX	B	141	12/13	0.95	0.12	22,29,60,61	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

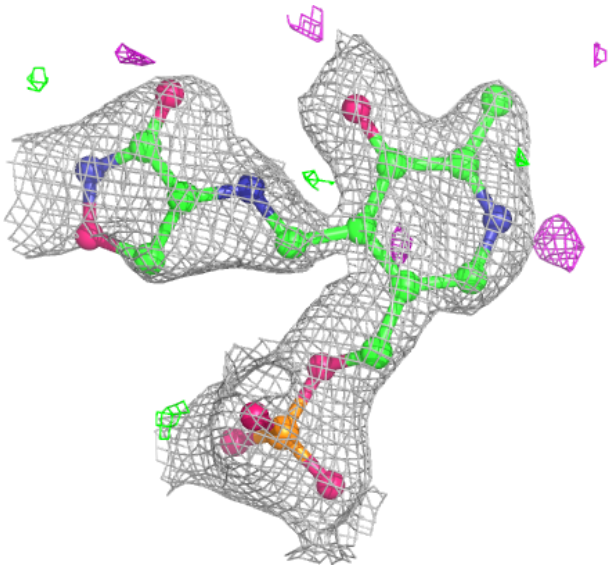
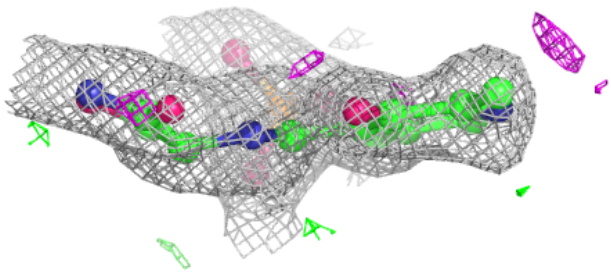
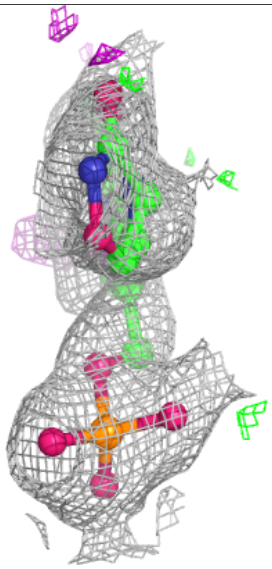
6.4 Ligands (i)

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	NA	C	404	1/1	0.90	0.18	34,34,34,34	0
3	NA	B	402	1/1	0.94	0.08	31,31,31,31	0
2	DCS	D	401	22/22	0.95	0.13	31,51,64,75	0
2	DCS	A	401	22/22	0.96	0.15	18,37,55,67	0
3	NA	A	402	1/1	0.96	0.07	31,31,31,31	0
2	DCS	B	401	22/22	0.96	0.13	18,34,53,55	0
2	DCS	C	401	22/22	0.96	0.11	21,39,44,54	0
4	CL	D	403	1/1	0.96	0.09	35,35,35,35	0
3	NA	D	402	1/1	0.97	0.16	26,26,26,26	0
4	CL	B	404	1/1	0.98	0.13	29,29,29,29	0
4	CL	B	403	1/1	0.98	0.12	20,20,20,20	0
3	NA	C	402	1/1	0.99	0.07	28,28,28,28	0
3	NA	C	403	1/1	0.99	0.05	33,33,33,33	0
4	CL	A	403	1/1	0.99	0.12	17,17,17,17	0
4	CL	C	405	1/1	1.00	0.18	15,15,15,15	0

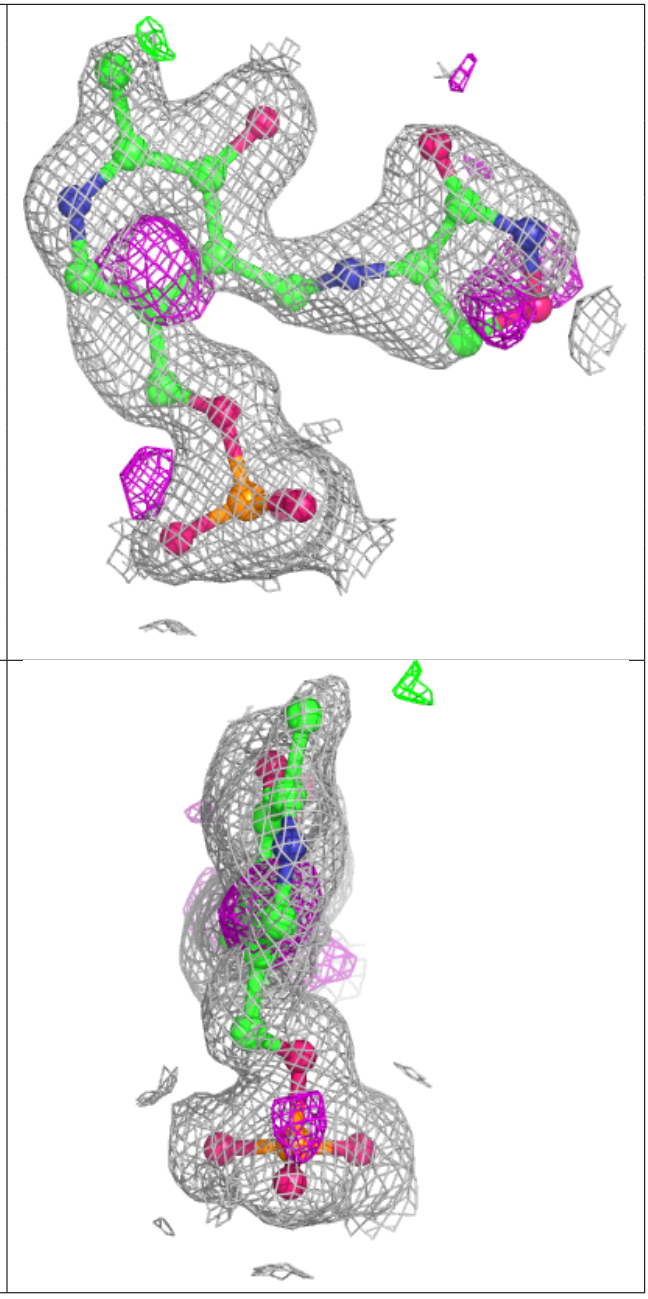
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

Electron density around DCS 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)	
	

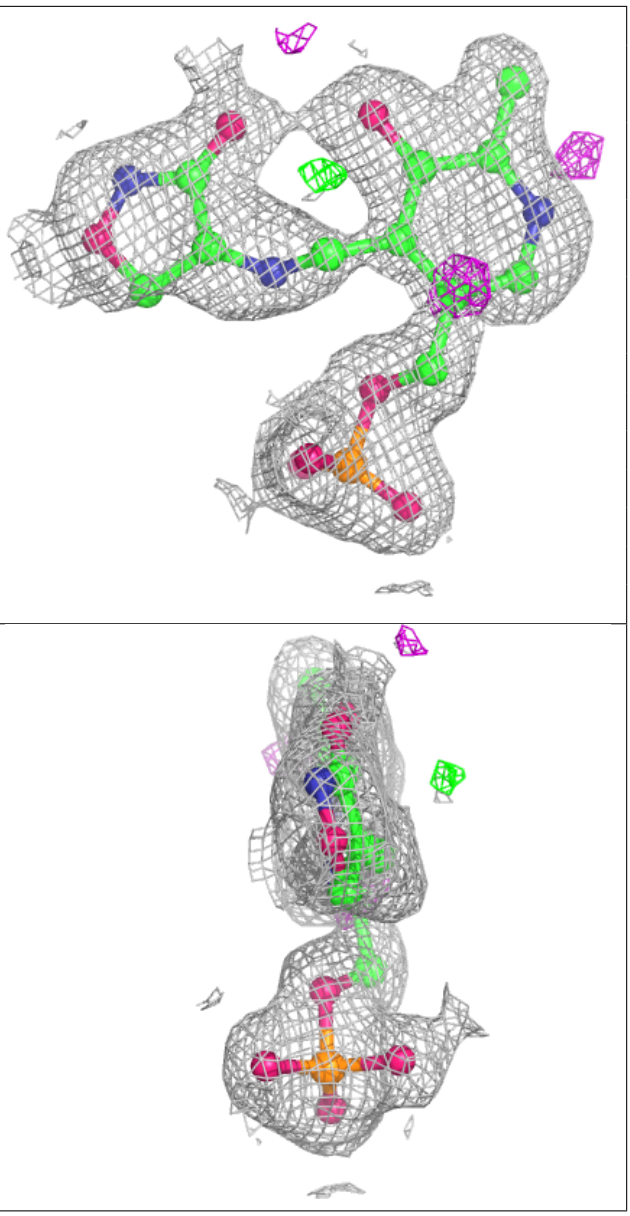
Electron density around DCS A 401:

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



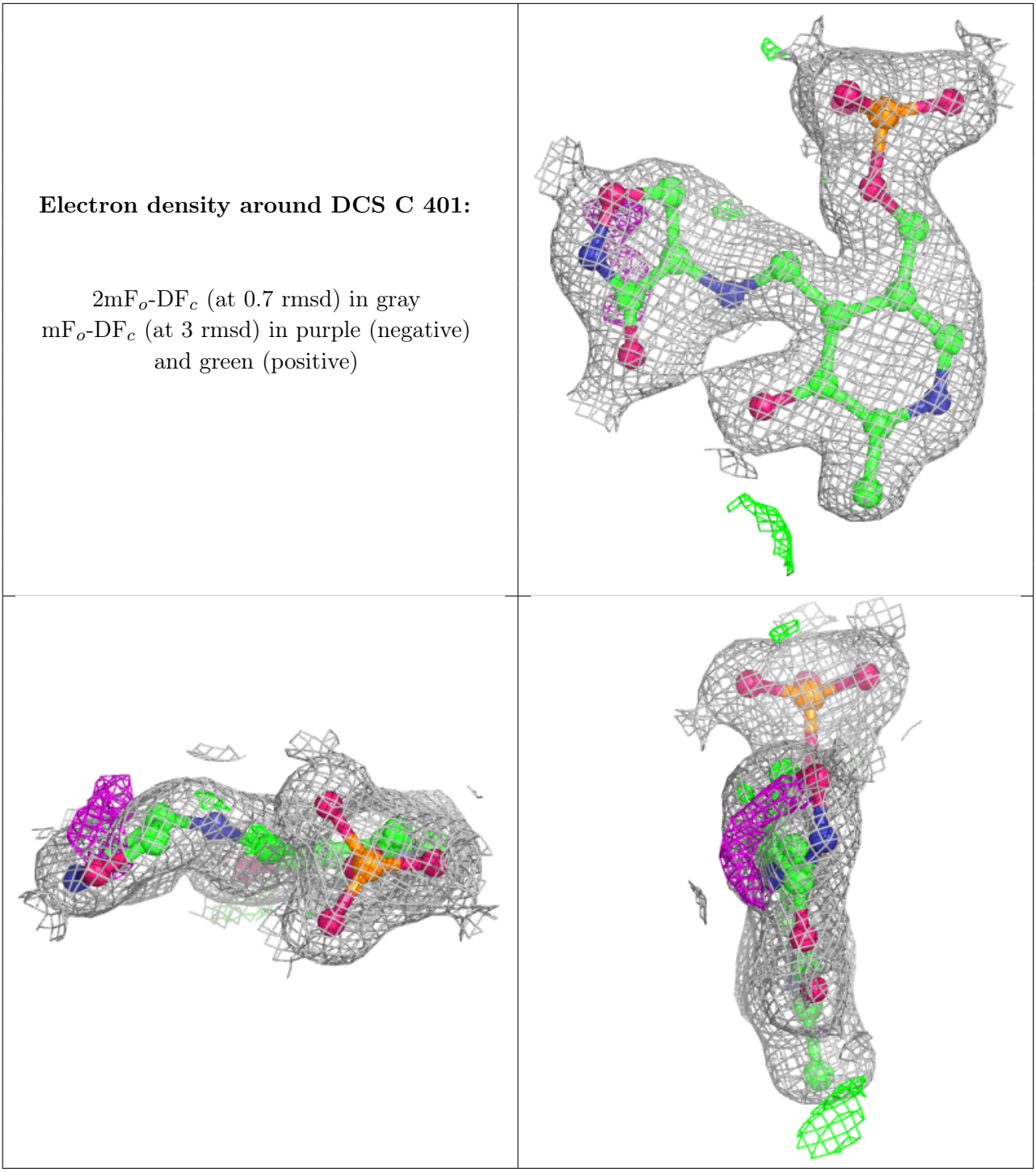
Electron density around DCS B 401:

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



Electron density around DCS 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)



6.5 Other polymers (i)

There are no such residues in this entry.