Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 08:17 PM JST

PDB ID	:	7F1V
Title	:	Crystal structure of Pseudomonas putida methionine gamma-lyase Q349S mutant with L-homocysteine intermediates
Authors	:	Okawa, A.; Handa, H.; Yasuda, E.; Murota, M.; Kudo, D.; Tamura, T.; Shiba, T.; Inagaki, K.
Deposited on	:	2021-06-09
Resolution	:	2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

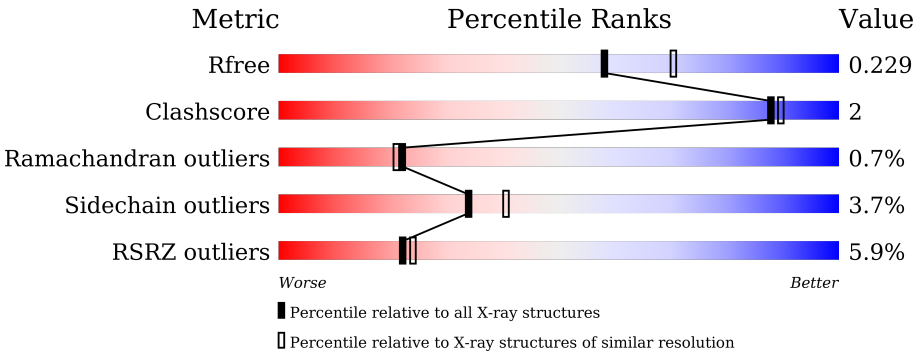
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	398	7% 94% 5% •
1	C	398	7% 90% 7% ••
2	B	398	4% 91% 7% ••
2	D	398	5% 89% 8% ••

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12101 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 L-methionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			2975	1876	527	555	17			
1	C	392	Total	C	N	O	S	0	0	0
			2948	1861	521	549	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	SER	GLN	engineered mutation	UNP P13254
C	349	SER	GLN	engineered mutation	UNP P13254

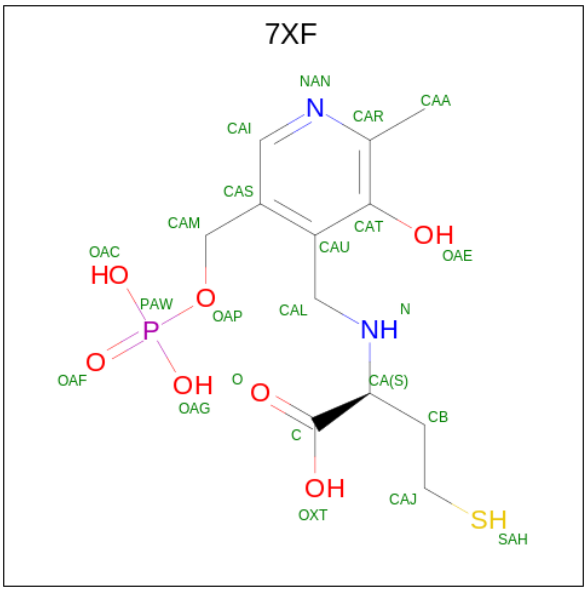
- Molecule 2 is a protein called L-methionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	392	Total	C	N	O	P	S	0	0	0
			2963	1869	522	554	1	17			
2	D	392	Total	C	N	O	P	S	0	0	0
			2963	1869	522	554	1	17			

There are 2 discrepancies between the modelled and reference sequences:

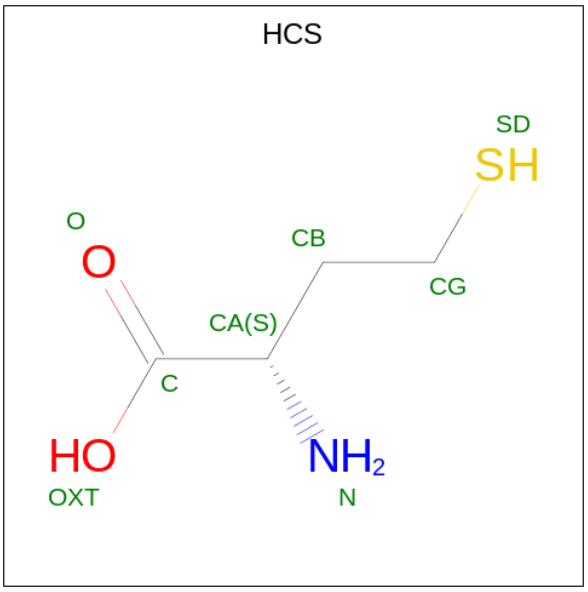
Chain	Residue	Modelled	Actual	Comment	Reference
B	349	SER	GLN	engineered mutation	UNP P13254
D	349	SER	GLN	engineered mutation	UNP P13254

- Molecule 3 is (2 {S})-2-[[2-methyl-3-oxidanyl-5-(phosphonooxymethyl)pyridin-4-yl]methylamino]-4-sulfanyl-butanoic acid (three-letter code: 7XF) (formula: $C_{12}H_{19}N_2O_7PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			23	12	2	7	1	1		
3	C	1	Total	C	N	O	P	S	0	0
			23	12	2	7	1	1		

- Molecule 4 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (three-letter code: HCS) (formula: $C_4H_9NO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			8	4	1	2	1		

- Molecule 5 is water.

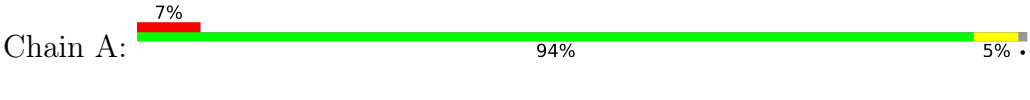
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	63	Total O 63 63	0	0
5	B	54	Total O 54 54	0	0
5	C	33	Total O 33 33	0	0
5	D	48	Total O 48 48	0	0

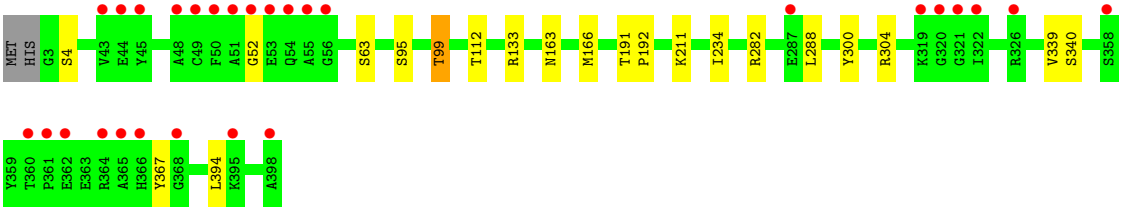
3 Residue-property plots (i)

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: L-methionine gamma-lyase

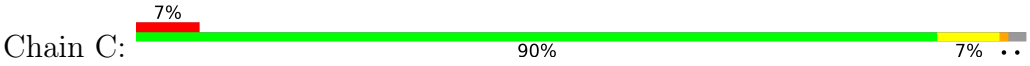
Chain A:

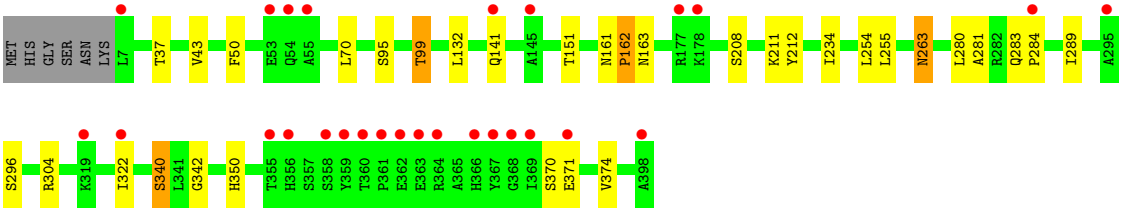




• Molecule 1: L-methionine gamma-lyase

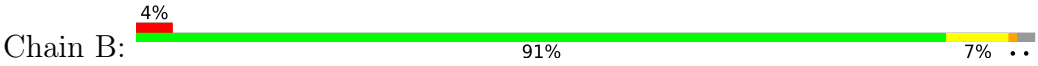
Chain C:

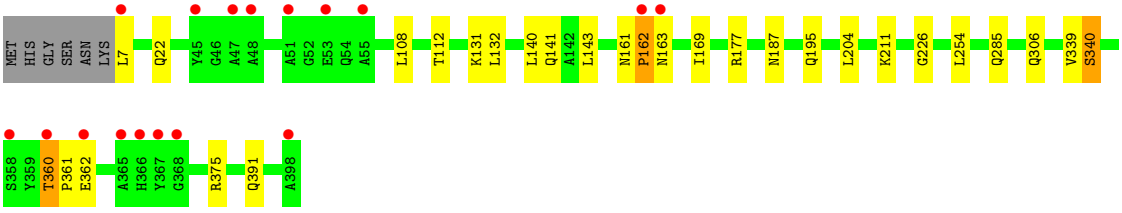




• Molecule 2: L-methionine gamma-lyase

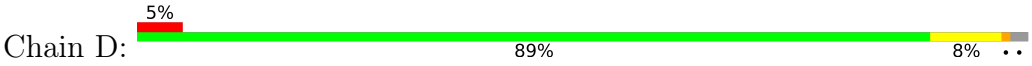
Chain B:

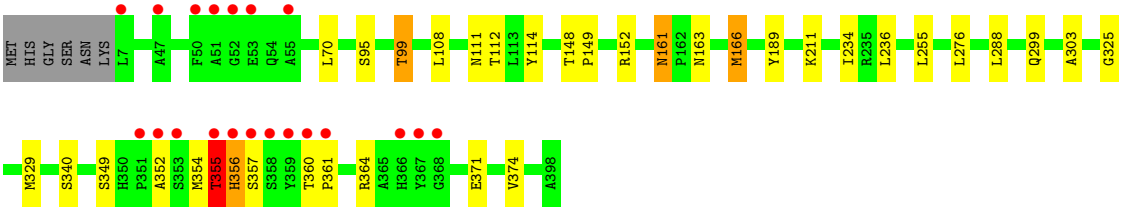




• Molecule 2: L-methionine gamma-lyase

Chain D:




MET
HIS
GLY
SER
ASN
LYS
L7
A47
F50
A51
G52
E53
Q54
A55
L70
S95
T99
L108
N111
T112
L113
Y114
T148
P149
R152
N161
P162
N163
M166
Y189
K211
I234
R235
L236
L255
L276
L288
Q299
A303
G325
M329
S340
S349
H350
P351
A352
S353
M354
T355
H356
S357
S358
Y359
T360
P361
R364
A365
H366
Y367
G368
E371
V374
A398

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	154.07Å 152.30Å 80.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.25 19.97 – 2.25	Depositor EDS
% Data completeness (in resolution range)	87.7 (19.97-2.25) 87.9 (19.97-2.25)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.14 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.188 , 0.227 0.194 , 0.229	Depositor DCC
R_{free} test set	3961 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 27.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12101	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7XF, HCS, LLP

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	0.50	0/3039	0.69	2/4124 (0.0%)
1	C	0.48	0/3012	0.68	0/4089
2	B	0.49	0/3002	0.70	0/4075
2	D	0.49	0/3002	0.70	0/4075
All	All	0.49	0/12055	0.69	2/16363 (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
2	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	LYS	CD-CE-NZ	5.34	123.98	111.70
1	A	282	ARG	NE-CZ-NH2	5.14	122.87	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	356	HIS	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	2975	0	2942	6	0
1	C	2948	0	2918	16	0
2	B	2963	0	2921	9	0
2	D	2963	0	2921	21	0
3	A	23	0	0	0	0
3	C	23	0	0	0	0
4	D	8	0	8	1	0
5	A	63	0	0	0	0
5	B	54	0	0	1	0
5	C	33	0	0	0	0
5	D	48	0	0	1	0
All	All	12101	0	11710	47	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 2.

All (47) 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)
2:B:162:PRO:N	2:B:163:ASN:HA	1.97	0.80
1:A:99:THR:HG21	1:A:234:ILE:HA	1.66	0.78
1:C:99:THR:HG21	1:C:234:ILE:HA	1.72	0.71
1:C:281:ALA:HA	1:C:289:ILE:HD11	1.78	0.65
2:D:99:THR:HG21	2:D:234:ILE:HA	1.78	0.65
2:B:112:THR:HG21	2:B:162:PRO:HB3	1.79	0.64
2:B:169:ILE:H	2:B:306:GLN:HE22	1.50	0.59
1:A:112:THR:HG22	1:A:367:TYR:O	2.02	0.59
2:D:166:MET:H	2:D:299:GLN:HE22	1.51	0.58
2:D:356:HIS:HB3	2:D:364:ARG:CZ	2.35	0.56
1:C:37:THR:HG22	5:D:517:HOH:O	2.08	0.53
1:C:50:PHE:CD1	2:D:355:THR:HG23	2.44	0.52
2:D:166:MET:CE	2:D:303:ALA:HB2	2.40	0.52
2:D:161:ASN:HB3	2:D:189:TYR:OH	2.10	0.51
1:A:300:TYR:CZ	1:A:304:ARG:HD2	2.47	0.50
1:A:95:SER:O	1:A:99:THR:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:ASN:HB3	2:D:189:TYR:CZ	2.48	0.48
2:D:95:SER:O	2:D:99:THR:CG2	2.62	0.47
2:D:70:LEU:HD21	2:D:255:LEU:HD23	1.95	0.47
1:C:95:SER:O	1:C:99:THR:HG23	2.15	0.46
1:C:43:VAL:HG12	2:D:354:MET:CE	2.45	0.46
1:C:43:VAL:HG12	2:D:354:MET:HE3	1.97	0.46
1:A:339:VAL:HG22	5:B:432:HOH:O	2.15	0.45
1:C:208:SER:OG	1:C:211:LYS:NZ	2.43	0.45
2:D:161:ASN:CB	2:D:189:TYR:OH	2.63	0.45
2:D:354:MET:O	2:D:356:HIS:N	2.50	0.45
1:C:370:SER:OG	1:C:371:GLU:N	2.50	0.44
2:D:352:ALA:HB2	2:D:371:GLU:HA	2.00	0.44
1:C:212:TYR:CE1	1:C:342:GLY:HA2	2.52	0.44
2:D:360:THR:HG22	2:D:361:PRO:HD2	2.00	0.44
1:C:50:PHE:CE1	2:D:355:THR:HG23	2.53	0.43
2:B:204:LEU:HD23	2:B:226:GLY:HA3	2.00	0.43
1:C:263:ASN:H	1:C:263:ASN:HD22	1.65	0.43
1:C:70:LEU:HD21	1:C:255:LEU:HD23	2.00	0.42
2:D:114:TYR:CA	2:D:161:ASN:HD21	2.32	0.42
2:D:114:TYR:CE1	4:D:401:HCS:HG2	2.54	0.42
2:B:360:THR:HG22	2:B:361:PRO:HD2	2.00	0.42
2:B:108:LEU:HD23	2:B:143:LEU:CD2	2.49	0.42
2:D:325:GLY:O	2:D:329:MET:HG2	2.19	0.42
2:B:339:VAL:O	2:B:340:SER:CB	2.68	0.41
1:A:191:THR:HB	1:A:192:PRO:HD2	2.03	0.41
2:D:329:MET:HE1	2:D:349:SER:HA	2.03	0.41
1:C:283:GLN:HA	1:C:284:PRO:HD3	1.97	0.41
2:B:254:LEU:HD21	1:C:254:LEU:HD21	2.02	0.40
2:B:187:ASN:ND2	2:B:195:GLN:HE21	2.19	0.40
2:D:148:THR:HB	2:D:149:PRO:HD2	2.04	0.40
1:C:161:ASN:HA	1:C:162:PRO:HA	1.92	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	394/398 (99%)	378 (96%)	14 (4%)	2 (0%)	29	29
1	C	390/398 (98%)	373 (96%)	14 (4%)	3 (1%)	19	17
2	B	389/398 (98%)	375 (96%)	11 (3%)	3 (1%)	19	17
2	D	389/398 (98%)	379 (97%)	7 (2%)	3 (1%)	19	17
All	All	1562/1592 (98%)	1505 (96%)	46 (3%)	11 (1%)	22	21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	161	ASN
2	D	355	THR
2	D	357	SER
2	B	340	SER
1	A	52	GLY
1	A	340	SER
1	C	151	THR
1	C	340	SER
2	D	340	SER
2	B	162	PRO
1	C	162	PRO

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	305/307 (99%)	297 (97%)	8 (3%)	46	55
1	C	302/307 (98%)	290 (96%)	12 (4%)	31	37
2	B	301/306 (98%)	289 (96%)	12 (4%)	31	37
2	D	301/306 (98%)	288 (96%)	13 (4%)	29	33
All	All	1209/1226 (99%)	1164 (96%)	45 (4%)	34	40

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	63	SER
1	A	99	THR
1	A	133	ARG
1	A	163	ASN
1	A	166	MET
1	A	288	LEU
1	A	394	LEU
2	B	7	LEU
2	B	22	GLN
2	B	131	LYS
2	B	132	LEU
2	B	140	LEU
2	B	141	GLN
2	B	177	ARG
2	B	285	GLN
2	B	360	THR
2	B	362	GLU
2	B	375	ARG
2	B	391	GLN
1	C	99	THR
1	C	132	LEU
1	C	141	GLN
1	C	163	ASN
1	C	263	ASN
1	C	280	LEU
1	C	296	SER
1	C	304	ARG
1	C	322	ILE
1	C	340	SER
1	C	350	HIS
1	C	374	VAL
2	D	99	THR
2	D	108	LEU
2	D	111	ASN
2	D	112	THR
2	D	152	ARG
2	D	161	ASN
2	D	163	ASN
2	D	166	MET
2	D	236	LEU
2	D	276	LEU

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Mol	Chain	Res	Type
2	D	288	LEU
2	D	355	THR
2	D	374	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	22	GLN
1	A	34	GLN
1	A	187	ASN
1	A	195	GLN
1	A	237	GLN
1	A	274	GLN
1	A	330	ASN
2	B	34	GLN
2	B	57	HIS
2	B	141	GLN
2	B	187	ASN
2	B	250	HIS
2	B	285	GLN
2	B	299	GLN
2	B	306	GLN
2	B	309	GLN
1	C	68	ASN
1	C	207	HIS
1	C	250	HIS
1	C	263	ASN
1	C	309	GLN
1	C	333	GLN
1	C	350	HIS
2	D	64	ASN
2	D	111	ASN
2	D	161	ASN
2	D	274	GLN
2	D	299	GLN
2	D	306	GLN
2	D	309	GLN
2	D	330	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

2 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	$\#\|Z\| > 2$
2	LLP	B	211	2	23,24,25	3.14	5 (21%)	25,32,34	1.76	9 (36%)
2	LLP	D	211	2	23,24,25	2.86	5 (21%)	25,32,34	1.53	4 (16%)

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	LLP	B	211	2	-	6/16/17/19	0/1/1/1
2	LLP	D	211	2	-	4/16/17/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	211	LLP	C3-C2	8.31	1.49	1.40
2	B	211	LLP	C4-C5	7.49	1.51	1.42
2	D	211	LLP	C3-C2	7.34	1.48	1.40
2	D	211	LLP	C4-C5	6.54	1.50	1.42
2	D	211	LLP	C4'-NZ	6.29	1.48	1.27
2	B	211	LLP	C4'-NZ	6.22	1.48	1.27
2	B	211	LLP	C4-C3	5.96	1.49	1.40
2	D	211	LLP	C4-C3	5.25	1.48	1.40
2	B	211	LLP	C4-C4'	4.07	1.54	1.46
2	D	211	LLP	C4-C4'	3.96	1.54	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	211	LLP	C3-C4-C5	-3.41	115.64	118.26
2	B	211	LLP	OP3-P-OP4	-3.30	97.95	106.73
2	D	211	LLP	CD-CE-NZ	3.04	118.37	110.93
2	B	211	LLP	C6-N1-C2	2.99	124.70	119.17
2	B	211	LLP	C3-C4-C5	-2.93	116.01	118.26
2	B	211	LLP	OP4-P-OP1	-2.76	98.72	106.47
2	D	211	LLP	C6-N1-C2	2.68	124.13	119.17
2	B	211	LLP	CD-CE-NZ	2.37	116.73	110.93
2	B	211	LLP	OP3-P-OP1	2.16	119.13	110.68
2	B	211	LLP	C4-C4'-NZ	-2.13	114.54	124.31
2	B	211	LLP	OP2-P-OP1	2.09	118.85	110.68
2	D	211	LLP	OP3-P-OP4	-2.08	101.20	106.73
2	B	211	LLP	C5-C4-C4'	2.02	124.89	121.56

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	211	LLP	O-C-CA-CB
2	D	211	LLP	O-C-CA-CB
2	B	211	LLP	C4-C4'-NZ-CE
2	D	211	LLP	C4-C4'-NZ-CE
2	D	211	LLP	CG-CD-CE-NZ
2	B	211	LLP	CG-CD-CE-NZ
2	B	211	LLP	CA-CB-CG-CD
2	D	211	LLP	CA-CB-CG-CD
2	B	211	LLP	CD-CE-NZ-C4'
2	B	211	LLP	C3-C4-C4'-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	7XF	C	401	-	23,23,23	2.07	4 (17%)	27,32,32	2.07	9 (33%)
4	HCS	D	401	-	6,7,7	1.15	1 (16%)	7,8,8	2.24	3 (42%)
3	7XF	A	401	1	23,23,23	1.99	6 (26%)	27,32,32	2.47	14 (51%)

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	7XF	C	401	-	-	8/18/18/18	0/1/1/1
4	HCS	D	401	-	-	3/7/7/7	-
3	7XF	A	401	1	-	6/18/18/18	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	7XF	CAA-CAR	-6.08	1.40	1.50
3	A	401	7XF	CAA-CAR	-5.65	1.40	1.50
3	A	401	7XF	CAL-CAU	4.25	1.57	1.51
3	C	401	7XF	CAL-CAU	4.17	1.57	1.51
3	C	401	7XF	CAR-NAN	3.62	1.40	1.33
3	A	401	7XF	CAR-NAN	2.60	1.38	1.33
4	D	401	HCS	OXT-C	-2.38	1.22	1.30
3	A	401	7XF	PAW-OAG	-2.32	1.45	1.54
3	A	401	7XF	PAW-OAC	-2.32	1.45	1.54
3	C	401	7XF	PAW-OAG	-2.23	1.46	1.54
3	A	401	7XF	CA-C	2.05	1.58	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	7XF	OAC-PAW-OAP	-4.67	94.31	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	7XF	CAL-N-CA	4.58	122.61	113.92
3	A	401	7XF	CB-CAJ-SAH	-4.42	109.14	113.74
3	A	401	7XF	CAL-CAU-CAS	4.10	124.27	119.71
3	A	401	7XF	OAC-PAW-OAP	-4.04	95.97	106.73
4	D	401	HCS	CB-CA-N	3.83	120.22	110.17
3	A	401	7XF	OAG-PAW-OAP	-3.52	97.35	106.73
3	A	401	7XF	OAP-PAW-OAF	-3.51	96.62	106.47
3	C	401	7XF	CB-CAJ-SAH	-3.48	110.11	113.74
3	C	401	7XF	OAG-PAW-OAP	-3.34	97.84	106.73
3	C	401	7XF	OAC-PAW-OAG	3.26	120.08	107.64
4	D	401	HCS	CB-CG-SD	3.12	116.99	113.74
3	A	401	7XF	CAT-CAU-CAS	-2.98	115.86	118.72
3	C	401	7XF	CAL-CAU-CAS	2.78	122.80	119.71
3	A	401	7XF	CAT-CAR-NAN	-2.75	117.22	120.77
3	C	401	7XF	CAL-N-CA	2.71	119.06	113.92
3	A	401	7XF	OAC-PAW-OAG	2.60	117.58	107.64
3	A	401	7XF	CB-CA-C	2.49	116.36	110.35
4	D	401	HCS	OXT-C-O	-2.38	118.69	124.09
3	C	401	7XF	CAT-CAR-NAN	-2.33	117.76	120.77
3	C	401	7XF	OAP-PAW-OAF	-2.32	99.96	106.47
3	A	401	7XF	OAG-PAW-OAF	2.28	119.62	110.68
3	A	401	7XF	CAU-CAT-CAR	2.23	123.48	120.06
3	A	401	7XF	CAM-CAS-CAI	-2.21	115.73	119.37
3	A	401	7XF	OAC-PAW-OAF	2.08	118.83	110.68
3	C	401	7XF	OAC-PAW-OAF	2.03	118.61	110.68

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	7XF	N-CAL-CAU-CAS
3	A	401	7XF	N-CAL-CAU-CAT
3	A	401	7XF	SAH-CAJ-CB-CA
3	C	401	7XF	C-CA-N-CAL
3	C	401	7XF	N-CA-CB-CAJ
4	D	401	HCS	CA-CB-CG-SD
3	C	401	7XF	N-CAL-CAU-CAS
3	C	401	7XF	C-CA-CB-CAJ
3	C	401	7XF	SAH-CAJ-CB-CA
3	A	401	7XF	C-CA-N-CAL
3	C	401	7XF	N-CAL-CAU-CAT
3	C	401	7XF	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
3	C	401	7XF	OXT-C-CA-CB
3	A	401	7XF	CB-CA-N-CAL
4	D	401	HCS	N-CA-CB-CG
4	D	401	HCS	C-CA-CB-CG
3	A	401	7XF	C-CA-CB-CAJ

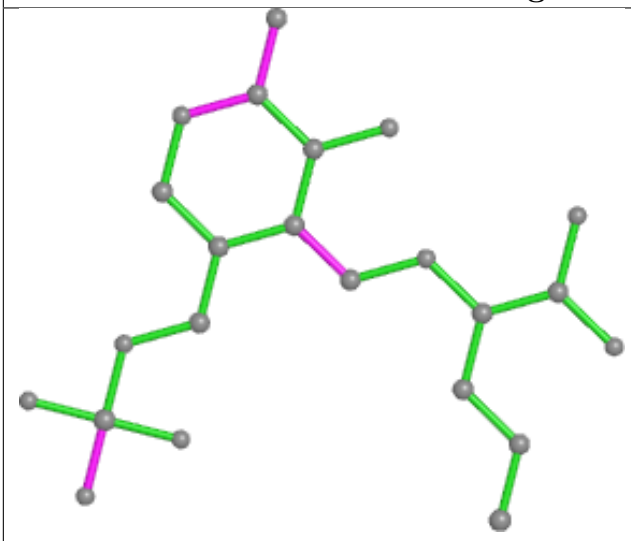
There are no ring outliers.

1 monomer is involved in 1 short contact:

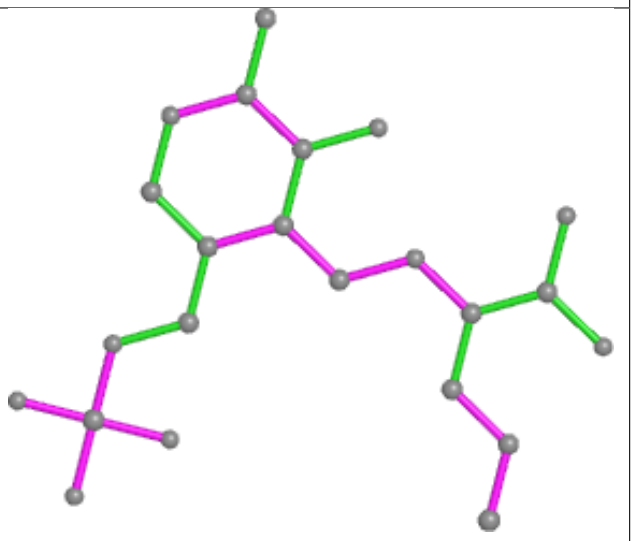
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	HCS	1	0

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.

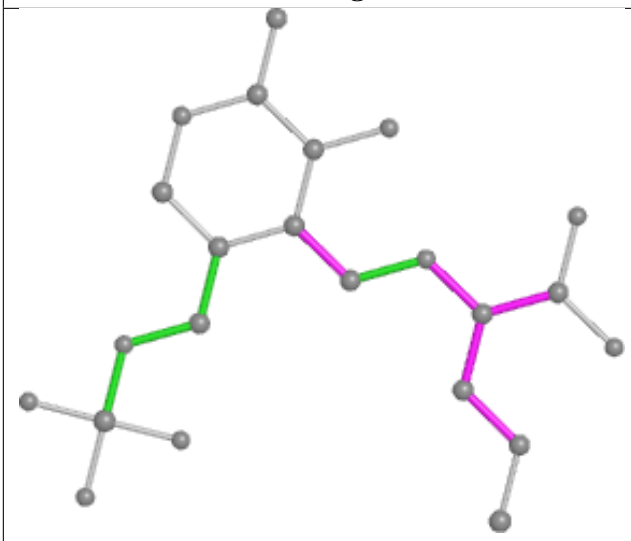
Ligand 7XF C 401



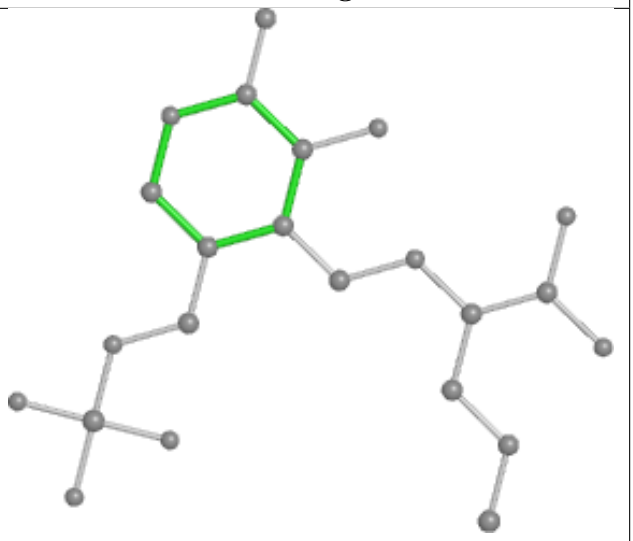
Bond lengths



Bond angles

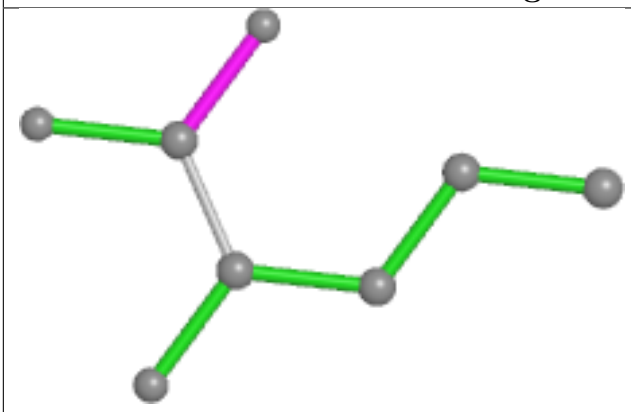


Torsions

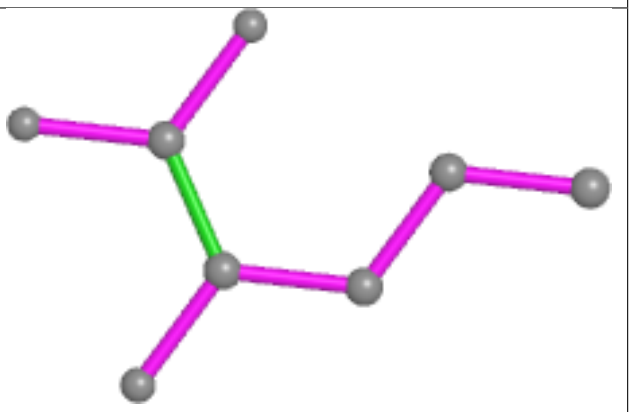


Rings

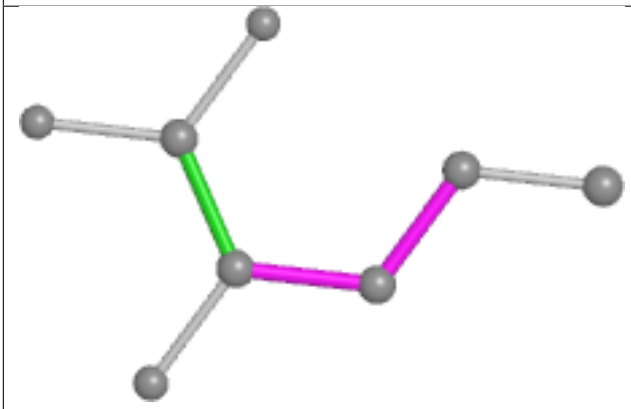
Ligand HCS D 401



Bond lengths



Bond angles



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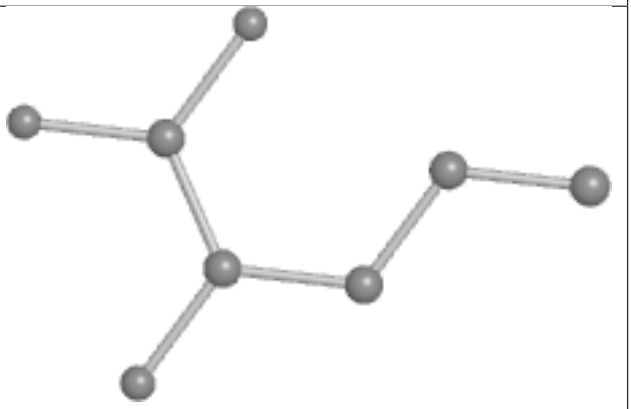
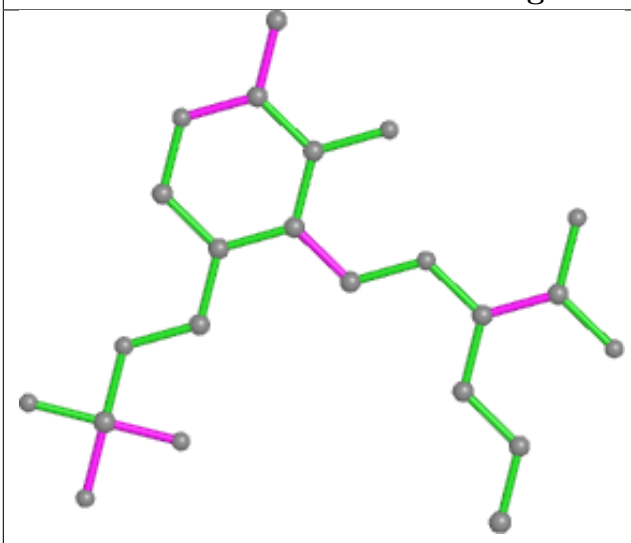
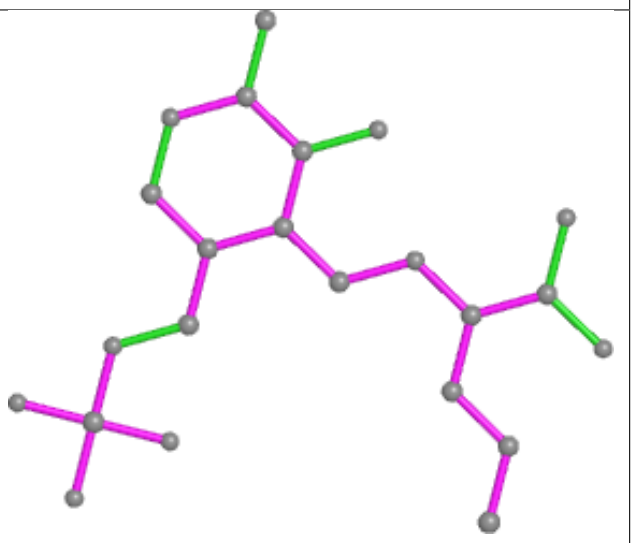


Rings

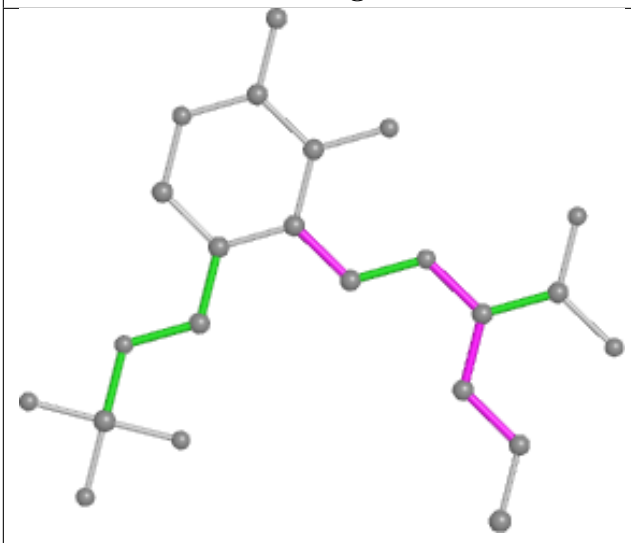
Ligand 7XF A 401



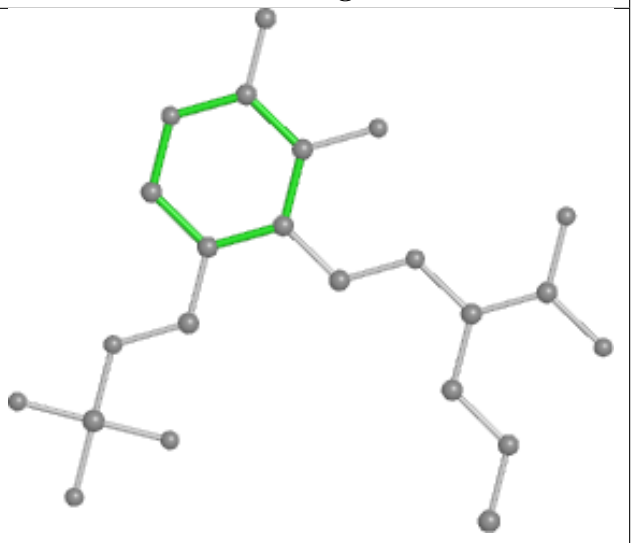
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	396/398 (99%)	-0.05	28 (7%)	16	17	18, 30, 82, 126	0
1	C	392/398 (98%)	-0.01	27 (6%)	16	18	20, 38, 82, 112	0
2	B	391/398 (98%)	-0.16	17 (4%)	35	37	20, 33, 72, 110	0
2	D	391/398 (98%)	-0.21	20 (5%)	28	30	19, 31, 74, 97	0
All	All	1570/1592 (98%)	-0.11	92 (5%)	22	24	18, 33, 78, 126	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	GLY	8.6
1	A	55	ALA	7.3
1	C	55	ALA	7.3
1	C	367	TYR	6.0
1	A	51	ALA	5.9
1	C	366	HIS	5.6
2	B	162	PRO	5.6
1	C	360	THR	5.6
2	B	360	THR	5.6
1	C	368	GLY	5.5
2	D	51	ALA	5.5
1	A	398	ALA	5.4
2	B	367	TYR	5.1
1	A	361	PRO	5.0
2	D	366	HIS	4.9
2	D	360	THR	4.9
1	A	366	HIS	4.9
1	A	362	GLU	4.6
1	A	322	ILE	4.6
1	A	44	GLU	4.3
2	B	368	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	365	ALA	4.2
2	D	357	SER	4.2
1	C	363	GLU	4.2
1	A	48	ALA	4.1
2	D	55	ALA	4.1
2	B	55	ALA	4.1
2	D	47	ALA	4.0
1	A	365	ALA	3.9
1	A	54	GLN	3.8
1	A	358	SER	3.7
2	B	366	HIS	3.7
1	C	362	GLU	3.6
1	C	319	LYS	3.6
2	B	362	GLU	3.6
1	A	53	GLU	3.5
1	C	358	SER	3.5
1	C	361	PRO	3.5
1	C	398	ALA	3.5
2	D	361	PRO	3.4
1	A	45	TYR	3.3
2	D	50	PHE	3.3
1	C	177	ARG	3.3
1	C	322	ILE	3.3
2	B	358	SER	3.3
2	D	52	GLY	3.2
1	A	56	GLY	3.2
2	D	358	SER	3.1
1	C	356	HIS	3.0
2	B	53	GLU	3.0
2	D	53	GLU	3.0
1	C	145	ALA	3.0
2	B	398	ALA	3.0
2	D	368	GLY	2.9
1	C	53	GLU	2.9
2	B	47	ALA	2.8
1	A	360	THR	2.8
1	C	359	TYR	2.8
2	B	51	ALA	2.7
1	A	395	LYS	2.7
2	D	367	TYR	2.6
1	A	364	ARG	2.6
2	D	352	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	7	LEU	2.5
1	C	54	GLN	2.5
2	D	355	THR	2.5
1	C	371	GLU	2.4
1	A	368	GLY	2.4
2	B	7	LEU	2.4
1	A	319	LYS	2.4
2	D	359	TYR	2.4
1	C	295	ALA	2.4
1	A	287	GLU	2.3
1	A	50	PHE	2.3
2	D	7	LEU	2.3
1	A	43	VAL	2.3
2	D	356	HIS	2.2
1	A	326	ARG	2.2
1	A	49	CYS	2.2
1	C	369	ILE	2.2
2	D	351	PRO	2.2
2	B	48	ALA	2.2
2	D	353	SER	2.2
1	A	321	GLY	2.1
2	B	45	TYR	2.1
1	C	364	ARG	2.1
1	C	141	GLN	2.1
1	C	355	THR	2.1
2	B	163	ASN	2.1
1	C	284	PRO	2.1
1	A	320	GLY	2.1
1	C	178	LYS	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LLP	D	211	24/25	0.94	0.11	22,30,35,40	0
2	LLP	B	211	24/25	0.95	0.14	22,32,38,40	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

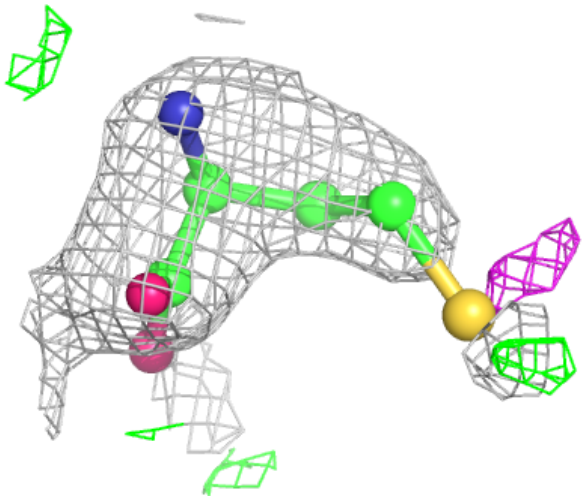
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

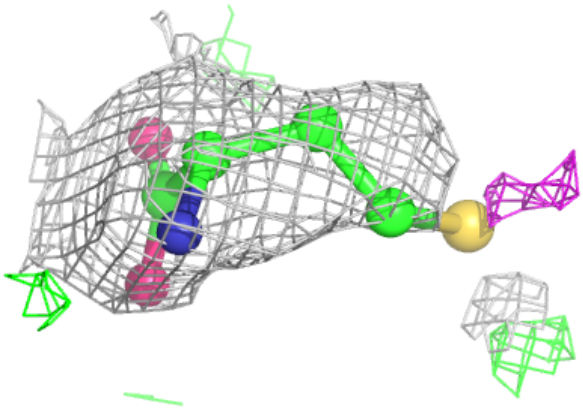
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	HCS	D	401	8/8	0.73	0.27	67,69,78,91	0
3	7XF	C	401	23/23	0.94	0.16	30,44,70,89	0
3	7XF	A	401	23/23	0.96	0.11	24,36,52,70	0

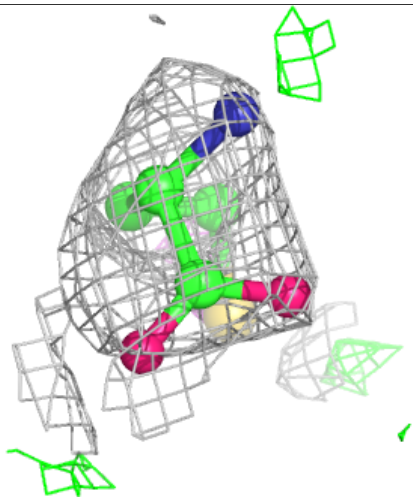
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HCS 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)

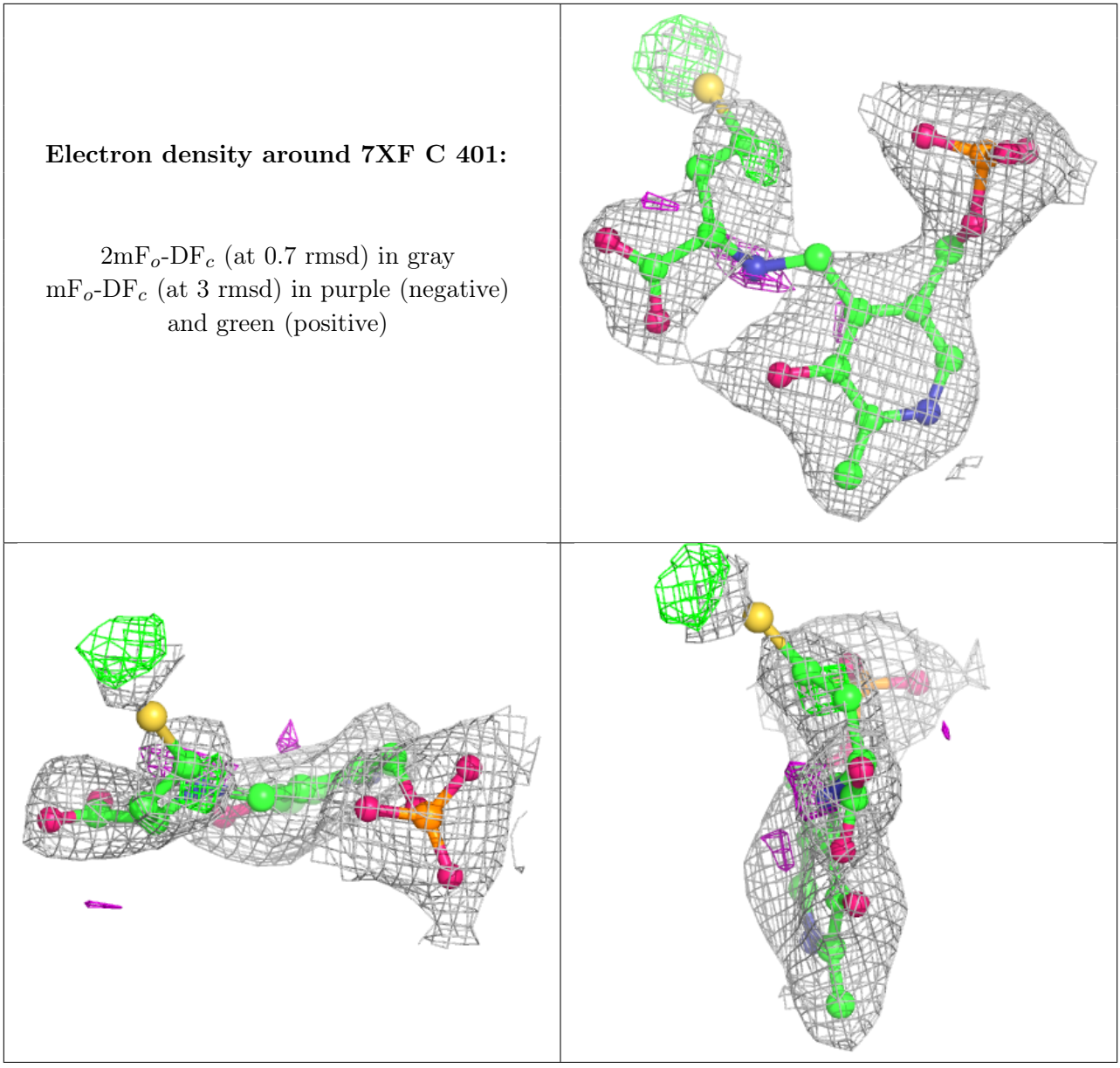






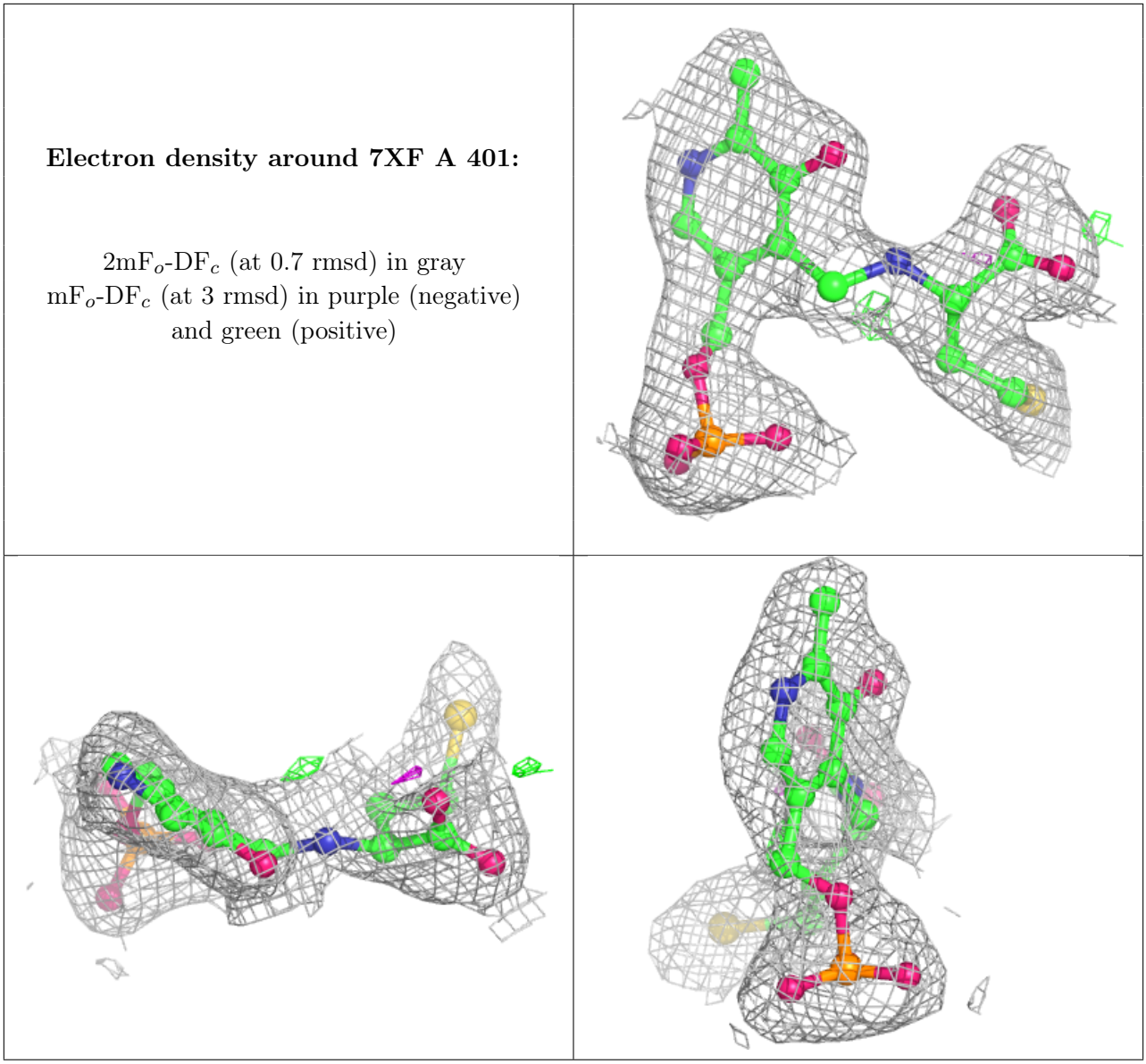
Electron density around 7XF C 401:

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



Electron density around 7XF 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)



6.5 Other polymers

There are no such residues in this entry.