Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2024 – 12:10 PM EDT

PDB ID	:	8VHE
Title	:	Crystal Structure of Human IDH1 R132Q in Complex with NADPH-TCEP Adduct
Authors	:	Mealka, M.; Sohl, C.D.; Huxford, T.
Deposited on	:	2023-12-31
Resolution	:	2.16 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:

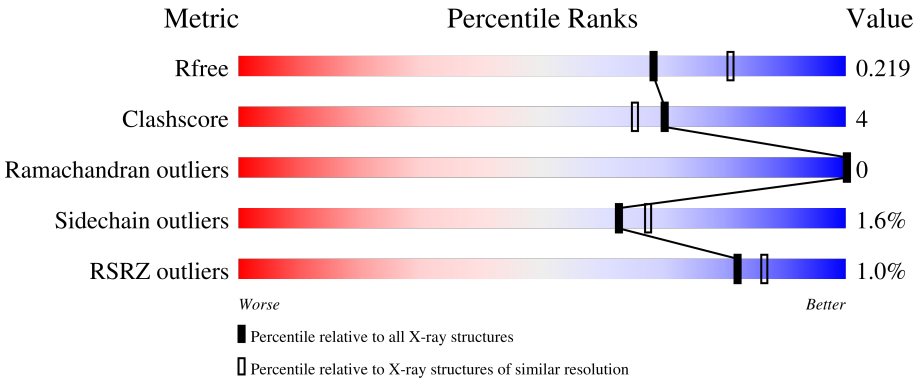
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	2% 88% 8%
1	B	430	% 90% 7%
1	C	430	85% 11%
1	D	430	87% 9%

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
3	GOL	B	504	-	-	X	-
3	GOL	C	502	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14414 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	2	0
			3286	2088	555	624	19			
1	B	421	Total	C	N	O	S	0	2	0
			3336	2116	567	634	19			
1	C	414	Total	C	N	O	S	0	1	0
			3285	2088	555	622	20			
1	D	411	Total	C	N	O	S	0	0	0
			3247	2064	547	618	18			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP O75874
A	-14	HIS	-	expression tag	UNP O75874
A	-13	HIS	-	expression tag	UNP O75874
A	-12	HIS	-	expression tag	UNP O75874
A	-11	HIS	-	expression tag	UNP O75874
A	-10	HIS	-	expression tag	UNP O75874
A	-9	SER	-	expression tag	UNP O75874
A	-8	SER	-	expression tag	UNP O75874
A	-7	GLY	-	expression tag	UNP O75874
A	-6	LEU	-	expression tag	UNP O75874
A	-5	VAL	-	expression tag	UNP O75874
A	-4	PRO	-	expression tag	UNP O75874
A	-3	ARG	-	expression tag	UNP O75874
A	-2	GLY	-	expression tag	UNP O75874
A	-1	SER	-	expression tag	UNP O75874
A	0	HIS	-	expression tag	UNP O75874
A	132	GLN	ARG	engineered mutation	UNP O75874
B	-15	HIS	-	expression tag	UNP O75874
B	-14	HIS	-	expression tag	UNP O75874
B	-13	HIS	-	expression tag	UNP O75874
B	-12	HIS	-	expression tag	UNP O75874

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP O75874
B	-10	HIS	-	expression tag	UNP O75874
B	-9	SER	-	expression tag	UNP O75874
B	-8	SER	-	expression tag	UNP O75874
B	-7	GLY	-	expression tag	UNP O75874
B	-6	LEU	-	expression tag	UNP O75874
B	-5	VAL	-	expression tag	UNP O75874
B	-4	PRO	-	expression tag	UNP O75874
B	-3	ARG	-	expression tag	UNP O75874
B	-2	GLY	-	expression tag	UNP O75874
B	-1	SER	-	expression tag	UNP O75874
B	0	HIS	-	expression tag	UNP O75874
B	132	GLN	ARG	engineered mutation	UNP O75874
C	-15	HIS	-	expression tag	UNP O75874
C	-14	HIS	-	expression tag	UNP O75874
C	-13	HIS	-	expression tag	UNP O75874
C	-12	HIS	-	expression tag	UNP O75874
C	-11	HIS	-	expression tag	UNP O75874
C	-10	HIS	-	expression tag	UNP O75874
C	-9	SER	-	expression tag	UNP O75874
C	-8	SER	-	expression tag	UNP O75874
C	-7	GLY	-	expression tag	UNP O75874
C	-6	LEU	-	expression tag	UNP O75874
C	-5	VAL	-	expression tag	UNP O75874
C	-4	PRO	-	expression tag	UNP O75874
C	-3	ARG	-	expression tag	UNP O75874
C	-2	GLY	-	expression tag	UNP O75874
C	-1	SER	-	expression tag	UNP O75874
C	0	HIS	-	expression tag	UNP O75874
C	132	GLN	ARG	engineered mutation	UNP O75874
D	-15	HIS	-	expression tag	UNP O75874
D	-14	HIS	-	expression tag	UNP O75874
D	-13	HIS	-	expression tag	UNP O75874
D	-12	HIS	-	expression tag	UNP O75874
D	-11	HIS	-	expression tag	UNP O75874
D	-10	HIS	-	expression tag	UNP O75874
D	-9	SER	-	expression tag	UNP O75874
D	-8	SER	-	expression tag	UNP O75874
D	-7	GLY	-	expression tag	UNP O75874
D	-6	LEU	-	expression tag	UNP O75874
D	-5	VAL	-	expression tag	UNP O75874
D	-4	PRO	-	expression tag	UNP O75874

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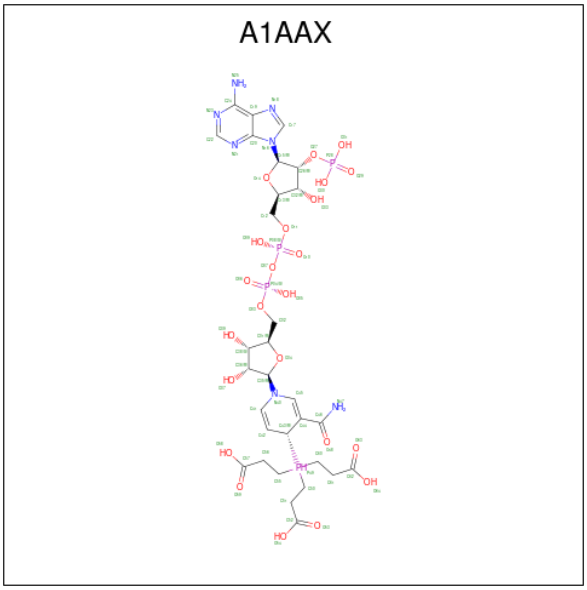
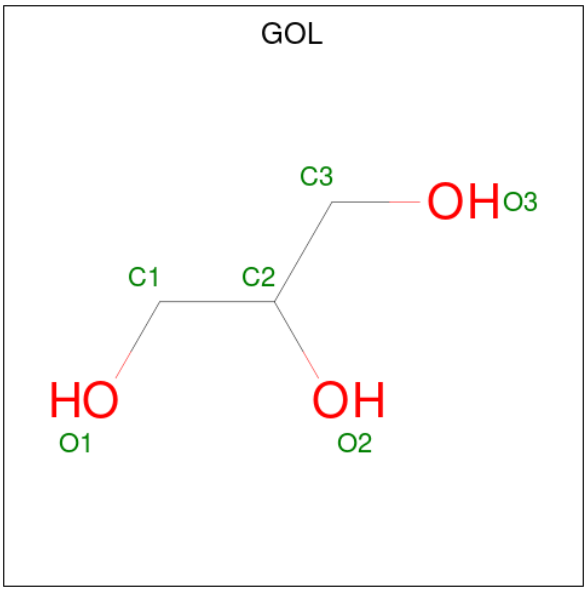
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	ARG	-	expression tag	UNP O75874
D	-2	GLY	-	expression tag	UNP O75874
D	-1	SER	-	expression tag	UNP O75874
D	0	HIS	-	expression tag	UNP O75874
D	132	GLN	ARG	engineered mutation	UNP O75874

- Molecule 2 is 3,3',3''-({(4R)-1-[(2R,3R,4S,5R)-5-({[(S)-{[(S)-{[(2R,3R,4R,5R)-5-(6-amino-9H-purin-9-yl)-3-hydroxy-4-(phosphonooxy)oxolan-2-yl]methoxy}(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]oxy}methyl)-3,4-dihydroxyoxolan-2-yl]-3-carbamoyl-1,4-dihydropyridin-4-yl}-lambda 5 -phosphanetriyl)tripropanoic acid (three-letter code: A1AAX) (formula: $C_{30}H_{45}N_7O_{23}P_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			64	30	7	23	4		
2	B	1	Total	C	N	O	P	0	0
			64	30	7	23	4		
2	C	1	Total	C	N	O	P	0	0
			64	30	7	23	4		
2	D	1	Total	C	N	O	P	0	0
			64	30	7	23	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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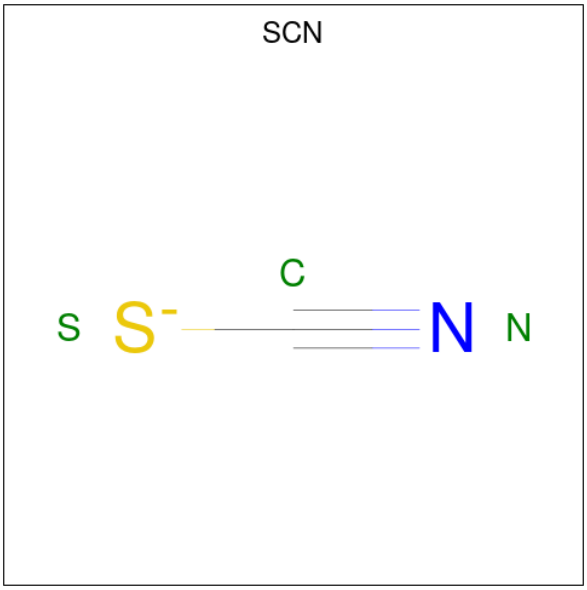
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0

- Molecule 6 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N S 3 1 1 1	0	0
6	C	1	Total C N S 3 1 1 1	0	0
6	D	1	Total C N S 3 1 1 1	0	0

- Molecule 7 is water.

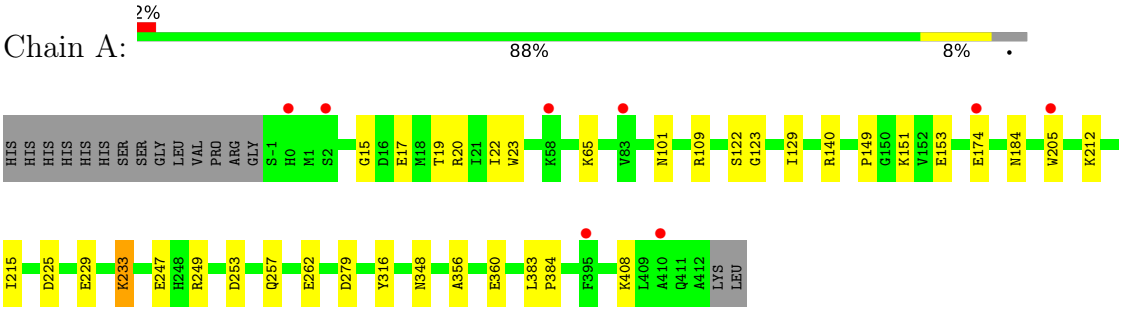
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	201	Total O 201 201	0	0
7	B	254	Total O 254 254	0	0
7	C	254	Total O 254 254	0	0
7	D	224	Total O 224 224	0	0

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.

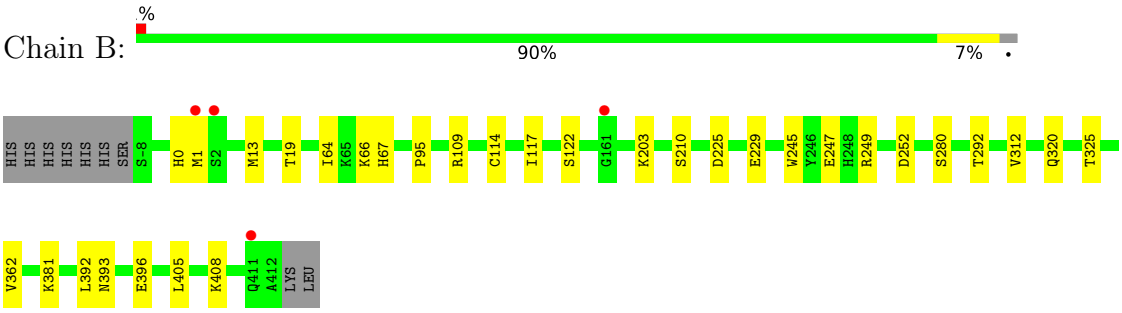
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain A:



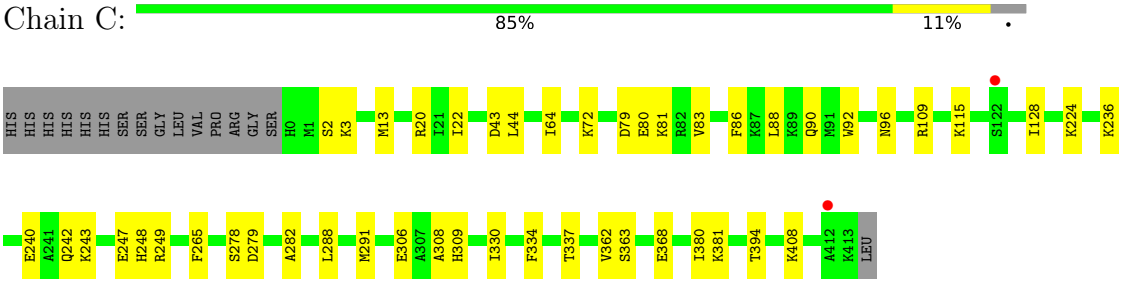
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain B:



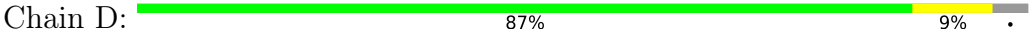
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

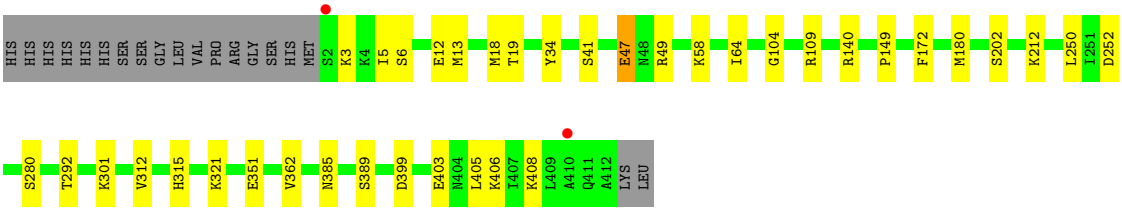
Chain C:



• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain D:




HIS
HIS
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HIS
SER
SER
GLY
LEU
VAL
PRO
ARG
GLY
SER
HIS
MET
S2
K3
K4
I5
S6
E12
M13
M18
T19
Y34
S41
E47
N48
R49
K58
I64
G104
R109
R140
P149
F172
M180
S202
K212
L250
I251
D252
S280
T292
K301
V312
H315
K321
E351
V362
N385
S389
D399
E403
N404
L405
K406
I407
K408
L409
A410
Q411
A412
LYS
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.30Å 107.35Å 109.94Å 90.00° 99.19° 90.00°	Depositor
Resolution (Å)	108.53 – 2.16 108.53 – 2.16	Depositor EDS
% Data completeness (in resolution range)	97.8 (108.53-2.16) 97.8 (108.53-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.171 , 0.223 0.169 , 0.219	Depositor DCC
R_{free} test set	5063 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14414	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 4.60% 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: CA, GOL, CL, SCN, A1AAX

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	0.41	0/3355	0.57	0/4526
1	B	0.44	0/3406	0.59	0/4594
1	C	0.41	0/3354	0.58	0/4522
1	D	0.40	0/3315	0.58	0/4473
All	All	0.42	0/13430	0.58	0/18115

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3286	0	3236	23	0
1	B	3336	0	3299	19	0
1	C	3285	0	3243	33	0
1	D	3247	0	3194	19	0
2	A	64	0	0	0	0
2	B	64	0	0	1	0
2	C	64	0	0	1	0
2	D	64	0	0	0	0
3	A	18	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	22	4	0
3	C	6	0	6	4	0
3	D	12	0	14	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	B	3	0	0	0	0
6	C	3	0	0	1	0
6	D	3	0	0	0	0
7	A	201	0	0	1	0
7	B	254	0	0	1	0
7	C	254	0	0	1	0
7	D	224	0	0	5	0
All	All	14414	0	13036	95	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 4.

All (95) 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:58:LYS:NZ	7:D:601:HOH:O	2.14	0.77
1:C:308:ALA:HB1	3:C:502:GOL:H32	1.69	0.73
1:C:288:LEU:HG	1:C:309:HIS:HB3	1.74	0.70
1:A:65:LYS:HE2	3:A:503:GOL:H11	1.76	0.68
1:A:101:ASN:OD1	1:A:140:ARG:NH1	2.27	0.67
1:C:86:PHE:HB2	1:C:88:LEU:CD1	2.25	0.67
1:A:151:LYS:HE3	1:A:153:GLU:CD	2.18	0.64
1:D:104:GLY:HA3	3:D:501:GOL:H2	1.80	0.64
1:C:224:LYS:HG3	1:C:248:HIS:CD2	2.36	0.61
1:C:362:VAL:HG23	1:C:408:LYS:HD2	1.82	0.61
1:B:225:ASP:O	1:B:229:GLU:HG2	2.02	0.60
1:C:278:SER:OG	3:C:502:GOL:H11	2.01	0.59
1:D:362:VAL:HG23	1:D:408:LYS:HD3	1.85	0.58
1:C:330:ILE:HD12	1:C:363:SER:HB3	1.85	0.57
1:A:279:ASP:OD2	1:B:252:ASP:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLU:OE1	3:B:504:GOL:H32	2.07	0.55
1:C:115:LYS:HG3	1:C:368:GLU:OE2	2.06	0.55
1:D:6:SER:HB2	7:D:610:HOH:O	2.07	0.55
1:C:22:ILE:HD11	1:C:394:THR:HG23	1.88	0.54
1:B:66:LYS:HE2	1:B:67:HIS:NE2	2.23	0.54
1:A:22:ILE:HD12	1:A:23:TRP:N	2.22	0.54
1:D:3:LYS:NZ	7:D:610:HOH:O	2.41	0.54
1:C:291:MET:HB3	1:C:308:ALA:HB3	1.89	0.54
1:A:109:ARG:HB3	7:A:663:HOH:O	2.09	0.52
1:B:245:TRP:CZ2	3:B:504:GOL:H11	2.44	0.52
1:A:140:ARG:HG3	1:A:140:ARG:HH11	1.75	0.51
1:C:13:MET:HB3	1:C:44:LEU:HG	1.92	0.51
1:A:17:GLU:HG2	1:A:316:TYR:CD2	2.46	0.51
1:B:245:TRP:CD1	3:B:504:GOL:H31	2.46	0.50
1:D:47:GLU:CD	1:D:47:GLU:H	2.14	0.50
1:C:334:PHE:HA	1:C:337:THR:OG1	2.12	0.50
1:A:247:GLU:OE1	1:A:249:ARG:NH1	2.43	0.50
1:A:19:THR:HA	1:A:22:ILE:HG13	1.93	0.50
1:A:229:GLU:O	1:A:233:LYS:HE2	2.13	0.49
1:C:288:LEU:HB2	7:C:813:HOH:O	2.13	0.49
1:C:90:GLN:HG3	1:C:92:TRP:CH2	2.47	0.48
1:A:149:PRO:HG3	1:A:174:GLU:O	2.13	0.48
1:C:247:GLU:OE1	1:C:249:ARG:NH1	2.46	0.48
1:B:203:LYS:HB3	1:B:203:LYS:HE3	1.46	0.48
1:C:80:GLU:H	1:C:80:GLU:CD	2.17	0.48
1:C:79:ASP:O	1:C:83:VAL:HG23	2.14	0.48
1:D:399:ASP:O	1:D:403:GLU:HG3	2.14	0.48
1:C:279:ASP:CG	3:C:502:GOL:H12	2.34	0.47
1:A:109:ARG:NH1	3:A:504:GOL:H12	2.30	0.46
1:C:96:ASN:HA	6:C:503:SCN:N	2.31	0.46
1:D:212:LYS:HD2	1:D:250:LEU:HD11	1.98	0.46
1:C:242:GLN:C	1:C:243:LYS:HG2	2.35	0.46
1:A:140:ARG:NH1	1:A:140:ARG:HG3	2.31	0.45
1:B:114:CYS:HB2	1:B:117:ILE:HG12	1.98	0.45
2:C:501:A1AAX:O30	2:C:501:A1AAX:O33	2.35	0.45
1:B:362:VAL:HG21	1:B:405:LEU:HA	1.99	0.45
1:D:49:ARG:HD2	7:D:665:HOH:O	2.16	0.45
1:A:129:ILE:HD12	1:A:205:TRP:HZ3	1.82	0.44
1:A:225:ASP:O	1:A:229:GLU:HG3	2.17	0.44
2:B:501:A1AAX:O33	2:B:501:A1AAX:O29	2.36	0.44
1:B:210:SER:HA	1:B:249:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:VAL:HG23	1:B:408:LYS:HD2	2.00	0.44
1:C:13:MET:CE	1:C:64:ILE:HD11	2.47	0.44
1:C:72:LYS:NZ	1:C:306:GLU:OE2	2.46	0.44
1:C:20:ARG:NH2	1:C:43:ASP:OD1	2.51	0.44
1:A:253[B]:ASP:O	1:A:257:GLN:HG3	2.17	0.43
1:D:5:ILE:HG12	1:D:351:GLU:HB3	1.99	0.43
1:D:13:MET:CE	1:D:64:ILE:HD11	2.48	0.43
1:D:362:VAL:HG21	1:D:405:LEU:HA	2.00	0.43
1:D:109:ARG:HA	1:D:292:THR:O	2.19	0.43
1:A:356:ALA:O	1:A:360:GLU:HG3	2.19	0.43
1:B:325:THR:O	1:B:393:ASN:HB2	2.19	0.43
1:C:128:ILE:HG12	1:C:265:PHE:CZ	2.53	0.43
1:D:149:PRO:HA	1:D:172:PHE:O	2.19	0.43
1:C:236:LYS:O	1:C:240:GLU:HG3	2.20	0.42
1:D:321:LYS:HB2	1:D:321:LYS:HE3	1.77	0.42
1:C:3:LYS:HD3	1:C:3:LYS:HA	1.86	0.42
1:A:212:LYS:HE3	1:A:215:ILE:HG13	2.02	0.42
1:C:109:ARG:NE	3:C:502:GOL:H31	2.35	0.42
1:B:381:LYS:HB3	1:B:381:LYS:HE2	1.87	0.42
1:C:380:ILE:HG22	1:C:381:LYS:HG2	2.01	0.41
1:C:81:LYS:H	1:C:81:LYS:HG2	1.72	0.41
1:A:15:GLY:O	1:A:20:ARG:HD2	2.21	0.41
1:C:22:ILE:HD13	1:C:22:ILE:HA	1.77	0.41
1:A:383:LEU:N	1:A:384:PRO:HD2	2.36	0.41
1:B:95:PRO:HD2	7:B:601:HOH:O	2.21	0.41
1:D:389:SER:HB2	7:D:622:HOH:O	2.21	0.41
1:A:123:GLY:O	1:A:262:GLU:HA	2.21	0.41
1:A:253[A]:ASP:O	1:A:257:GLN:HG3	2.21	0.41
1:B:245:TRP:NE1	3:B:504:GOL:H31	2.36	0.41
1:C:282:ALA:HB2	1:C:291:MET:HG2	2.02	0.40
1:C:330:ILE:CD1	1:C:363:SER:HB3	2.50	0.40
1:B:13:MET:HE1	1:B:64:ILE:HD11	2.03	0.40
1:C:86:PHE:HB2	1:C:88:LEU:HD12	2.01	0.40
1:B:109:ARG:HA	1:B:292:THR:O	2.21	0.40
1:B:66:LYS:HE2	1:B:67:HIS:CE1	2.57	0.40
1:D:12:GLU:OE2	1:D:41:SER:OG	2.29	0.40
1:D:18:MET:HG2	1:D:315:HIS:HB2	2.04	0.40
1:B:392:LEU:HB3	1:B:396:GLU:HB2	2.03	0.40
1:D:34:TYR:OH	1:D:406:LYS:HE3	2.21	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	414/430 (96%)	401 (97%)	13 (3%)	0	100	100
1	B	421/430 (98%)	408 (97%)	13 (3%)	0	100	100
1	C	413/430 (96%)	400 (97%)	13 (3%)	0	100	100
1	D	409/430 (95%)	393 (96%)	16 (4%)	0	100	100
All	All	1657/1720 (96%)	1602 (97%)	55 (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	349/364 (96%)	344 (99%)	5 (1%)	67	72
1	B	357/364 (98%)	350 (98%)	7 (2%)	55	59
1	C	349/364 (96%)	348 (100%)	1 (0%)	92	95
1	D	344/364 (94%)	334 (97%)	10 (3%)	42	42
All	All	1399/1456 (96%)	1376 (98%)	23 (2%)	62	67

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	SER
1	A	184	ASN

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Mol	Chain	Res	Type
1	A	233	LYS
1	A	348	ASN
1	A	408	LYS
1	B	0	HIS
1	B	1	MET
1	B	19	THR
1	B	122	SER
1	B	280	SER
1	B	312	VAL
1	B	320	GLN
1	C	2	SER
1	D	19	THR
1	D	47	GLU
1	D	140	ARG
1	D	180	MET
1	D	202	SER
1	D	252	ASP
1	D	280	SER
1	D	301	LYS
1	D	312	VAL
1	D	385	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	ASN
1	C	171	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	A1AAX	A	501	5	58,68,68	2.51	18 (31%)	73,103,103	1.43	8 (10%)
3	GOL	D	504	5	5,5,5	1.20	1 (20%)	5,5,5	0.65	0
3	GOL	C	502	5	5,5,5	1.11	0	5,5,5	1.31	0
2	A1AAX	C	501	5	58,68,68	2.36	18 (31%)	73,103,103	1.37	8 (10%)
2	A1AAX	B	501	5	58,68,68	2.16	16 (27%)	73,103,103	1.31	8 (10%)
2	A1AAX	D	502	5	58,68,68	2.33	17 (29%)	73,103,103	1.37	8 (10%)
3	GOL	A	504	5	5,5,5	1.03	0	5,5,5	0.78	0
3	GOL	D	501	-	5,5,5	1.09	0	5,5,5	0.89	0
6	SCN	B	503	-	1,2,2	0.56	0	0,1,1	-	-
3	GOL	A	503	-	5,5,5	0.92	0	5,5,5	1.01	0
3	GOL	B	505	5	5,5,5	0.91	0	5,5,5	0.96	0
6	SCN	C	503	-	1,2,2	0.85	0	0,1,1	-	-
3	GOL	B	504	-	5,5,5	0.75	0	5,5,5	0.86	0
3	GOL	B	502	-	5,5,5	0.87	0	5,5,5	1.04	0
6	SCN	D	503	-	1,2,2	0.89	0	0,1,1	-	-
3	GOL	A	502	-	5,5,5	1.06	0	5,5,5	1.07	0

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	A1AAX	A	501	5	-	13/48/104/104	0/5/5/5
3	GOL	D	504	5	-	0/4/4/4	-
3	GOL	C	502	5	-	4/4/4/4	-
2	A1AAX	C	501	5	-	17/48/104/104	0/5/5/5
2	A1AAX	B	501	5	-	15/48/104/104	0/5/5/5
2	A1AAX	D	502	5	-	11/48/104/104	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	504	5	-	2/4/4/4	-
3	GOL	D	501	-	-	2/4/4/4	-
3	GOL	A	503	-	-	4/4/4/4	-
3	GOL	B	505	5	-	1/4/4/4	-
3	GOL	B	504	-	-	0/4/4/4	-
3	GOL	B	502	-	-	2/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1AAX	P49-C50	7.79	1.92	1.80
2	C	501	A1AAX	P49-C60	7.60	1.91	1.80
2	D	502	A1AAX	P49-C50	7.06	1.90	1.80
2	D	502	A1AAX	P49-C55	6.83	1.90	1.80
2	B	501	A1AAX	P49-C60	6.33	1.89	1.80
2	A	501	A1AAX	P49-C60	6.23	1.89	1.80
2	C	501	A1AAX	P49-C50	6.08	1.89	1.80
2	D	502	A1AAX	P49-C60	5.97	1.89	1.80
2	C	501	A1AAX	P49-C55	5.95	1.89	1.80
2	A	501	A1AAX	P49-C55	5.61	1.88	1.80
2	A	501	A1AAX	P04-O03	5.59	1.81	1.59
2	B	501	A1AAX	P49-C55	5.50	1.88	1.80
2	D	502	A1AAX	P04-O03	5.38	1.81	1.59
2	A	501	A1AAX	P49-C43	5.35	1.90	1.84
2	B	501	A1AAX	P04-O03	5.21	1.80	1.59
2	B	501	A1AAX	P49-C50	5.21	1.88	1.80
2	C	501	A1AAX	P04-O03	5.17	1.80	1.59
2	A	501	A1AAX	C35-N40	4.35	1.58	1.46
2	C	501	A1AAX	C35-N40	4.30	1.58	1.46
2	A	501	A1AAX	C61-C62	4.29	1.60	1.50
2	A	501	A1AAX	P28-O27	4.11	1.67	1.59
2	D	502	A1AAX	C35-N40	4.07	1.57	1.46
2	C	501	A1AAX	C61-C62	3.84	1.59	1.50
2	B	501	A1AAX	P28-O27	3.48	1.65	1.59
2	D	502	A1AAX	C61-C62	3.41	1.58	1.50
2	D	502	A1AAX	P08-O11	3.39	1.73	1.59
2	C	501	A1AAX	C56-C57	3.25	1.58	1.50
2	B	501	A1AAX	C56-C57	3.22	1.58	1.50
2	B	501	A1AAX	C61-C62	3.18	1.58	1.50
2	A	501	A1AAX	P08-O11	3.18	1.72	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	A1AAX	P08-O11	3.10	1.71	1.59
2	D	502	A1AAX	P28-O27	3.08	1.65	1.59
2	C	501	A1AAX	P28-O27	2.99	1.65	1.59
2	A	501	A1AAX	C22-N23	2.93	1.39	1.33
2	C	501	A1AAX	C22-N23	2.88	1.39	1.33
2	C	501	A1AAX	O03-C02	-2.84	1.33	1.44
2	B	501	A1AAX	C45-C44	2.82	1.38	1.34
2	A	501	A1AAX	C56-C57	2.80	1.57	1.50
2	B	501	A1AAX	O27-C26	-2.76	1.34	1.44
2	C	501	A1AAX	O27-C26	-2.74	1.34	1.44
2	D	502	A1AAX	O27-C26	-2.74	1.34	1.44
2	A	501	A1AAX	O27-C26	-2.73	1.34	1.44
2	B	501	A1AAX	C22-N23	2.72	1.39	1.33
2	C	501	A1AAX	P08-O11	2.69	1.70	1.59
2	B	501	A1AAX	C41-C42	2.69	1.39	1.33
2	C	501	A1AAX	C20-N21	2.66	1.39	1.35
2	A	501	A1AAX	C45-C44	2.65	1.38	1.34
2	D	502	A1AAX	C22-N23	2.63	1.38	1.33
2	D	502	A1AAX	C45-C44	2.57	1.38	1.34
2	D	502	A1AAX	C56-C57	2.51	1.56	1.50
2	C	501	A1AAX	C46-N47	2.50	1.40	1.33
2	D	502	A1AAX	C41-C42	2.49	1.38	1.33
2	B	501	A1AAX	O03-C02	-2.48	1.35	1.44
2	B	501	A1AAX	C35-N40	2.47	1.53	1.46
2	B	501	A1AAX	C46-N47	2.45	1.39	1.33
2	C	501	A1AAX	C45-C44	2.44	1.38	1.34
2	C	501	A1AAX	C51-C52	2.43	1.56	1.50
2	D	502	A1AAX	O03-C02	-2.43	1.35	1.44
2	A	501	A1AAX	C41-C42	2.42	1.38	1.33
2	A	501	A1AAX	C46-N47	2.40	1.39	1.33
2	A	501	A1AAX	O03-C02	-2.40	1.35	1.44
2	D	502	A1AAX	C46-N47	2.36	1.39	1.33
2	C	501	A1AAX	C41-C42	2.35	1.38	1.33
2	A	501	A1AAX	C20-N21	2.28	1.38	1.35
2	D	502	A1AAX	C20-N21	2.28	1.38	1.35
2	C	501	A1AAX	C24-N25	2.14	1.41	1.34
2	B	501	A1AAX	C20-N21	2.14	1.38	1.35
2	A	501	A1AAX	C51-C52	2.09	1.55	1.50
3	D	504	GOL	C3-C2	2.08	1.60	1.51
2	D	502	A1AAX	C51-C52	2.01	1.55	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	A1AAX	C32-C26-C15	-4.17	95.06	102.89
2	D	502	A1AAX	C32-C26-C15	-4.13	95.12	102.89
2	A	501	A1AAX	C32-C26-C15	-4.08	95.22	102.89
2	B	501	A1AAX	C32-C26-C15	-4.00	95.37	102.89
2	C	501	A1AAX	O27-P28-O29	-3.96	94.12	109.39
2	B	501	A1AAX	C19-C24-N25	3.29	125.36	120.35
2	A	501	A1AAX	O48-C46-N47	-3.23	115.33	122.88
2	D	502	A1AAX	O48-C46-N47	-3.17	115.46	122.88
2	B	501	A1AAX	O48-C46-N47	-3.16	115.48	122.88
2	A	501	A1AAX	C19-C24-N25	3.16	125.15	120.35
2	C	501	A1AAX	O48-C46-N47	-3.08	115.69	122.88
2	C	501	A1AAX	O03-P04-O06	-2.87	97.86	109.07
2	A	501	A1AAX	O03-P04-O06	-2.83	98.01	109.07
2	D	502	A1AAX	C19-C24-N25	2.82	124.64	120.35
2	A	501	A1AAX	C44-C45-N40	2.78	125.94	122.84
2	D	502	A1AAX	O03-P04-O06	-2.78	98.22	109.07
2	D	502	A1AAX	O27-P28-O29	-2.76	98.72	109.39
2	B	501	A1AAX	O27-P28-O29	-2.76	98.73	109.39
2	A	501	A1AAX	O27-P28-O29	-2.73	98.86	109.39
2	B	501	A1AAX	O03-P04-O06	-2.68	98.59	109.07
2	A	501	A1AAX	O31-P28-O30	2.58	117.49	107.64
2	D	502	A1AAX	C44-C45-N40	2.55	125.68	122.84
2	D	502	A1AAX	O31-P28-O30	2.52	117.27	107.64
2	B	501	A1AAX	O31-P28-O30	2.46	117.05	107.64
2	C	501	A1AAX	C19-C24-N25	2.45	124.07	120.35
2	D	502	A1AAX	O53-C52-C51	-2.35	115.55	123.08
2	C	501	A1AAX	O34-C35-C36	-2.29	101.65	106.64
2	A	501	A1AAX	C50-P49-C43	2.28	117.80	110.08
2	B	501	A1AAX	O53-C52-C51	-2.20	116.00	123.08
2	C	501	A1AAX	O31-P28-O30	2.13	115.78	107.64
2	C	501	A1AAX	O30-P28-O29	2.09	118.87	110.68
2	B	501	A1AAX	O05-P04-O06	2.01	122.19	112.24

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1AAX	C51-C50-P49-C43
2	A	501	A1AAX	C56-C55-P49-C50
2	C	501	A1AAX	C02-O03-P04-O05
2	C	501	A1AAX	C02-O03-P04-O06
2	C	501	A1AAX	C12-O11-P08-O10
3	A	503	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	503	GOL	O1-C1-C2-C3
3	A	504	GOL	O1-C1-C2-C3
3	B	502	GOL	C1-C2-C3-O3
3	C	502	GOL	O1-C1-C2-C3
3	D	501	GOL	O1-C1-C2-O2
3	D	501	GOL	O1-C1-C2-C3
2	A	501	A1AAX	C51-C50-P49-C55
2	B	501	A1AAX	C51-C50-P49-C43
2	D	502	A1AAX	C51-C50-P49-C43
3	A	503	GOL	C1-C2-C3-O3
3	C	502	GOL	C1-C2-C3-O3
2	A	501	A1AAX	C55-C56-C57-O59
2	B	501	A1AAX	C50-C51-C52-O53
2	C	501	A1AAX	C50-C51-C52-O54
2	D	502	A1AAX	C50-C51-C52-O53
3	B	502	GOL	O2-C2-C3-O3
3	C	502	GOL	O1-C1-C2-O2
2	A	501	A1AAX	C51-C50-P49-C60
3	A	504	GOL	O1-C1-C2-O2
3	C	502	GOL	O2-C2-C3-O3
2	B	501	A1AAX	P08-O07-P04-O06
2	B	501	A1AAX	C50-C51-C52-O54
2	B	501	A1AAX	C60-C61-C62-O63
2	D	502	A1AAX	C50-C51-C52-O54
2	A	501	A1AAX	C56-C55-P49-C60
3	A	502	GOL	O2-C2-C3-O3
2	A	501	A1AAX	P08-O07-P04-O03
2	B	501	A1AAX	P08-O07-P04-O03
2	D	502	A1AAX	P08-O07-P04-O03
2	C	501	A1AAX	C51-C50-P49-C60
2	C	501	A1AAX	C02-O03-P04-O07
2	C	501	A1AAX	C12-O11-P08-O07
3	A	503	GOL	O2-C2-C3-O3
3	B	505	GOL	O2-C2-C3-O3
2	B	501	A1AAX	C60-C61-C62-O64
2	C	501	A1AAX	C50-C51-C52-O53
2	C	501	A1AAX	C60-C61-C62-O63
2	C	501	A1AAX	C60-C61-C62-O64
2	A	501	A1AAX	C02-O03-P04-O06
2	C	501	A1AAX	C12-O11-P08-O09
2	B	501	A1AAX	C51-C50-P49-C60
2	D	502	A1AAX	C51-C50-P49-C60

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Mol	Chain	Res	Type	Atoms
2	B	501	A1AAX	P49-C55-C56-C57
2	D	502	A1AAX	P49-C55-C56-C57
2	C	501	A1AAX	C15-C26-O27-P28
2	A	501	A1AAX	C36-C35-N40-C45
2	C	501	A1AAX	C36-C35-N40-C45
2	A	501	A1AAX	O34-C35-N40-C45
2	B	501	A1AAX	O34-C35-N40-C45
2	C	501	A1AAX	O34-C35-N40-C45
2	D	502	A1AAX	O34-C35-N40-C45
2	B	501	A1AAX	C36-C35-N40-C45
2	D	502	A1AAX	C36-C35-N40-C45
2	D	502	A1AAX	C56-C55-P49-C60
2	C	501	A1AAX	C51-C50-P49-C43
2	D	502	A1AAX	C61-C60-P49-C43
2	B	501	A1AAX	O34-C01-C02-O03
2	B	501	A1AAX	C55-C56-C57-O58
3	A	502	GOL	C1-C2-C3-O3
2	A	501	A1AAX	C55-C56-C57-O58
2	C	501	A1AAX	C55-C56-C57-O58
2	A	501	A1AAX	C02-O03-P04-O05
2	B	501	A1AAX	C45-C44-C46-N47
2	B	501	A1AAX	C02-O03-P04-O06
2	D	502	A1AAX	C61-C60-P49-C50
2	A	501	A1AAX	C36-C35-N40-C41
2	C	501	A1AAX	C36-C35-N40-C41

There are no ring outliers.

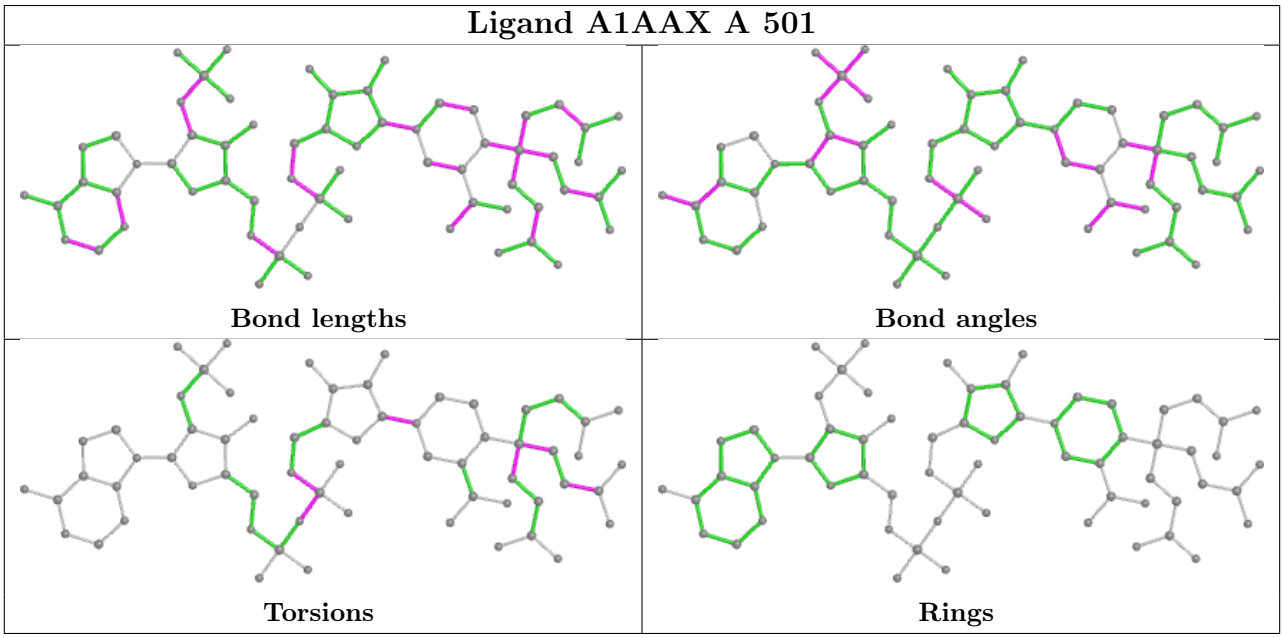
8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	GOL	4	0
2	C	501	A1AAX	1	0
2	B	501	A1AAX	1	0
3	A	504	GOL	1	0
3	D	501	GOL	1	0
3	A	503	GOL	1	0
6	C	503	SCN	1	0
3	B	504	GOL	4	0

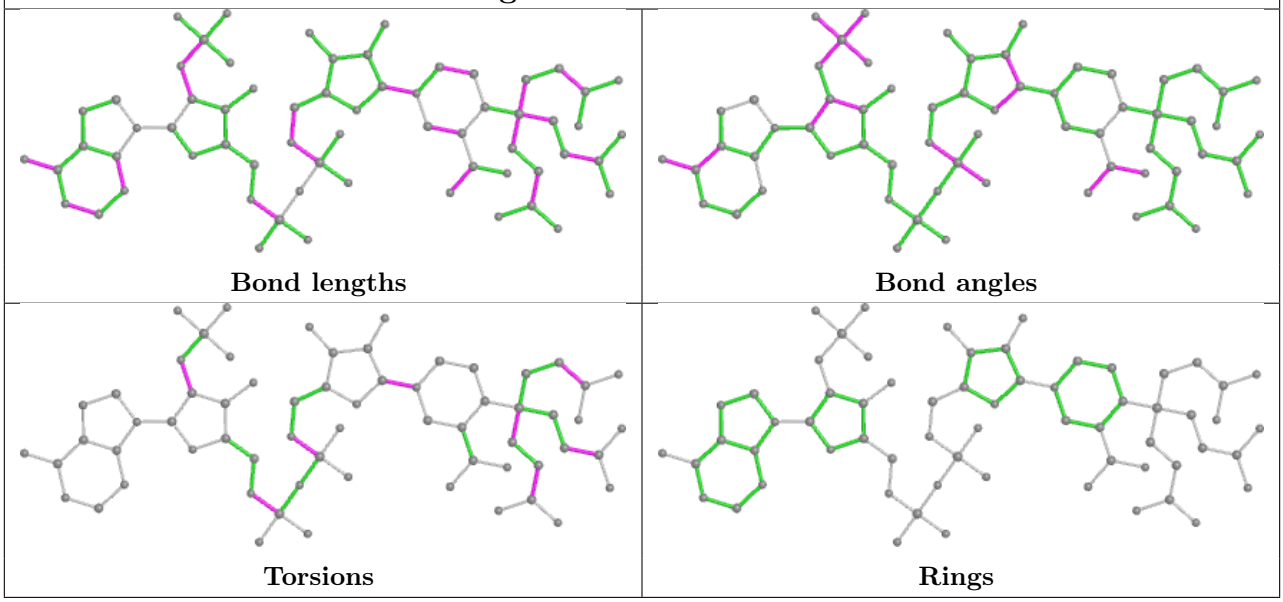
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

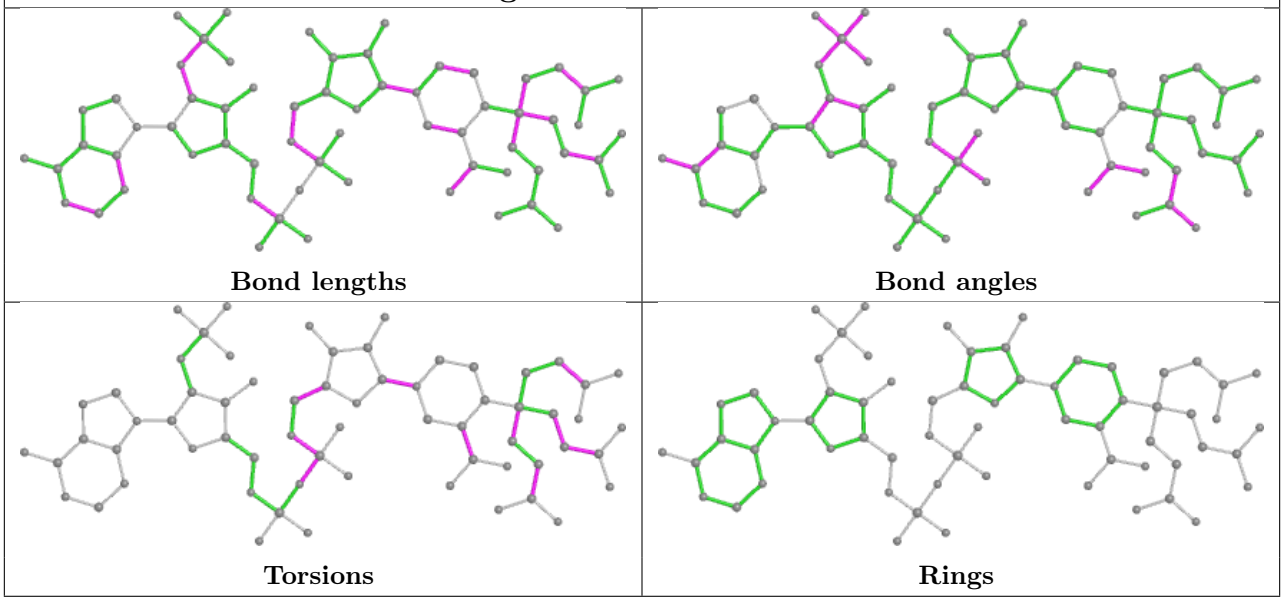
Ligand A1AAX A 501



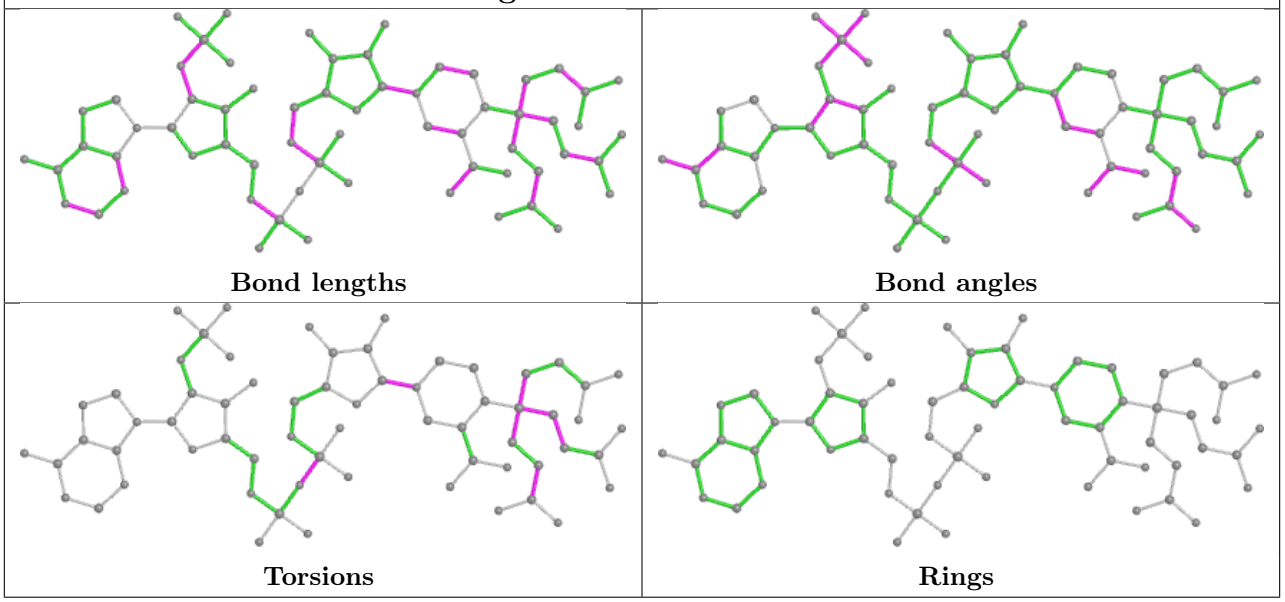
Ligand A1AAX C 501



Ligand A1AAX B 501



Ligand A1AAX D 502



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	414/430 (96%)	0.19	8 (1%)	66	74	24, 42, 65, 84	0
1	B	421/430 (97%)	0.07	4 (0%)	82	86	24, 35, 52, 79	0
1	C	414/430 (96%)	0.06	2 (0%)	91	93	25, 35, 53, 78	0
1	D	411/430 (95%)	0.10	2 (0%)	91	93	26, 40, 55, 81	0
All	All	1660/1720 (96%)	0.10	16 (0%)	82	86	24, 38, 58, 84	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	HIS	3.7
1	D	2	SER	3.3
1	A	58	LYS	3.1
1	A	395	PHE	2.8
1	A	174	GLU	2.8
1	B	2	SER	2.7
1	A	410	ALA	2.7
1	D	410	ALA	2.6
1	A	83	VAL	2.5
1	C	412	ALA	2.5
1	B	161	GLY	2.4
1	C	122	SER	2.4
1	B	411	GLN	2.3
1	A	2	SER	2.2
1	B	1	MET	2.1
1	A	205	TRP	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

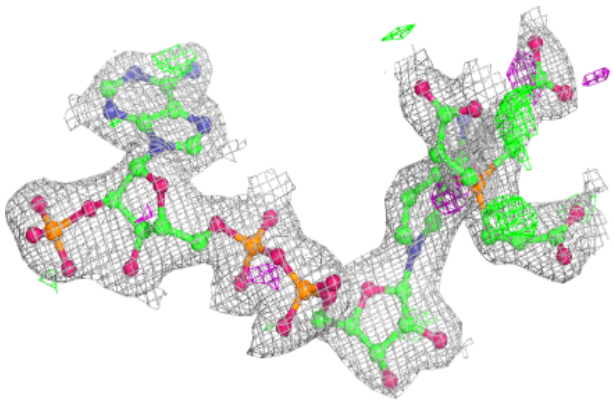
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

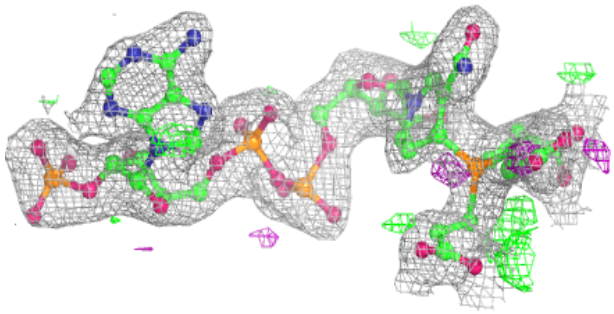
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	D	501	6/6	0.64	0.29	49,53,55,56	0
6	SCN	D	503	3/3	0.73	0.26	55,55,56,72	0
3	GOL	A	502	6/6	0.74	0.21	47,51,58,62	0
3	GOL	C	502	6/6	0.81	0.24	39,44,46,49	0
3	GOL	A	503	6/6	0.86	0.20	45,54,58,62	0
3	GOL	B	502	6/6	0.89	0.18	46,51,53,61	0
3	GOL	B	504	6/6	0.90	0.19	50,53,56,57	0
4	CL	A	505	1/1	0.90	0.16	60,60,60,60	0
3	GOL	A	504	6/6	0.90	0.28	44,46,48,49	0
6	SCN	C	503	3/3	0.92	0.32	47,47,51,63	0
3	GOL	D	504	6/6	0.93	0.18	34,35,37,38	0
2	A1AAX	A	501	64/64	0.94	0.15	39,50,59,61	0
6	SCN	B	503	3/3	0.94	0.12	49,49,49,61	0
3	GOL	B	505	6/6	0.95	0.18	29,35,35,35	0
2	A1AAX	C	501	64/64	0.96	0.12	29,38,49,55	0
2	A1AAX	D	502	64/64	0.96	0.12	36,42,48,51	0
5	CA	A	506	1/1	0.96	0.06	38,38,38,38	0
2	A1AAX	B	501	64/64	0.97	0.12	26,33,38,42	0
4	CL	C	504	1/1	0.98	0.16	44,44,44,44	0
4	CL	D	505	1/1	0.98	0.14	53,53,53,53	0
5	CA	D	506	1/1	0.99	0.08	33,33,33,33	0
4	CL	B	506	1/1	0.99	0.14	38,38,38,38	0
5	CA	B	507	1/1	0.99	0.10	29,29,29,29	0
5	CA	C	505	1/1	0.99	0.08	33,33,33,33	0

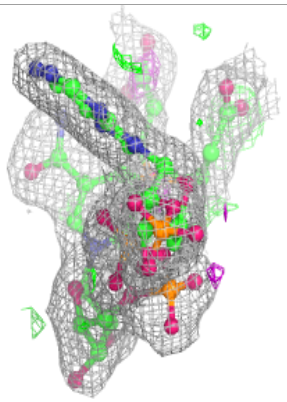
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1AAX 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)

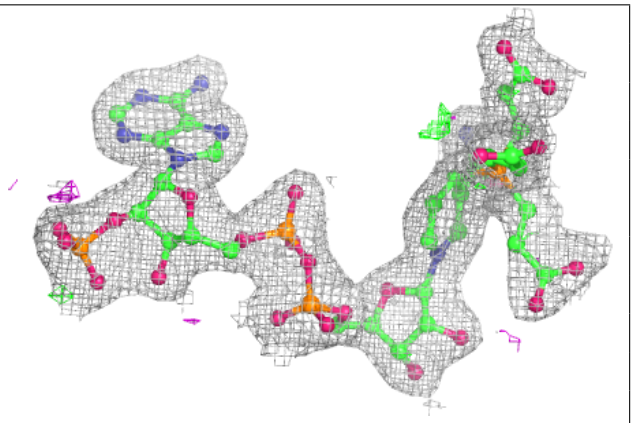


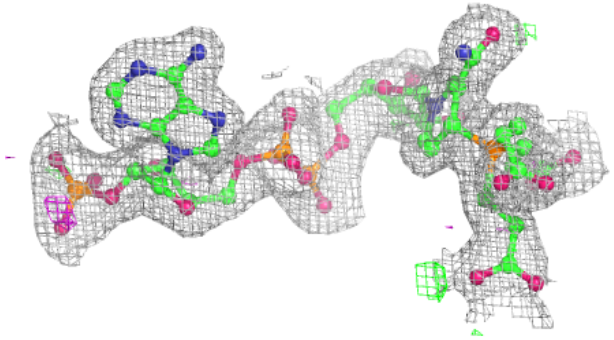


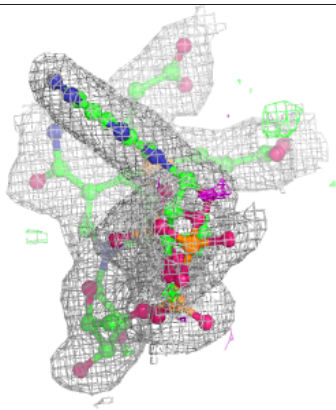


Electron density around A1AAX C 501:

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

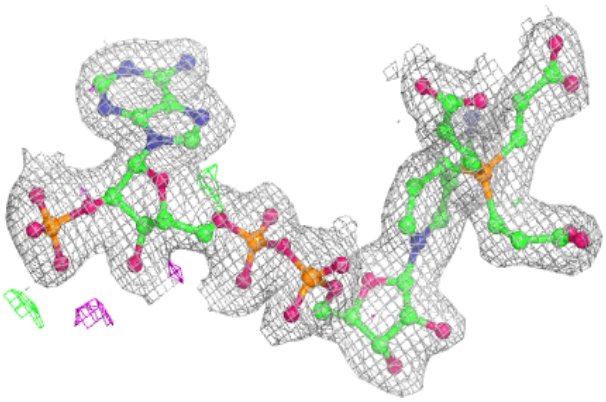


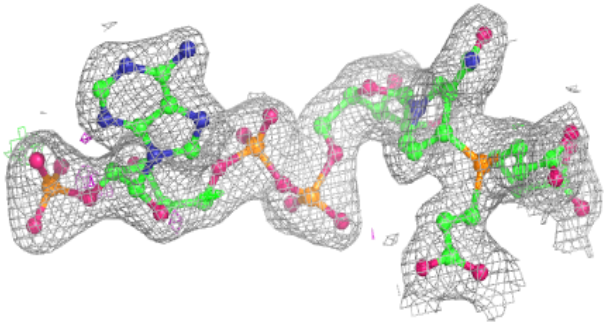


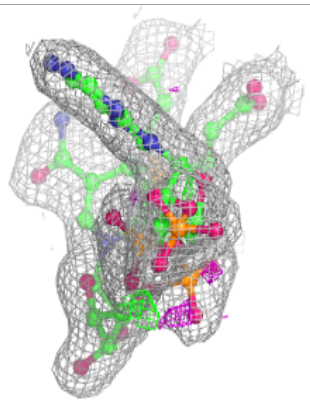


Electron density around A1AAX D 502:

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

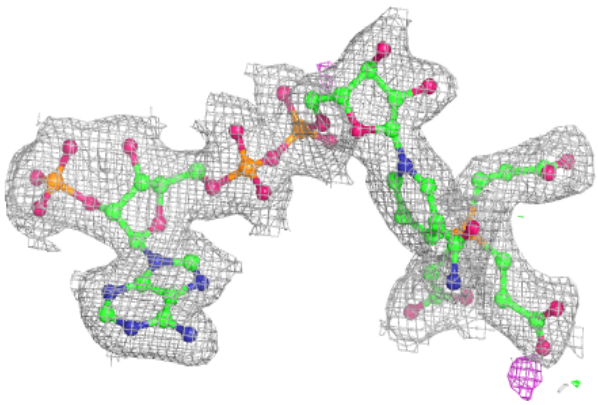


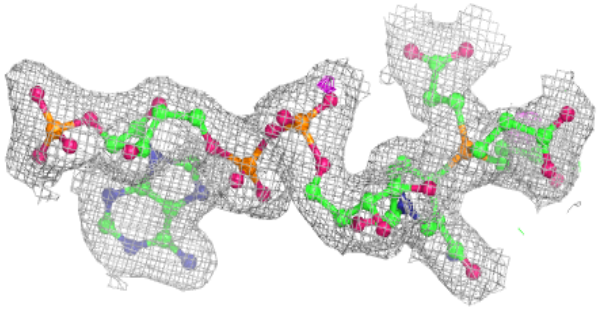


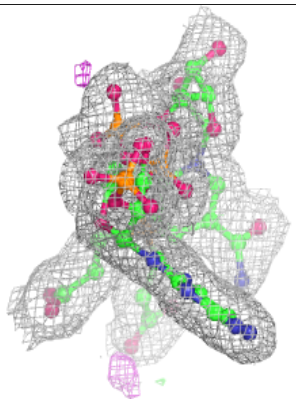


Electron density around A1AAX B 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.