Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 03:55 PM EDT

PDB ID	:	3VCY
Title	:	Structure of MurA (UDP-N-acetylglucosamine enolpyruvyl transferase), from Vibrio fischeri in complex with substrate UDP-N-acetylglucosamine and the drug fosfomycin.
Authors	:	Bensen, D.C.; Rodriguez, S.; Nix, J.; Cunningham, M.L.; Tari, L.W.
Deposited on	:	2012-01-04
Resolution	:	1.93 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:

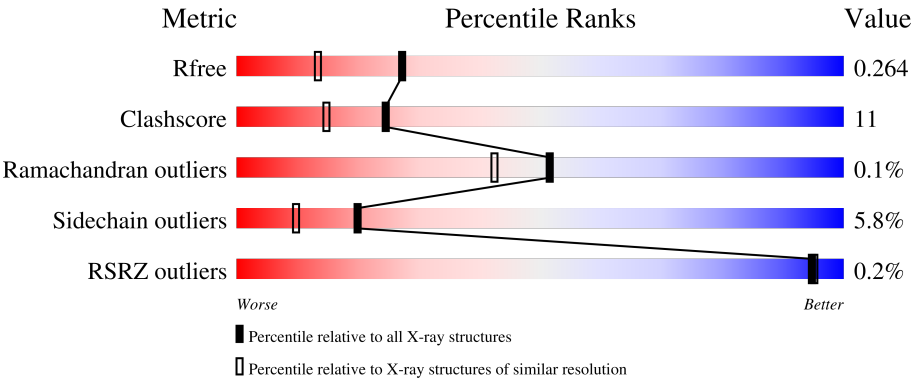
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 1.93 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	430	77% 19%
1	B	430	78% 18%
1	C	430	79% 16%
1	D	430	77% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FFQ	C	500	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13938 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 UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	5	0
			3123	1958	542	604	19			
1	B	419	Total	C	N	O	S	0	5	0
			3125	1958	544	604	19			
1	C	419	Total	C	N	O	S	0	8	0
			3142	1967	545	611	19			
1	D	419	Total	C	N	O	S	0	9	0
			3145	1973	544	609	19			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	TYR	SEE REMARK 999	UNP B5F9P4
A	423	LEU	-	expression tag	UNP B5F9P4
A	424	GLU	-	expression tag	UNP B5F9P4
A	425	HIS	-	expression tag	UNP B5F9P4
A	426	HIS	-	expression tag	UNP B5F9P4
A	427	HIS	-	expression tag	UNP B5F9P4
A	428	HIS	-	expression tag	UNP B5F9P4
A	429	HIS	-	expression tag	UNP B5F9P4
A	430	HIS	-	expression tag	UNP B5F9P4
B	2	ASP	TYR	SEE REMARK 999	UNP B5F9P4
B	423	LEU	-	expression tag	UNP B5F9P4
B	424	GLU	-	expression tag	UNP B5F9P4
B	425	HIS	-	expression tag	UNP B5F9P4
B	426	HIS	-	expression tag	UNP B5F9P4
B	427	HIS	-	expression tag	UNP B5F9P4
B	428	HIS	-	expression tag	UNP B5F9P4
B	429	HIS	-	expression tag	UNP B5F9P4
B	430	HIS	-	expression tag	UNP B5F9P4
C	2	ASP	TYR	SEE REMARK 999	UNP B5F9P4
C	423	LEU	-	expression tag	UNP B5F9P4
C	424	GLU	-	expression tag	UNP B5F9P4

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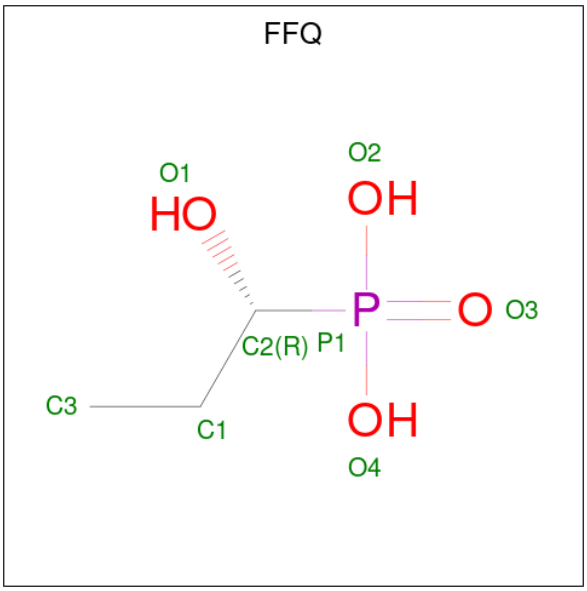
Chain	Residue	Modelled	Actual	Comment	Reference
C	425	HIS	-	expression tag	UNP B5F9P4
C	426	HIS	-	expression tag	UNP B5F9P4
C	427	HIS	-	expression tag	UNP B5F9P4
C	428	HIS	-	expression tag	UNP B5F9P4
C	429	HIS	-	expression tag	UNP B5F9P4
C	430	HIS	-	expression tag	UNP B5F9P4
D	2	ASP	TYR	SEE REMARK 999	UNP B5F9P4
D	423	LEU	-	expression tag	UNP B5F9P4
D	424	GLU	-	expression tag	UNP B5F9P4
D	425	HIS	-	expression tag	UNP B5F9P4
D	426	HIS	-	expression tag	UNP B5F9P4
D	427	HIS	-	expression tag	UNP B5F9P4
D	428	HIS	-	expression tag	UNP B5F9P4
D	429	HIS	-	expression tag	UNP B5F9P4
D	430	HIS	-	expression tag	UNP B5F9P4

- Molecule 2 is [(1R)-1-hydroxypropyl]phosphonic acid (three-letter code: FFQ) (formula: $C_3H_9O_4P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			8	3	4	1		
2	B	1	Total	C	O	P	0	0
			8	3	4	1		
2	C	1	Total	C	O	P	0	0
			8	3	4	1		

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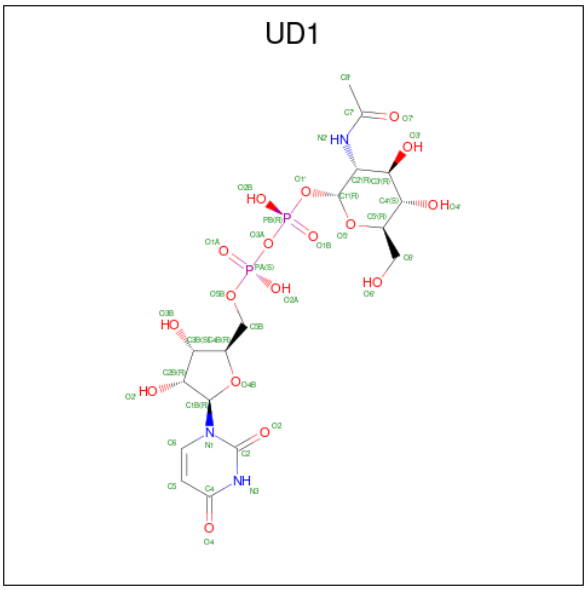
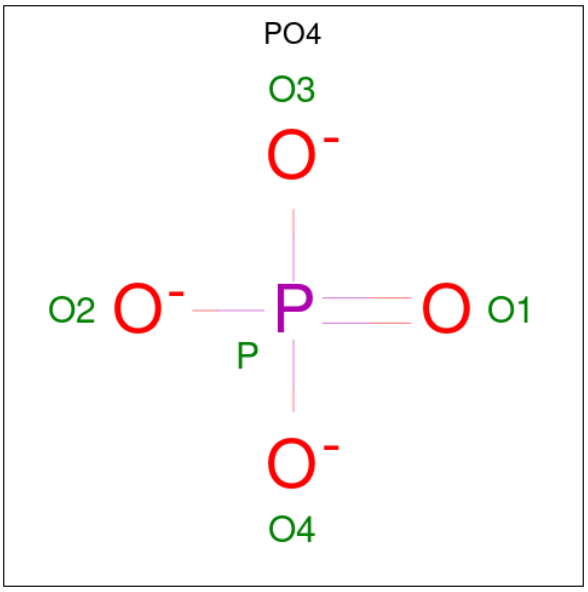
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O P 8 3 4 1	0	0

- Molecule 3 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



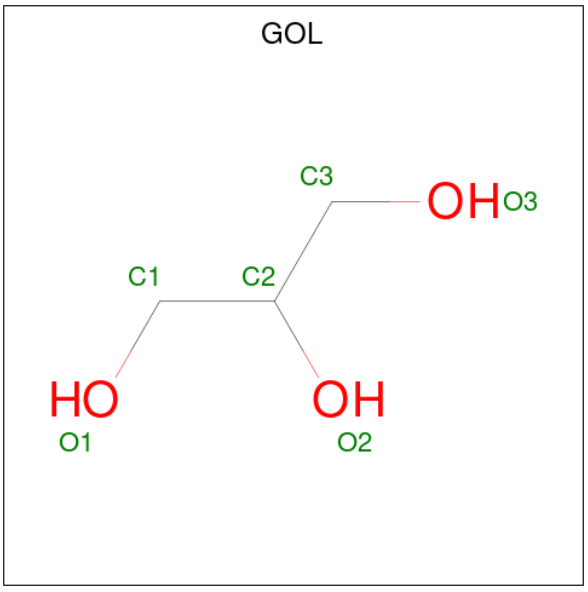
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 39 17 3 17 2	0	0
3	B	1	Total C N O P 39 17 3 17 2	0	0
3	C	1	Total C N O P 39 17 3 17 2	0	0
3	D	1	Total C N O P 39 17 3 17 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

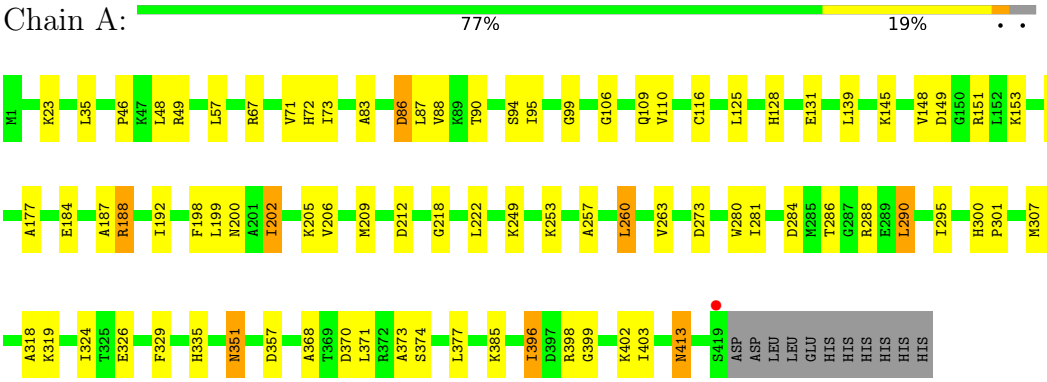
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	281	Total O 281 281	0	0
6	B	258	Total O 258 258	0	0
6	C	304	Total O 304 304	0	0
6	D	328	Total O 328 328	0	0

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.

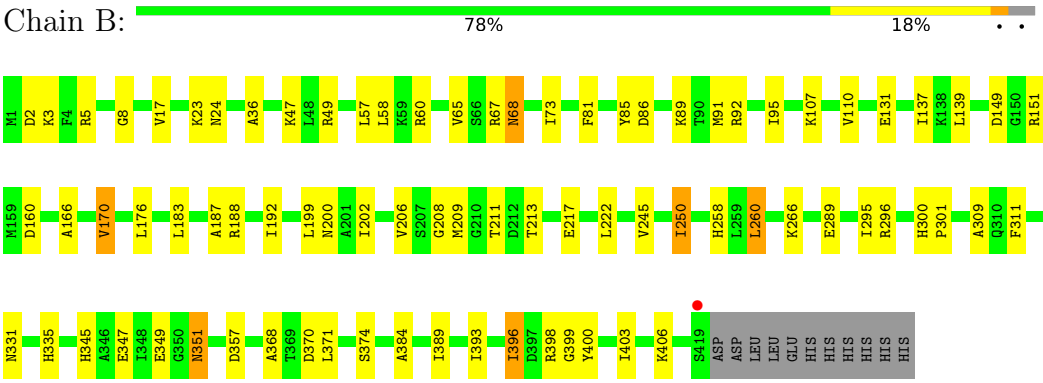
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain A:



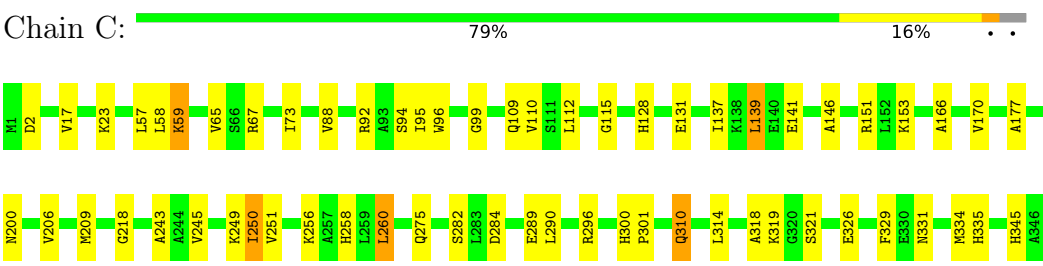
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain B:



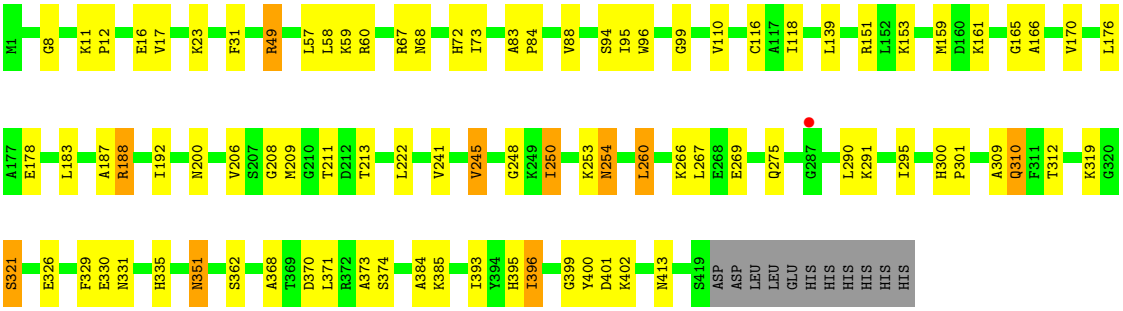
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain C:



• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.60Å 118.51Å 92.51Å 90.00° 116.48° 90.00°	Depositor
Resolution (Å)	27.90 – 1.93 27.90 – 1.93	Depositor EDS
% Data completeness (in resolution range)	96.9 (27.90-1.93) 96.9 (27.90-1.93)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.199 , 0.261 0.202 , 0.264	Depositor DCC
R_{free} test set	6151 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 26.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13938	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: GOL, UD1, PO4, FFQ

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	0.54	1/3180 (0.0%)	0.70	3/4305 (0.1%)
1	B	0.54	0/3183	0.68	1/4309 (0.0%)
1	C	0.54	1/3208 (0.0%)	0.67	1/4341 (0.0%)
1	D	0.53	1/3215 (0.0%)	0.65	1/4353 (0.0%)
All	All	0.54	3/12786 (0.0%)	0.68	6/17308 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	96	TRP	CD2-CE2	5.50	1.48	1.41
1	D	96	TRP	CD2-CE2	5.34	1.47	1.41
1	A	280	TRP	CD2-CE2	5.04	1.47	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	LEU	CA-CB-CG	7.61	132.79	115.30
1	B	260	LEU	CA-CB-CG	7.00	131.39	115.30
1	C	260	LEU	CA-CB-CG	6.95	131.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	260	LEU	CA-CB-CG	6.86	131.08	115.30
1	A	151	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	151	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	ARG	Peptide
1	C	67	ARG	Peptide
1	D	67	ARG	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	3123	0	3185	79	0
1	B	3125	0	3181	62	0
1	C	3142	0	3199	69	0
1	D	3145	0	3209	74	0
2	A	8	0	6	1	0
2	B	8	0	6	1	0
2	C	8	0	6	1	0
2	D	8	0	6	0	0
3	A	39	0	25	0	0
3	B	39	0	25	0	0
3	C	39	0	25	0	0
3	D	39	0	25	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	1	0
6	A	281	0	0	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	258	0	0	8	0
6	C	304	0	0	25	0
6	D	328	0	0	26	0
All	All	13938	0	12930	281	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 11.

All (281) 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:A:212:ASP:HB3	6:A:832:HOH:O	1.29	1.24
1:A:286:THR:HG22	6:A:801:HOH:O	1.36	1.23
1:A:184:GLU:HG3	6:A:859:HOH:O	1.49	1.13
1:A:202:ILE:HB	6:A:847:HOH:O	1.49	1.11
1:B:199:LEU:O	1:B:202:ILE:HG22	1.55	1.06
1:A:374:SER:HB3	1:A:396[B]:ILE:HG12	1.38	1.05
1:B:208:GLY:O	1:B:211:THR:HG22	1.59	1.00
1:A:310:GLN:H	1:A:310:GLN:HE21	1.03	0.98
1:C:73:ILE:CG1	6:C:738:HOH:O	2.10	0.98
1:D:200:ASN:HD21	1:D:206:VAL:H	1.11	0.98
1:C:310:GLN:H	1:C:310:GLN:HE21	0.99	0.98
1:D:351:ASN:H	1:D:351:ASN:HD22	1.06	0.96
1:C:351:ASN:HD22	1:C:351:ASN:H	1.11	0.96
1:D:310:GLN:H	1:D:310:GLN:HE21	1.05	0.95
1:B:200:ASN:HD21	1:B:206:VAL:H	1.11	0.95
1:A:351:ASN:H	1:A:351:ASN:HD22	1.08	0.94
1:B:368:ALA:HB1	1:B:374:SER:OG	1.69	0.93
1:D:241:VAL:HG23	6:D:924:HOH:O	1.68	0.93
1:C:365:GLN:HB3	6:C:620:HOH:O	1.69	0.91
1:C:73:ILE:HG12	6:C:738:HOH:O	1.66	0.91
1:C:200:ASN:HD21	1:C:206:VAL:H	1.14	0.90
1:D:211[A]:THR:HG21	6:D:848:HOH:O	1.73	0.88
1:D:393:ILE:O	1:D:396:ILE:HG22	1.72	0.88
1:A:200:ASN:HD21	1:A:206:VAL:H	1.24	0.85
1:A:368:ALA:HB1	1:A:374:SER:OG	1.77	0.85
1:C:331:ASN:ND2	6:C:633:HOH:O	2.10	0.83
1:B:211:THR:HG23	1:B:213:THR:H	1.42	0.83
1:C:73:ILE:HG13	6:C:738:HOH:O	1.76	0.82
1:C:151:ARG:HD3	6:C:869:HOH:O	1.80	0.81
1:A:88:VAL:HG22	1:A:94[A]:SER:OG	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:GLN:H	1:C:310:GLN:NE2	1.80	0.79
1:C:351:ASN:HD22	1:C:351:ASN:N	1.78	0.79
1:A:374:SER:HB3	1:A:396[B]:ILE:CG1	2.13	0.79
1:A:374:SER:CB	1:A:396[B]:ILE:HG12	2.14	0.77
1:D:211[A]:THR:HG23	1:D:213:THR:H	1.49	0.77
1:B:188:ARG:HH12	1:D:188:ARG:CZ	1.97	0.77
1:D:245:VAL:HB	6:D:923:HOH:O	1.84	0.77
1:A:311:PHE:HD1	6:A:772:HOH:O	1.70	0.75
1:C:351:ASN:H	1:C:351:ASN:ND2	1.86	0.74
1:A:145:LYS:HE2	6:A:881:HOH:O	1.86	0.74
1:D:208:GLY:O	1:D:211[A]:THR:HG22	1.88	0.73
1:B:36:ALA:HB2	1:B:202:ILE:HD11	1.71	0.73
1:A:310:GLN:HB2	6:A:772:HOH:O	1.87	0.73
1:D:310:GLN:HE21	1:D:310:GLN:N	1.83	0.72
1:A:99:GLY:HA3	6:A:880:HOH:O	1.87	0.72
1:D:395:HIS:HD2	6:D:871:HOH:O	1.71	0.72
1:C:112:LEU:HB3	6:C:602:HOH:O	1.88	0.71
1:A:95:ILE:HA	1:A:110[A]:VAL:HG11	1.73	0.71
1:D:368:ALA:HB1	1:D:374:SER:OG	1.92	0.70
1:A:83:ALA:HB3	1:A:110[B]:VAL:HG23	1.74	0.69
1:C:112:LEU:CB	6:C:602:HOH:O	2.39	0.69
1:A:351:ASN:H	1:A:351:ASN:ND2	1.87	0.69
6:C:855:HOH:O	1:D:331:ASN:HB2	1.91	0.69
1:D:151:ARG:HD3	6:D:884:HOH:O	1.93	0.68
1:D:275:GLN:HG2	6:D:881:HOH:O	1.92	0.68
1:C:17:VAL:HG12	1:C:250:ILE:HD11	1.76	0.68
1:B:17:VAL:HG12	1:B:250:ILE:HD11	1.75	0.67
1:D:17:VAL:HG12	1:D:250:ILE:HD11	1.76	0.67
1:D:310:GLN:H	1:D:310:GLN:NE2	1.87	0.67
1:D:351:ASN:H	1:D:351:ASN:ND2	1.86	0.67
1:A:368:ALA:CB	1:A:374:SER:OG	2.43	0.66
1:C:256:LYS:HD3	1:C:258:HIS:CE1	2.30	0.66
1:B:151:ARG:HD2	1:B:176:LEU:O	1.95	0.66
1:A:109:GLN:HG2	1:A:145:LYS:HG2	1.78	0.66
1:A:310:GLN:HE21	1:A:310:GLN:N	1.85	0.66
1:D:319:LYS:NZ	6:D:768:HOH:O	2.11	0.66
1:B:370:ASP:OD1	6:B:825:HOH:O	2.14	0.65
1:C:139:LEU:HD21	6:C:602:HOH:O	1.95	0.65
1:B:351:ASN:HD22	1:B:351:ASN:H	1.42	0.65
1:D:88:VAL:HG22	1:D:94[A]:SER:OG	1.96	0.65
1:D:326:GLU:HG3	1:D:329:PHE:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:GLU:HG3	1:B:329:PHE:O	1.98	0.64
1:A:95:ILE:HA	1:A:110[B]:VAL:HG21	1.80	0.64
1:D:371:LEU:HD21	1:D:399:GLY:HA3	1.80	0.64
1:D:396:ILE:HD13	1:D:400:TYR:HB2	1.81	0.63
1:B:47:LYS:HE3	6:B:845:HOH:O	1.97	0.63
1:D:16:GLU:OE1	1:D:253:LYS:HE3	1.99	0.62
1:C:310:GLN:HE21	1:C:310:GLN:N	1.84	0.62
1:A:290:LEU:HD13	1:A:318:ALA:HB2	1.81	0.62
1:B:170:VAL:HG21	1:B:183:LEU:HD13	1.81	0.62
1:D:275:GLN:NE2	6:D:881:HOH:O	2.32	0.62
1:C:335:HIS:HB3	1:C:373:ALA:HB1	1.83	0.61
6:A:721:HOH:O	1:B:331:ASN:HB2	1.99	0.61
1:D:151:ARG:CD	6:D:884:HOH:O	2.48	0.61
1:B:200:ASN:ND2	1:B:206:VAL:H	1.92	0.61
1:C:334:MET:HG3	6:C:633:HOH:O	2.01	0.60
1:A:198:PHE:O	1:A:202:ILE:HG22	2.01	0.60
1:A:351:ASN:HD22	1:A:351:ASN:N	1.88	0.60
1:A:357:ASP:OD1	6:A:802:HOH:O	2.16	0.60
1:D:245:VAL:CB	6:D:923:HOH:O	2.47	0.60
1:A:49:ARG:HG3	1:A:398:ARG:HG2	1.83	0.59
1:C:371:LEU:HD21	1:C:399:GLY:HA3	1.83	0.59
1:A:326:GLU:HG3	1:A:329:PHE:O	2.02	0.59
1:D:395:HIS:CD2	6:D:871:HOH:O	2.51	0.58
1:A:273:ASP:HB2	1:A:288:ARG:HH22	1.69	0.57
1:D:241:VAL:CG2	6:D:924:HOH:O	2.40	0.57
1:A:187:ALA:HB3	1:A:192:ILE:CD1	2.34	0.57
6:B:705:HOH:O	1:D:295:ILE:HG12	2.04	0.57
1:A:165:GLY:HA3	5:A:503:GOL:O1	2.05	0.57
1:A:263:VAL:HG23	6:A:704:HOH:O	2.03	0.57
1:C:345:HIS:HD2	1:C:357:ASP:O	1.88	0.57
1:C:88:VAL:HG13	6:C:717:HOH:O	2.04	0.56
1:B:188:ARG:NH1	1:D:188:ARG:CZ	2.68	0.56
1:B:349:GLU:HG3	6:C:605:HOH:O	2.06	0.56
1:D:351:ASN:HD22	1:D:351:ASN:N	1.85	0.55
1:B:345:HIS:HD2	1:B:357:ASP:O	1.88	0.55
1:C:395:HIS:HD2	6:C:899:HOH:O	1.87	0.55
1:B:2:ASP:HB3	1:B:393:ILE:HD11	1.88	0.55
1:C:170:VAL:HG22	1:C:183:LEU:HD22	1.88	0.55
1:A:284:ASP:OD1	1:A:286:THR:HG23	2.07	0.55
1:A:187:ALA:HB3	1:A:192:ILE:HD13	1.89	0.54
1:C:58:LEU:HD13	1:C:73:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:VAL:HG22	1:B:183:LEU:HD22	1.88	0.54
1:A:202:ILE:HG12	1:A:222:LEU:HB3	1.90	0.54
1:A:371:LEU:CD1	1:A:399:GLY:HA3	2.37	0.54
1:C:413:ASN:C	1:C:413:ASN:HD22	2.11	0.54
1:C:88:VAL:HG22	1:C:94[A]:SER:OG	2.07	0.54
1:C:396:ILE:HD13	1:C:400:TYR:CD1	2.42	0.54
1:D:170:VAL:HG22	1:D:183:LEU:HD22	1.90	0.54
1:A:368:ALA:HB1	1:A:374:SER:HG	1.71	0.54
1:B:187:ALA:HB3	1:B:192:ILE:CD1	2.38	0.54
1:A:371:LEU:HD11	1:A:399:GLY:HA3	1.90	0.53
1:C:141:GLU:HG2	6:D:912:HOH:O	2.07	0.53
1:A:413:ASN:C	1:A:413:ASN:HD22	2.10	0.53
1:B:5:ARG:HG3	1:B:389:ILE:CD1	2.39	0.53
1:D:267:LEU:HD21	6:D:924:HOH:O	2.07	0.53
1:D:11:LYS:HE3	6:D:897:HOH:O	2.08	0.53
1:D:187:ALA:HB3	1:D:192:ILE:CD1	2.39	0.53
1:D:72:HIS:HE1	6:D:779:HOH:O	1.92	0.52
1:B:95:ILE:HA	1:B:110:VAL:HG11	1.91	0.52
1:D:321:SER:OG	6:D:833:HOH:O	2.18	0.52
1:D:335:HIS:HB3	1:D:373:ALA:HB1	1.90	0.52
1:C:128:HIS:HD2	1:C:131:GLU:OE1	1.93	0.52
1:D:99:GLY:HA3	6:D:841:HOH:O	2.07	0.52
1:C:170:VAL:HG21	1:C:183:LEU:HD13	1.92	0.52
1:A:273:ASP:HB2	1:A:288:ARG:NH2	2.24	0.52
1:A:35:LEU:HB3	1:A:222:LEU:HD12	1.91	0.51
1:D:153:LYS:NZ	1:D:178:GLU:OE1	2.43	0.51
1:C:95:ILE:HA	1:C:110:VAL:HG11	1.92	0.51
1:B:17:VAL:CG2	1:B:406:LYS:HD3	2.40	0.51
1:B:67:ARG:O	1:B:68:ASN:HB2	2.10	0.51
1:B:158:VAL:HG12	6:B:607:HOH:O	2.10	0.51
6:B:705:HOH:O	1:D:266:LYS:HG3	2.09	0.51
1:B:188:ARG:HH12	1:D:188:ARG:NH2	2.08	0.51
1:D:326:GLU:CG	1:D:329:PHE:O	2.58	0.51
1:D:401:ASP:OD1	1:D:402:LYS:HD2	2.10	0.51
1:B:166:ALA:O	1:B:170:VAL:HG13	2.11	0.50
1:B:258:HIS:CE1	6:B:832:HOH:O	2.64	0.50
1:D:58:LEU:HD13	1:D:73:ILE:HD12	1.93	0.50
1:A:128:HIS:HD2	1:A:131:GLU:OE1	1.94	0.50
1:A:300:HIS:CG	1:A:301:PRO:HA	2.46	0.50
1:B:58:LEU:HD13	1:B:73:ILE:HD12	1.94	0.50
1:B:85:TYR:CE2	1:B:89:LYS:HE3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:ILE:O	1:C:396:ILE:HG22	2.11	0.50
1:B:309:ALA:HA	1:B:335:HIS:CE1	2.46	0.50
1:D:373:ALA:HB2	6:D:714:HOH:O	2.11	0.50
1:A:205:LYS:HE2	6:A:837:HOH:O	2.11	0.50
1:B:295:ILE:HD11	1:B:311:PHE:CD2	2.47	0.50
1:A:253:LYS:HD2	6:A:653:HOH:O	2.10	0.49
1:A:335:HIS:CD2	1:A:335:HIS:H	2.29	0.49
1:A:373:ALA:O	1:A:377:LEU:HG	2.11	0.49
1:A:307:MET:HE3	6:A:772:HOH:O	2.12	0.49
1:C:256:LYS:HD3	1:C:258:HIS:HE1	1.76	0.49
1:A:71:VAL:HG12	1:A:73:ILE:HD11	1.95	0.49
1:A:86:ASP:O	1:A:90:THR:HG23	2.12	0.49
1:C:326:GLU:HG3	1:C:329:PHE:O	2.12	0.49
1:A:199:LEU:HA	1:A:202:ILE:CG2	2.43	0.48
1:D:396:ILE:CD1	1:D:400:TYR:HB2	2.42	0.48
1:A:310:GLN:H	1:A:310:GLN:NE2	1.88	0.48
1:C:166:ALA:O	1:C:170:VAL:HG13	2.13	0.48
1:A:177:ALA:O	1:A:218:GLY:HA3	2.13	0.48
1:A:188:ARG:NH1	6:A:656:HOH:O	2.44	0.48
1:D:396:ILE:HB	6:D:921:HOH:O	2.13	0.48
1:A:23:LYS:HB2	1:A:48:LEU:HD11	1.95	0.48
1:B:368:ALA:CB	1:B:374:SER:OG	2.53	0.48
1:C:112:LEU:HB2	6:C:602:HOH:O	2.09	0.48
1:A:295:ILE:HD11	1:A:311:PHE:CD2	2.49	0.47
1:C:290:LEU:HG	1:C:318:ALA:HB2	1.96	0.47
1:D:159:MET:HG2	1:D:183:LEU:HD11	1.96	0.47
1:C:92:ARG:O	1:C:95:ILE:HG22	2.14	0.47
1:D:245:VAL:CG2	6:D:923:HOH:O	2.63	0.47
1:B:396:ILE:HD12	1:B:403:ILE:HG21	1.95	0.47
1:B:86:ASP:HA	1:B:89:LYS:NZ	2.30	0.47
1:B:371:LEU:HD21	1:B:399:GLY:HA3	1.96	0.47
1:B:3:LYS:NZ	6:B:734:HOH:O	2.41	0.46
1:D:8:GLY:HA3	1:D:384:ALA:O	2.15	0.46
1:C:392:ARG:HD2	6:C:778:HOH:O	2.15	0.46
1:B:200:ASN:HD21	1:B:206:VAL:N	1.94	0.46
1:C:59:LYS:HD2	1:C:65:VAL:HB	1.98	0.46
1:D:166:ALA:O	1:D:170:VAL:HG13	2.15	0.46
1:A:307:MET:CE	6:A:772:HOH:O	2.63	0.46
1:D:83:ALA:HB3	1:D:110[A]:VAL:HG12	1.96	0.46
1:B:8:GLY:HA3	1:B:384:ALA:O	2.15	0.46
1:B:92:ARG:HG2	6:B:831:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:GLU:CG	1:B:329:PHE:O	2.64	0.45
1:B:345:HIS:CD2	1:B:357:ASP:O	2.69	0.45
1:B:65:VAL:HG13	1:B:73:ILE:HD13	1.99	0.45
1:C:115:GLY:HA3	6:D:820:HOH:O	2.17	0.45
1:A:257:ALA:HA	1:A:281:ILE:HD11	1.97	0.45
1:C:23:LYS:HE2	6:C:895:HOH:O	2.15	0.45
1:C:335:HIS:CD2	1:C:335:HIS:H	2.35	0.45
1:C:275:GLN:NE2	6:C:795:HOH:O	2.50	0.45
1:A:159:MET:HE3	6:A:633:HOH:O	2.17	0.45
1:A:249:LYS:HD2	6:A:798:HOH:O	2.17	0.45
1:B:81:PHE:CE2	1:B:107:LYS:HE3	2.51	0.45
1:C:88:VAL:CG1	6:C:717:HOH:O	2.62	0.45
1:B:396:ILE:HD13	1:B:400:TYR:HB2	1.99	0.45
1:A:309:ALA:HA	1:A:335:HIS:CE1	2.52	0.44
1:B:393:ILE:O	1:B:396:ILE:HG22	2.17	0.44
1:D:385:LYS:HD2	1:D:385:LYS:HA	1.81	0.44
1:B:371:LEU:CD2	1:B:399:GLY:HA3	2.47	0.44
1:A:23:LYS:HB2	1:A:48:LEU:CD1	2.47	0.44
1:B:23:LYS:NZ	1:B:24:ASN:OD1	2.46	0.44
1:C:243:ALA:HB2	1:C:250:ILE:CG2	2.48	0.44
1:C:249:LYS:HD2	1:C:284:ASP:CG	2.38	0.44
1:D:254:ASN:N	1:D:254:ASN:HD22	2.14	0.44
1:D:330:GLU:HG3	6:D:628:HOH:O	2.17	0.44
1:D:213:THR:HG23	6:D:766:HOH:O	2.17	0.44
2:B:500:FFQ:O4	2:B:500:FFQ:H3	2.17	0.44
1:C:99:GLY:HA3	6:C:799:HOH:O	2.16	0.44
1:C:296[A]:ARG:NH1	6:C:824:HOH:O	2.50	0.44
1:A:319:LYS:HE2	6:A:843:HOH:O	2.17	0.44
1:C:319:LYS:HA	1:C:319:LYS:HD3	1.82	0.44
1:D:165:GLY:HA3	5:D:503:GOL:O1	2.17	0.44
1:A:72:HIS:HD2	6:A:661:HOH:O	2.00	0.44
1:A:308:GLN:HG2	1:A:324:ILE:HG21	2.00	0.44
1:C:177:ALA:O	1:C:218:GLY:HA3	2.18	0.44
1:C:300:HIS:CG	1:C:301:PRO:HA	2.53	0.44
1:C:335:HIS:HD2	6:C:762:HOH:O	2.00	0.43
1:C:58:LEU:CD1	1:C:73:ILE:HD12	2.49	0.43
1:D:49:ARG:HB2	6:D:604:HOH:O	2.18	0.43
1:D:245:VAL:HG23	6:D:923:HOH:O	2.17	0.43
1:A:188:ARG:HH12	1:C:188:ARG:NH2	2.16	0.43
1:D:266:LYS:HD3	1:D:266:LYS:HA	1.76	0.43
1:C:137:ILE:HG12	1:C:146:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HD21	1:A:160:ASP:HB2	2.01	0.43
1:C:396:ILE:CD1	1:C:400:TYR:CD1	3.02	0.43
1:A:188:ARG:CZ	6:A:656:HOH:O	2.67	0.43
1:C:335:HIS:HB3	1:C:373:ALA:CB	2.49	0.43
1:B:266:LYS:HD3	1:B:266:LYS:HA	1.83	0.42
2:C:500:FFQ:H3	6:C:859:HOH:O	2.18	0.42
1:D:23:LYS:HD2	1:D:399:GLY:HA2	2.01	0.42
1:B:131:GLU:HG3	1:B:137:ILE:HD12	2.02	0.42
1:B:202:ILE:HG21	1:B:202:ILE:HD13	1.81	0.42
1:B:202:ILE:HG23	1:B:222:LEU:HD22	2.00	0.42
1:A:202:ILE:HD13	1:A:202:ILE:HG21	1.66	0.42
1:A:109:GLN:CG	1:A:145:LYS:HG2	2.47	0.42
1:B:351:ASN:HD22	1:B:351:ASN:N	2.14	0.42
1:D:300:HIS:CG	1:D:301:PRO:HA	2.54	0.42
1:A:396[A]:ILE:HD12	1:A:403:ILE:HG21	2.01	0.42
1:D:12:PRO:HB3	1:D:248:GLY:HA2	2.01	0.42
1:A:295:ILE:HD11	1:A:311:PHE:HD2	1.85	0.42
1:C:128:HIS:CE1	6:C:888:HOH:O	2.72	0.42
1:D:335:HIS:CD2	1:D:335:HIS:H	2.36	0.42
1:B:86:ASP:HA	1:B:89:LYS:HZ1	1.85	0.42
1:C:251:VAL:HG22	1:C:282:SER:HB3	2.02	0.42
1:B:335:HIS:H	1:B:335:HIS:CD2	2.38	0.41
1:B:91:MET:O	1:B:91:MET:HG3	2.20	0.41
1:C:314:LEU:C	1:C:314:LEU:HD23	2.40	0.41
1:A:311:PHE:CD1	6:A:772:HOH:O	2.55	0.41
1:C:326:GLU:CG	1:C:329:PHE:O	2.69	0.41
1:A:49:ARG:HG2	1:A:398:ARG:HA	2.01	0.41
1:D:49:ARG:H	1:D:49:ARG:HG2	1.77	0.41
1:A:116:CYS:HB2	2:A:500:FFQ:H20	1.90	0.41
1:D:60:ARG:NH2	1:D:84:PRO:HG2	2.36	0.41
1:D:309:ALA:O	1:D:312:THR:HB	2.19	0.41
1:B:49:ARG:HG2	1:B:398:ARG:HA	2.02	0.41
1:C:243:ALA:CB	1:C:250:ILE:HG22	2.50	0.41
1:C:345:HIS:CD2	1:C:357:ASP:O	2.70	0.41
1:A:106:GLY:HA2	1:A:148:VAL:HG12	2.03	0.41
1:B:296:ARG:HD2	1:D:161:LYS:HE3	2.03	0.41
1:C:243:ALA:HB2	1:C:250:ILE:HG22	2.02	0.41
1:D:116:CYS:SG	1:D:118:ILE:HG12	2.61	0.41
1:C:2:ASP:HB3	1:C:393:ILE:HD11	2.03	0.41
1:C:347:GLU:HG3	6:C:637:HOH:O	2.20	0.41
1:A:46:PRO:HB2	1:A:48:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:PHE:HE1	1:D:57:LEU:HD12	1.86	0.40
1:A:87:LEU:HD23	1:A:87:LEU:HA	1.74	0.40
1:B:17:VAL:HG23	1:B:406:LYS:HD3	2.03	0.40
1:B:300:HIS:CG	1:B:301:PRO:HA	2.56	0.40
1:D:176:LEU:HD21	1:D:222:LEU:HG	2.03	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	422/430 (98%)	415 (98%)	7 (2%)	0	100	100
1	B	422/430 (98%)	412 (98%)	9 (2%)	1 (0%)	47	38
1	C	425/430 (99%)	415 (98%)	10 (2%)	0	100	100
1	D	426/430 (99%)	417 (98%)	8 (2%)	1 (0%)	47	38
All	All	1695/1720 (98%)	1659 (98%)	34 (2%)	2 (0%)	51	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	ASN
1	D	68	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	330/336 (98%)	312 (94%)	18 (6%)	21 11
1	B	330/336 (98%)	313 (95%)	17 (5%)	23 13
1	C	333/336 (99%)	311 (93%)	22 (7%)	16 7
1	D	334/336 (99%)	314 (94%)	20 (6%)	19 9
All	All	1327/1344 (99%)	1250 (94%)	77 (6%)	20 10

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	86	ASP
1	A	139	LEU
1	A	149	ASP
1	A	153	LYS
1	A	188	ARG
1	A	202	ILE
1	A	209	MET
1	A	260	LEU
1	A	290	LEU
1	A	310	GLN
1	A	351	ASN
1	A	370	ASP
1	A	385	LYS
1	A	396[A]	ILE
1	A	396[B]	ILE
1	A	402	LYS
1	A	413	ASN
1	B	57	LEU
1	B	60	ARG
1	B	139	LEU
1	B	149	ASP
1	B	153	LYS
1	B	160	ASP
1	B	170	VAL
1	B	209	MET
1	B	217	GLU
1	B	245	VAL
1	B	250	ILE
1	B	260	LEU
1	B	289	GLU

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Mol	Chain	Res	Type
1	B	326	GLU
1	B	347	GLU
1	B	351	ASN
1	B	396	ILE
1	C	57	LEU
1	C	59	LYS
1	C	109	GLN
1	C	139	LEU
1	C	153	LYS
1	C	188	ARG
1	C	209	MET
1	C	245	VAL
1	C	250	ILE
1	C	260	LEU
1	C	289	GLU
1	C	310	GLN
1	C	321	SER
1	C	347	GLU
1	C	349[A]	GLU
1	C	349[B]	GLU
1	C	351	ASN
1	C	362	SER
1	C	370	ASP
1	C	396	ILE
1	C	402	LYS
1	C	413	ASN
1	D	49	ARG
1	D	59	LYS
1	D	95	ILE
1	D	139	LEU
1	D	188	ARG
1	D	209	MET
1	D	245	VAL
1	D	250	ILE
1	D	254	ASN
1	D	260	LEU
1	D	269	GLU
1	D	290	LEU
1	D	291	LYS
1	D	310	GLN
1	D	321	SER
1	D	351	ASN

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Mol	Chain	Res	Type
1	D	362	SER
1	D	370	ASP
1	D	396	ILE
1	D	413	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	200	ASN
1	A	254	ASN
1	A	308	GLN
1	A	310	GLN
1	A	335	HIS
1	A	345	HIS
1	A	351	ASN
1	A	395	HIS
1	A	413	ASN
1	B	109	GLN
1	B	132	GLN
1	B	200	ASN
1	B	254	ASN
1	B	308	GLN
1	B	335	HIS
1	B	345	HIS
1	B	351	ASN
1	B	365	GLN
1	C	72	HIS
1	C	128	HIS
1	C	200	ASN
1	C	254	ASN
1	C	275	GLN
1	C	308	GLN
1	C	310	GLN
1	C	331	ASN
1	C	335	HIS
1	C	345	HIS
1	C	351	ASN
1	C	413	ASN
1	D	72	HIS
1	D	200	ASN
1	D	254	ASN

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Mol	Chain	Res	Type
1	D	308	GLN
1	D	310	GLN
1	D	335	HIS
1	D	345	HIS
1	D	351	ASN
1	D	395	HIS
1	D	413	ASN
1	D	418	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)

16 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	FFQ	A	500	1	5,7,7	2.92	3 (60%)	7,10,10	0.94	0
5	GOL	D	503	-	5,5,5	0.35	0	5,5,5	0.75	0
2	FFQ	C	500	1	5,7,7	3.06	2 (40%)	7,10,10	1.72	2 (28%)
5	GOL	C	503	-	5,5,5	0.43	0	5,5,5	0.90	0
4	PO4	B	502	-	4,4,4	1.38	0	6,6,6	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FFQ	B	500	1	5,7,7	2.96	3 (60%)	7,10,10	1.32	2 (28%)
4	PO4	C	502	-	4,4,4	1.20	0	6,6,6	0.48	0
3	UD1	B	501	-	38,41,41	0.92	4 (10%)	57,62,62	1.37	5 (8%)
2	FFQ	D	500	1	5,7,7	2.93	2 (40%)	7,10,10	1.46	1 (14%)
5	GOL	A	503	-	5,5,5	0.25	0	5,5,5	0.95	0
5	GOL	B	503	-	5,5,5	0.28	0	5,5,5	0.81	0
4	PO4	D	502	-	4,4,4	1.26	0	6,6,6	0.85	0
4	PO4	A	502	-	4,4,4	1.12	0	6,6,6	0.39	0
3	UD1	C	501	-	38,41,41	0.82	1 (2%)	57,62,62	1.36	7 (12%)
3	UD1	D	501	-	38,41,41	0.92	1 (2%)	57,62,62	1.41	6 (10%)
3	UD1	A	501	-	38,41,41	0.88	3 (7%)	57,62,62	1.30	4 (7%)

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	FFQ	A	500	1	-	1/7/8/8	-
5	GOL	D	503	-	-	1/4/4/4	-
2	FFQ	C	500	1	-	6/7/8/8	-
5	GOL	C	503	-	-	1/4/4/4	-
2	FFQ	B	500	1	-	0/7/8/8	-
5	GOL	A	503	-	-	2/4/4/4	-
3	UD1	B	501	-	-	3/26/63/63	0/3/3/3
2	FFQ	D	500	1	-	6/7/8/8	-
5	GOL	B	503	-	-	2/4/4/4	-
3	UD1	C	501	-	-	3/26/63/63	0/3/3/3
3	UD1	D	501	-	-	3/26/63/63	0/3/3/3
3	UD1	A	501	-	-	4/26/63/63	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FFQ	P1-O2	4.68	1.62	1.54
2	C	500	FFQ	P1-O2	4.66	1.62	1.54
2	D	500	FFQ	P1-O4	4.60	1.62	1.54
2	C	500	FFQ	P1-O4	4.58	1.62	1.54
2	D	500	FFQ	P1-O2	4.52	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FFQ	P1-O4	4.46	1.61	1.54
2	B	500	FFQ	P1-O2	4.29	1.61	1.54
2	A	500	FFQ	P1-O4	4.04	1.61	1.54
3	D	501	UD1	C2-N1	2.81	1.43	1.38
3	B	501	UD1	C2-N1	2.61	1.42	1.38
3	B	501	UD1	C4-N3	-2.51	1.34	1.38
3	A	501	UD1	C2-N3	-2.33	1.33	1.38
2	B	500	FFQ	O1-C2	2.32	1.44	1.41
3	A	501	UD1	C4-N3	-2.24	1.34	1.38
3	B	501	UD1	C2-N3	-2.20	1.34	1.38
3	C	501	UD1	C2-N1	2.17	1.41	1.38
3	A	501	UD1	C6-C5	2.14	1.40	1.35
2	A	500	FFQ	O1-C2	2.05	1.44	1.41
3	B	501	UD1	C6-C5	2.00	1.39	1.35

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	UD1	C4-N3-C2	-4.72	120.35	126.58
3	D	501	UD1	C4-N3-C2	-4.72	120.36	126.58
3	D	501	UD1	N3-C2-N1	4.40	120.73	114.89
3	B	501	UD1	C4-N3-C2	-4.38	120.80	126.58
3	A	501	UD1	C5-C4-N3	4.25	121.19	114.84
3	B	501	UD1	N3-C2-N1	4.17	120.43	114.89
3	B	501	UD1	C5-C4-N3	4.04	120.89	114.84
3	A	501	UD1	C4-N3-C2	-3.93	121.40	126.58
3	C	501	UD1	C5-C4-N3	3.76	120.46	114.84
3	A	501	UD1	N3-C2-N1	3.67	119.77	114.89
3	C	501	UD1	N3-C2-N1	3.67	119.75	114.89
3	D	501	UD1	C5-C4-N3	3.63	120.26	114.84
3	D	501	UD1	O4-C4-C5	-3.55	118.92	125.16
3	C	501	UD1	O4-C4-C5	-3.41	119.17	125.16
2	C	500	FFQ	O3-P1-C2	-3.06	105.50	112.94
2	D	500	FFQ	O3-P1-C2	-3.05	105.52	112.94
3	C	501	UD1	PB-O3A-PA	-3.04	122.39	132.83
3	B	501	UD1	O4-C4-C5	-2.59	120.61	125.16
2	B	500	FFQ	O3-P1-C2	-2.43	107.03	112.94
3	A	501	UD1	O4-C4-C5	-2.42	120.91	125.16
3	D	501	UD1	O2-C2-N1	-2.32	119.71	122.79
3	C	501	UD1	O2-C2-N1	-2.31	119.71	122.79
3	C	501	UD1	C4'-C3'-C2'	-2.24	107.06	110.34
3	D	501	UD1	O2A-PA-O1A	2.19	123.06	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	FFQ	C3-C1-C2	-2.15	107.88	114.36
3	B	501	UD1	O2-C2-N3	-2.11	117.56	121.50
2	B	500	FFQ	O4-P1-O3	-2.04	108.32	113.45

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	FFQ	C3-C1-C2-O1
2	C	500	FFQ	C1-C2-P1-O2
2	C	500	FFQ	O1-C2-P1-O2
2	C	500	FFQ	C1-C2-P1-O3
2	C	500	FFQ	O1-C2-P1-O3
2	C	500	FFQ	C1-C2-P1-O4
2	C	500	FFQ	O1-C2-P1-O4
2	D	500	FFQ	C1-C2-P1-O2
2	D	500	FFQ	O1-C2-P1-O2
2	D	500	FFQ	C1-C2-P1-O3
2	D	500	FFQ	O1-C2-P1-O3
2	D	500	FFQ	C1-C2-P1-O4
2	D	500	FFQ	O1-C2-P1-O4
3	A	501	UD1	C5B-O5B-PA-O1A
3	A	501	UD1	C5B-O5B-PA-O2A
3	B	501	UD1	C5B-O5B-PA-O1A
3	B	501	UD1	C5B-O5B-PA-O2A
3	C	501	UD1	C5B-O5B-PA-O1A
3	C	501	UD1	C5B-O5B-PA-O2A
3	D	501	UD1	C5B-O5B-PA-O1A
3	D	501	UD1	C5B-O5B-PA-O2A
5	A	503	GOL	C1-C2-C3-O3
5	B	503	GOL	C1-C2-C3-O3
5	A	503	GOL	O2-C2-C3-O3
5	B	503	GOL	O2-C2-C3-O3
5	C	503	GOL	C1-C2-C3-O3
5	D	503	GOL	C1-C2-C3-O3
3	A	501	UD1	C5B-O5B-PA-O3A
3	B	501	UD1	C5B-O5B-PA-O3A
3	C	501	UD1	C5B-O5B-PA-O3A
3	D	501	UD1	C5B-O5B-PA-O3A
3	A	501	UD1	PB-O3A-PA-O2A

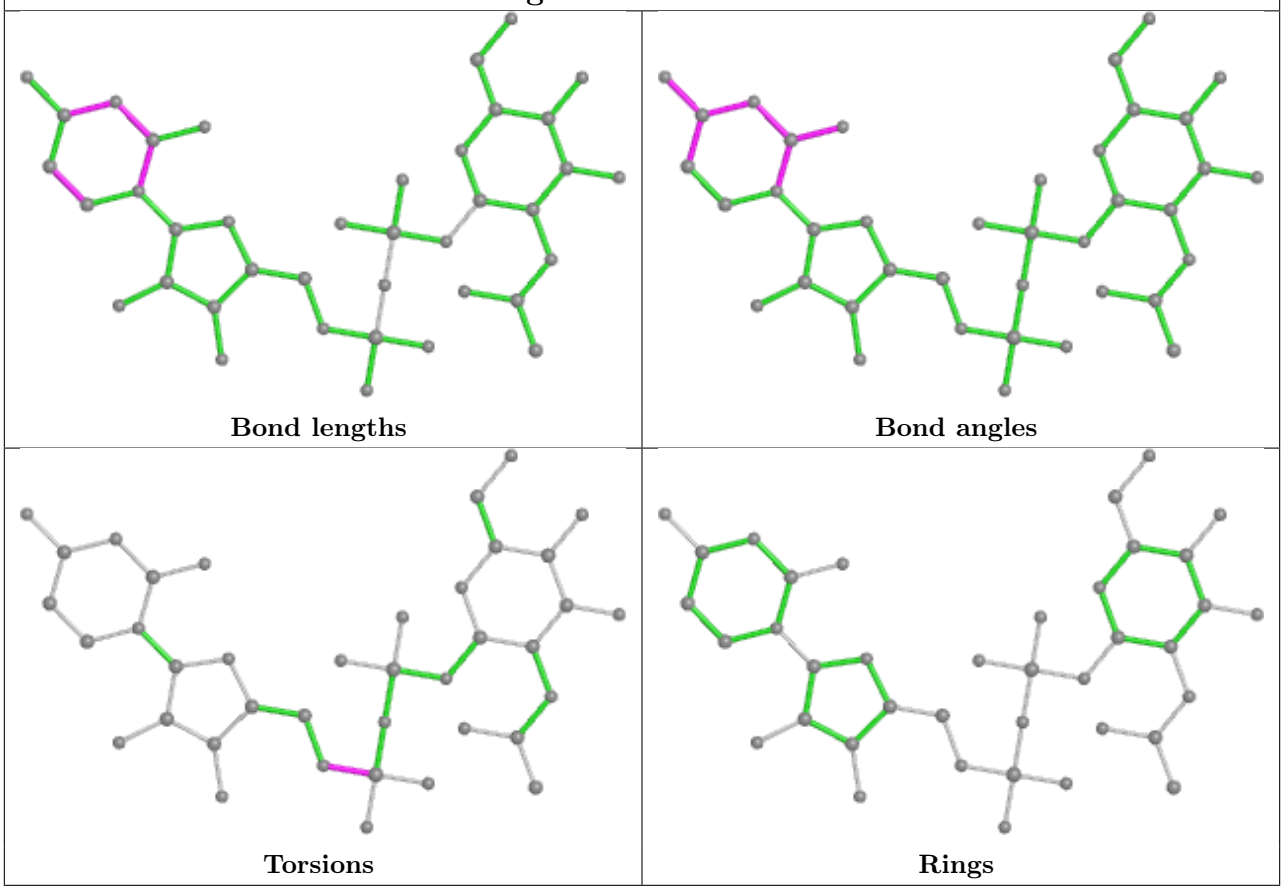
There are no ring outliers.

5 monomers are involved in 5 short contacts:

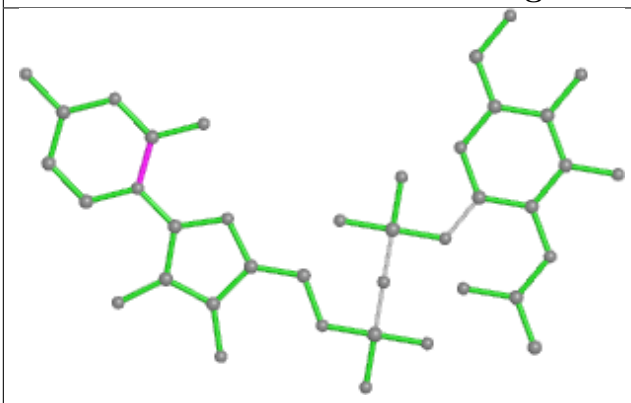
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	FFQ	1	0
5	D	503	GOL	1	0
2	C	500	FFQ	1	0
2	B	500	FFQ	1	0
5	A	503	GOL	1	0

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.

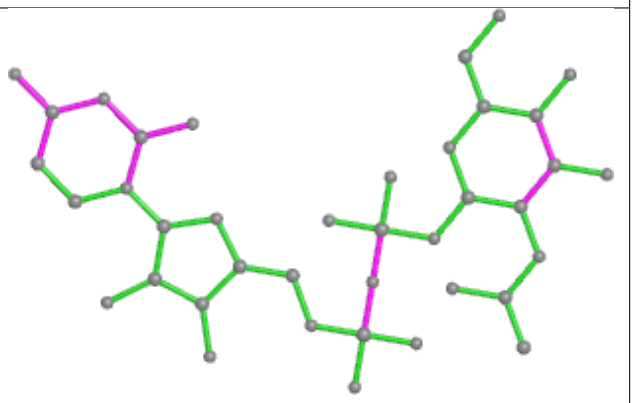
Ligand UD1 B 501



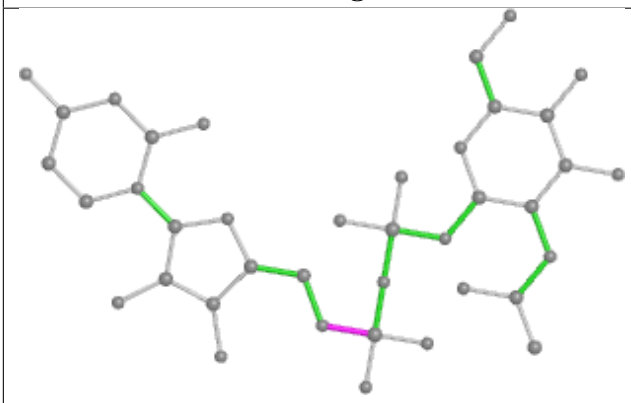
Ligand UD1 C 501



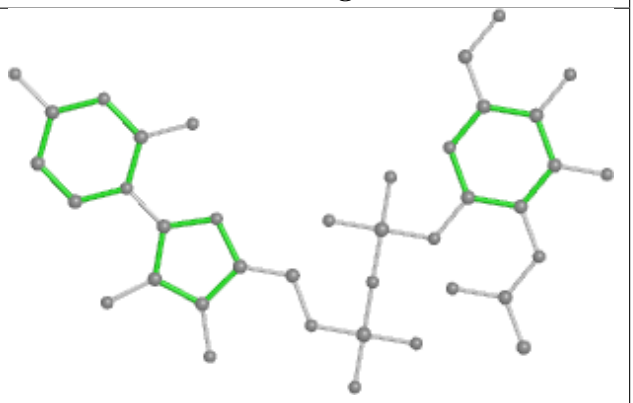
Bond lengths



Bond angles

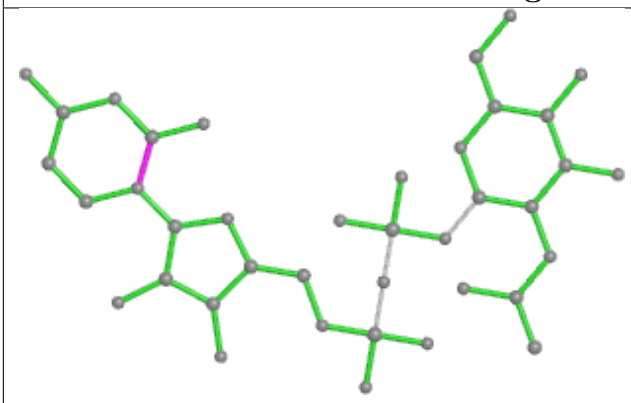


Torsions

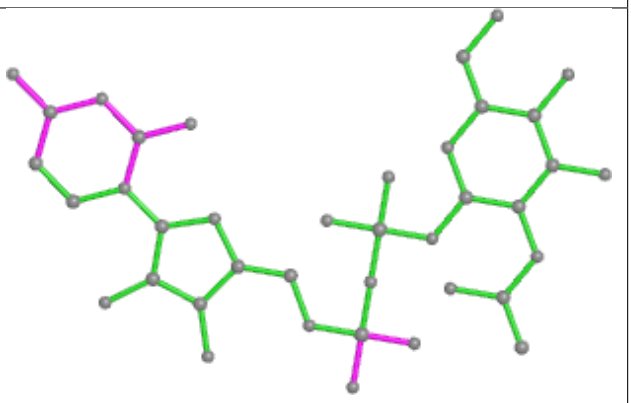


Rings

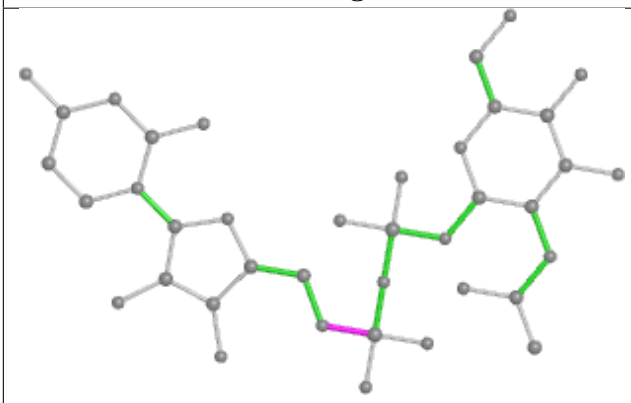
Ligand UD1 D 501



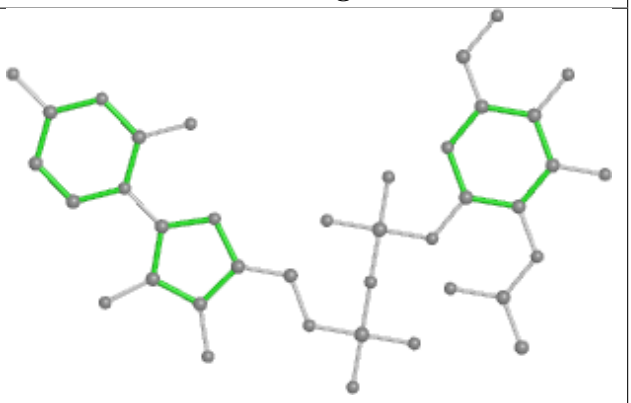
Bond lengths



Bond angles

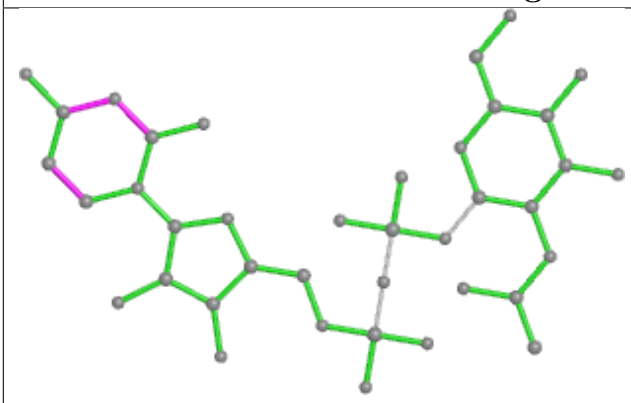


Torsions

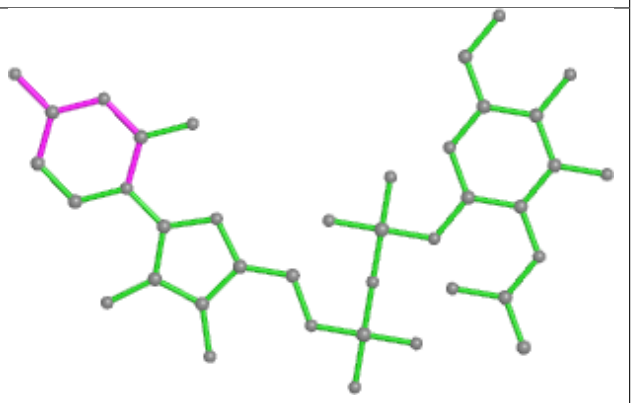


Rings

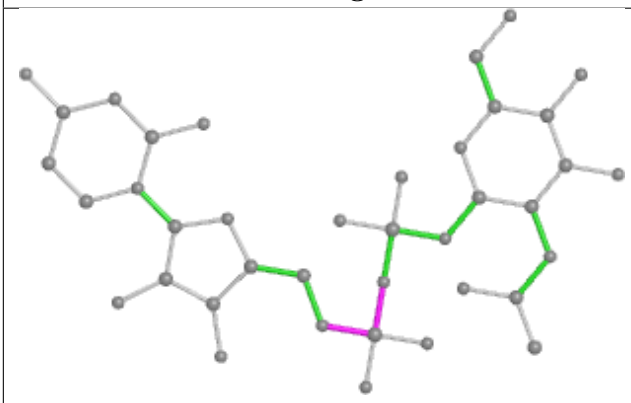
Ligand UD1 A 501



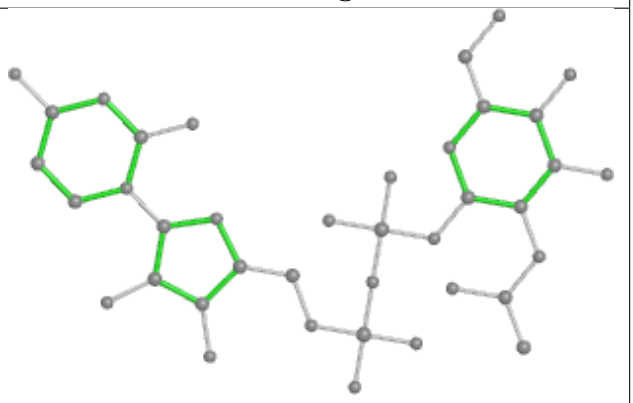
Bond lengths



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	419/430 (97%)	-0.53	1 (0%)	95	95	15, 23, 35, 59	0
1	B	419/430 (97%)	-0.49	1 (0%)	95	95	15, 25, 37, 58	0
1	C	419/430 (97%)	-0.52	0	100	100	15, 24, 35, 52	0
1	D	419/430 (97%)	-0.52	1 (0%)	95	95	14, 23, 34, 47	0
All	All	1676/1720 (97%)	-0.51	3 (0%)	95	95	14, 24, 35, 59	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	SER	3.1
1	B	419	SER	3.0
1	D	287	GLY	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

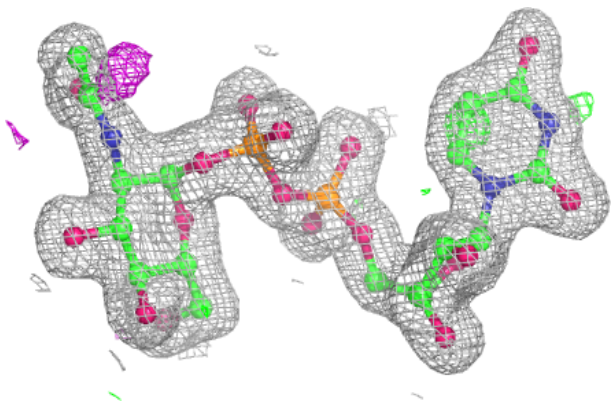
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

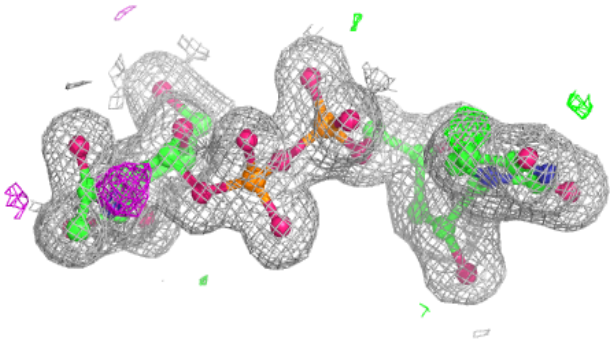
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FFQ	A	500	8/8	0.90	0.21	40,51,53,55	0
2	FFQ	C	500	8/8	0.90	0.14	37,47,51,52	0
2	FFQ	D	500	8/8	0.90	0.14	34,39,47,50	0
2	FFQ	B	500	8/8	0.91	0.16	35,46,51,52	0
5	GOL	B	503	6/6	0.95	0.10	22,24,26,28	0
5	GOL	A	503	6/6	0.96	0.10	22,23,24,25	0
5	GOL	C	503	6/6	0.96	0.09	23,24,25,25	0
5	GOL	D	503	6/6	0.96	0.09	21,22,22,22	0
4	PO4	C	502	5/5	0.98	0.11	29,29,32,32	0
4	PO4	D	502	5/5	0.98	0.11	28,30,32,34	0
3	UD1	A	501	39/39	0.98	0.08	15,19,21,24	0
3	UD1	B	501	39/39	0.98	0.07	17,19,24,26	0
3	UD1	C	501	39/39	0.98	0.07	19,20,22,23	0
3	UD1	D	501	39/39	0.98	0.07	16,19,22,24	0
4	PO4	A	502	5/5	0.99	0.11	30,33,37,37	0
4	PO4	B	502	5/5	0.99	0.09	27,31,33,35	0

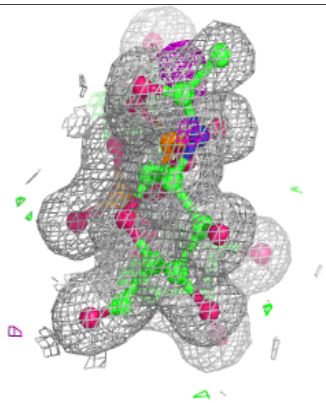
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UD1 A 501:

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

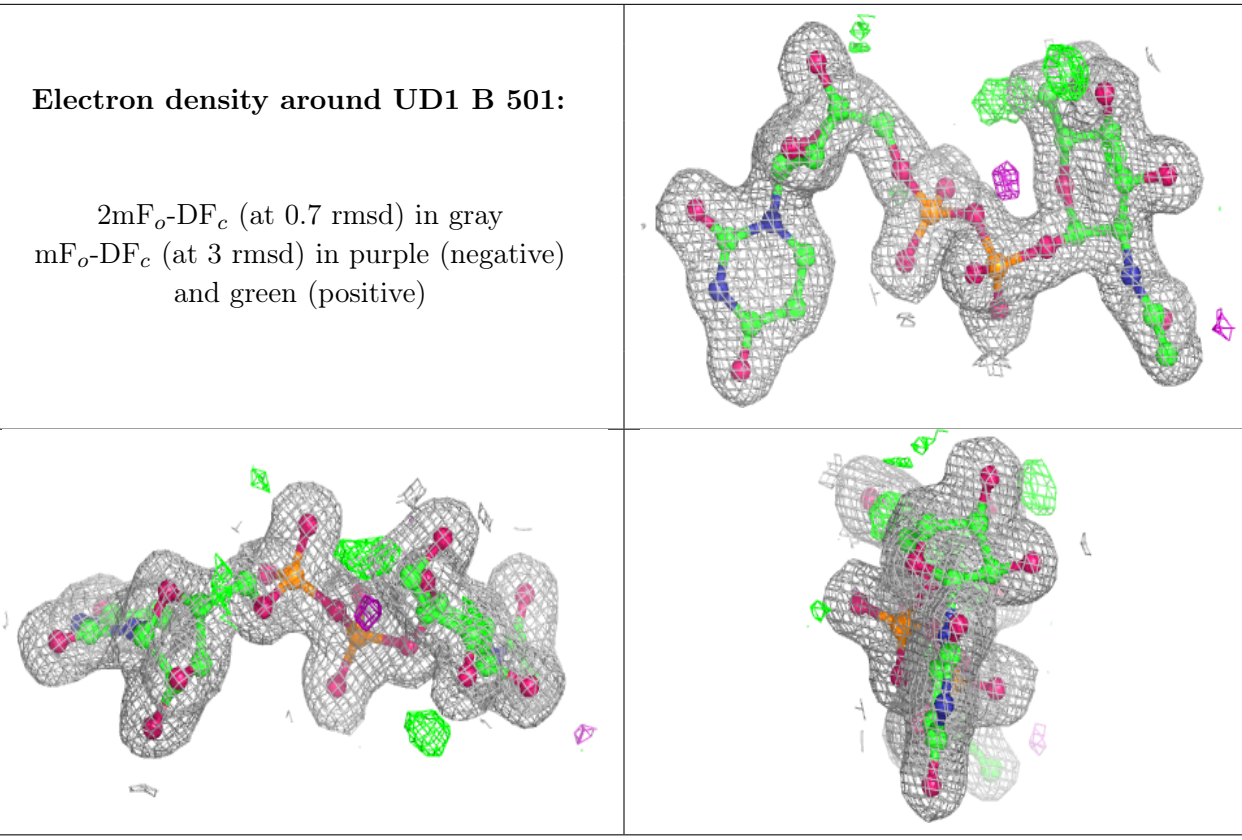






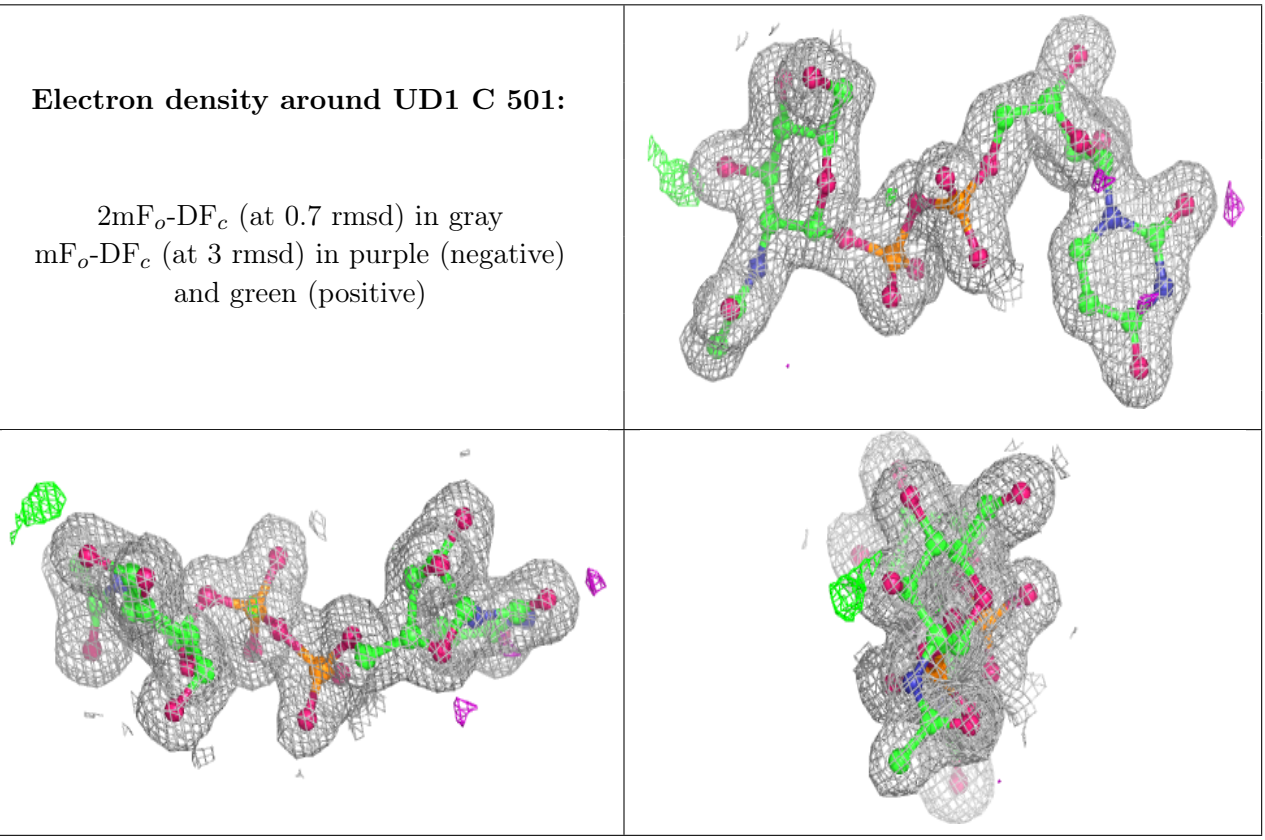
Electron density around UD1 B 501:

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



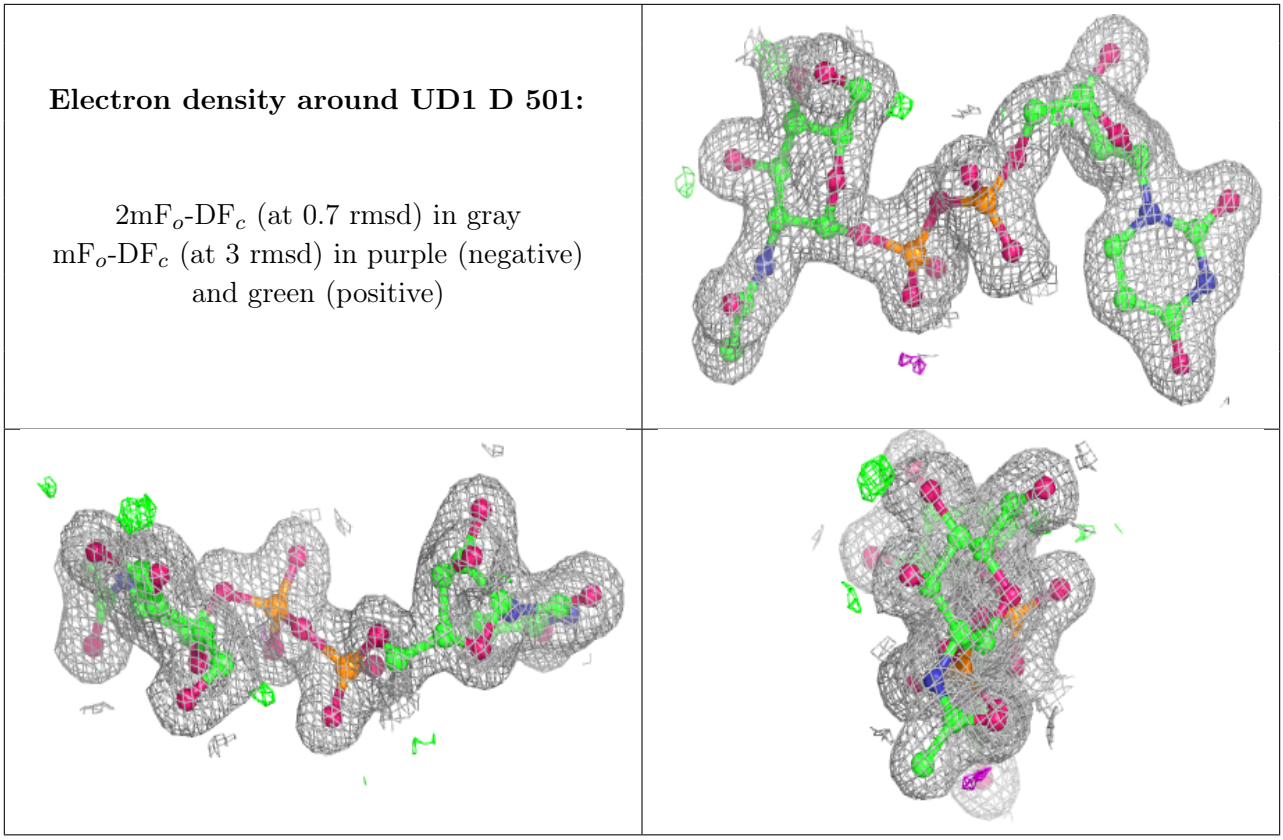
Electron density around UD1 C 501:

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



Electron density around UD1 D 501:

$2mF_o$-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.