



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 01:19 pm BST

PDB ID : 2IPJ
Title : Crystal structure of h3alpha-hydroxysteroid dehydrogenase type 3 mutant Y24A in complex with NADP+ and epi-testosterone
Authors : Faucher, F.; Cantin, L.; Pereira de Jesus-Tran, K.; Luu-the, V.; Labrie, F.; Breton, R.
Deposited on : 2006-10-12
Resolution : 1.80 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 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 : 2.11
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) : 2.11

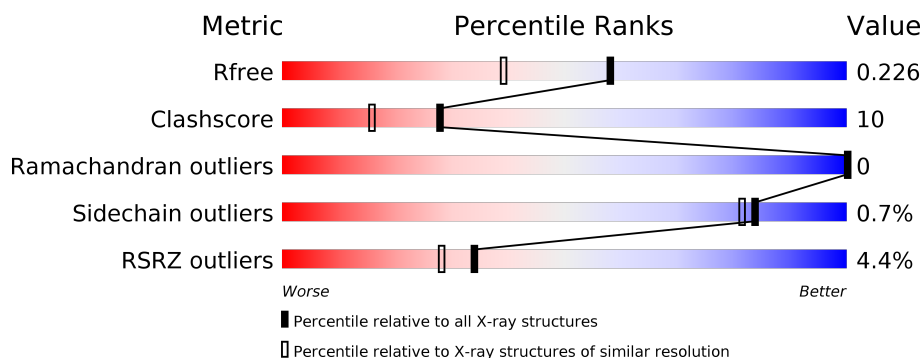
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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 $\leq 5\%$. 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	321	<div> <div>3%</div> <div>84%</div> <div>16%</div> </div>
1	B	321	<div> <div>6%</div> <div>83%</div> <div>17%</div> </div>

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	SO4	B	325	-	X	-	-
4	FFA	A	325	-	-	-	X
4	FFA	B	326	-	-	-	X
5	BME	A	326	-	-	X	-
5	BME	A	327	-	-	X	-
5	BME	B	327	-	-	X	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5998 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 Aldo-keto reductase family 1 member C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	4	0
			2597	1661	450	473	13			
1	B	321	Total	C	N	O	S	0	4	0
			2595	1661	448	473	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	TYR	CONFLICT	UNP P52895
B	24	ALA	TYR	CONFLICT	UNP P52895

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



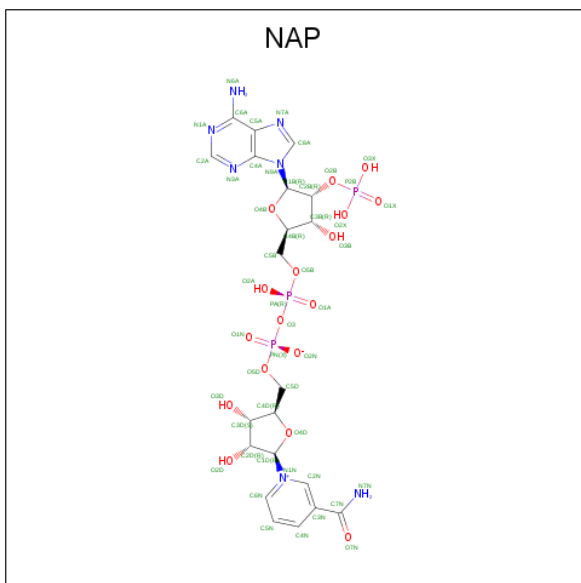
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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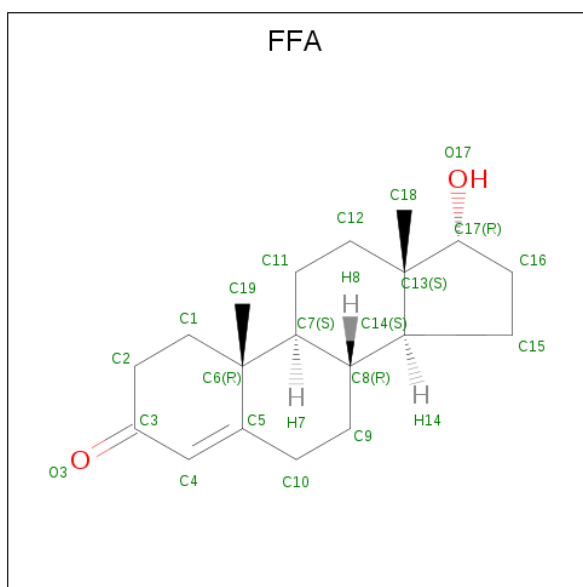
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $\text{C}_{21}\text{H}_{28}\text{N}_7\text{O}_{17}\text{P}_3$).



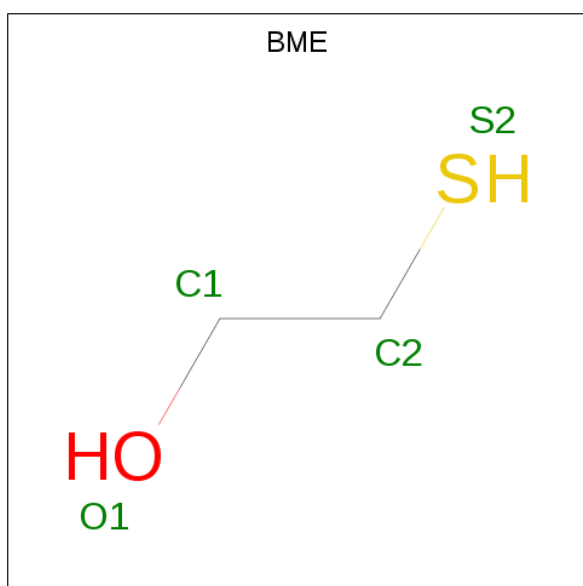
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is (10ALPHA,13ALPHA,14BETA,17ALPHA)-17-HYDROXYANDROST-4-EN-3-ONE (three-letter code: FFA) (formula: C₁₉H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	19	2		
4	B	1	Total	C	O	0	0
			21	19	2		

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O		0	0
			4	2	2			
6	A	1	Total	C	O		0	0
			4	2	2			
6	A	1	Total	C	O		0	0
			4	2	2			
6	B	1	Total	C	O		0	0
			4	2	2			
6	B	1	Total	C	O		0	0
			4	2	2			
6	B	1	Total	C	O		0	0
			4	2	2			

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	326	Total	O	0	0
			326	326		

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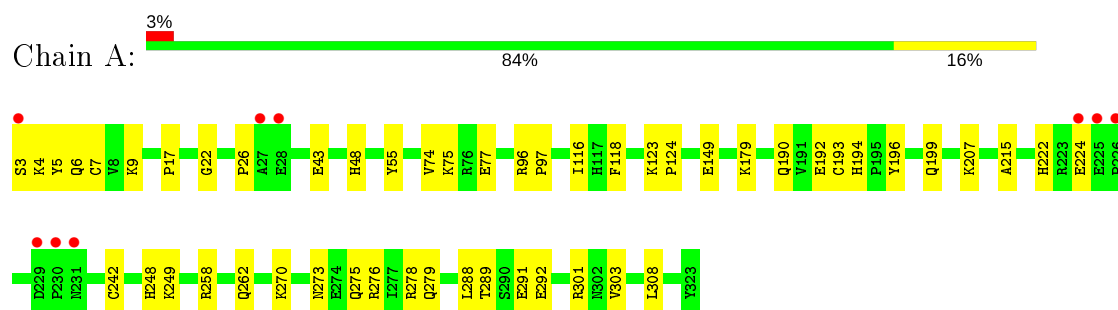
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	287	Total	O	0	0
			287	287		

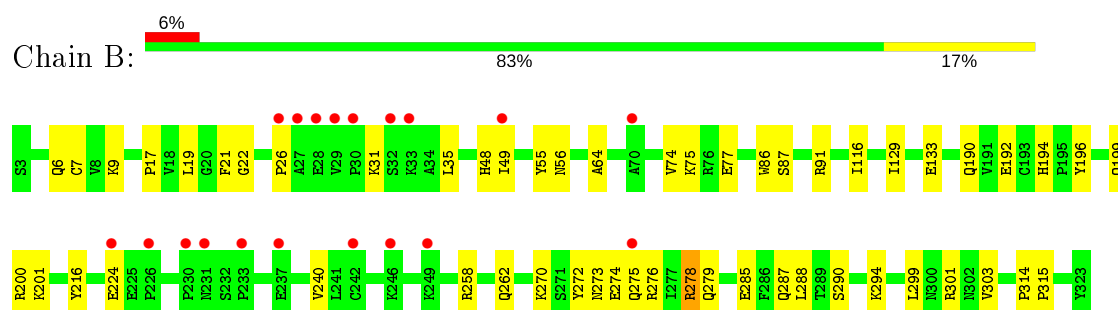
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Aldo-keto reductase family 1 member C2



- Molecule 1: Aldo-keto reductase family 1 member C2



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	144.79 Å 144.79 Å 203.88 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 1.80 19.98 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.98-1.80) 99.8 (19.98-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 1.80 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.228 0.203 , 0.226	Depositor DCC
R_{free} test set	3811 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5998	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SO4, NAP, EDO, FFA, BME

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	0.30	0/2657	0.56	1/3597 (0.0%)
1	B	0.32	0/2655	0.56	1/3594 (0.0%)
All	All	0.31	0/5312	0.56	2/7191 (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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	116	ILE	N-CA-C	-5.12	97.17	111.00
1	A	116	ILE	N-CA-C	-5.03	97.41	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	216	TYR	Sidechain

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	2597	0	2608	54	0
1	B	2595	0	2609	56	0
2	A	5	0	0	0	0
2	B	10	0	0	1	0
3	A	48	0	25	5	0
3	B	48	0	25	7	0
4	A	21	0	28	3	0
4	B	21	0	28	4	0
5	A	8	0	11	10	0
5	B	4	0	6	13	0
6	A	12	0	12	0	0
6	B	16	0	16	1	0
7	A	326	0	0	3	0
7	B	287	0	0	3	0
All	All	5998	0	5368	107	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 10.

All (107) 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:7[A]:CYS:SG	5:A:326:BME:S2	2.35	1.15
1:B:262:GLN:HE22	1:B:288:LEU:H	1.03	0.98
1:A:262:GLN:HE22	1:A:288:LEU:H	1.05	0.97
1:A:258:ARG:HE	1:A:262:GLN:HE21	1.09	0.92
1:B:7[A]:CYS:SG	5:B:327:BME:S2	2.63	0.92
1:B:258:ARG:HE	1:B:262:GLN:HE21	1.17	0.91
1:B:7[B]:CYS:SG	5:B:327:BME:C2	2.65	0.85
1:A:242[A]:CYS:SG	5:A:327:BME:S2	2.63	0.80
1:A:301:ARG:HG3	1:A:303:VAL:HG23	1.64	0.79
1:A:222:HIS:HD2	1:A:224:GLU:HB3	1.49	0.77
1:A:222:HIS:CD2	1:A:224:GLU:HB3	2.22	0.74
1:B:7[A]:CYS:SG	5:B:327:BME:H21	2.28	0.73
1:A:273:ASN:HD22	1:A:276:ARG:H	1.37	0.73
1:B:7[B]:CYS:SG	5:B:327:BME:S2	2.88	0.71
1:A:26:PRO:HB3	1:A:224:GLU:OE1	1.91	0.70
1:A:149:GLU:HG3	1:A:179:LYS:HE3	1.73	0.69
1:B:301:ARG:HG3	1:B:303:VAL:HG23	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LYS:HB3	1:A:77:GLU:OE2	1.93	0.69
1:A:242[B]:CYS:HG	5:A:327:BME:HS2	1.42	0.67
1:B:7[A]:CYS:HG	5:B:327:BME:C2	2.06	0.67
1:B:7[B]:CYS:SG	5:B:327:BME:H21	2.32	0.67
1:B:7[A]:CYS:SG	5:B:327:BME:C2	2.83	0.66
1:B:270:LYS:HE2	1:B:272:TYR:CD1	2.31	0.65
1:A:55:TYR:HE1	4:A:325:FFA:H122	1.63	0.63
1:A:6:GLN:HE21	1:B:9:LYS:H	1.44	0.62
1:B:279:GLN:NE2	3:B:2:NAP:H62A	1.98	0.62
1:A:55:TYR:CE1	4:A:325:FFA:H122	2.34	0.62
1:B:26:PRO:HB3	1:B:224:GLU:OE2	2.01	0.61
1:B:55:TYR:HE1	4:B:326:FFA:H122	1.66	0.61
1:A:7[A]:CYS:CB	5:A:326:BME:S2	2.81	0.60
1:A:6:GLN:NE2	1:B:9:LYS:H	1.99	0.60
3:A:1:NAP:C4N	4:A:325:FFA:H17	2.32	0.60
1:A:242[A]:CYS:HG	5:A:327:BME:HS2	0.61	0.60
1:B:7[A]:CYS:HG	5:B:327:BME:HS2	1.07	0.59
1:B:55:TYR:CE1	4:B:326:FFA:H122	2.38	0.59
1:A:279:GLN:NE2	3:A:1:NAP:H62A	2.01	0.58
1:B:262:GLN:HE22	1:B:288:LEU:N	1.87	0.58
1:A:43:GLU:HG2	7:A:604:HOH:O	2.03	0.58
1:A:7[A]:CYS:HB2	5:A:326:BME:S2	2.44	0.58
1:B:194:HIS:HD2	1:B:196:TYR:H	1.52	0.57
3:B:2:NAP:C4N	4:B:326:FFA:H17	2.35	0.56
1:A:301:ARG:HG3	1:A:303:VAL:CG2	2.35	0.56
1:A:273:ASN:HD21	1:A:275:GLN:HB3	1.70	0.56
1:A:270:LYS:O	3:A:1:NAP:H8A	2.06	0.55
1:B:278:ARG:HH11	1:B:278:ARG:HG3	1.71	0.55
1:A:262:GLN:HE22	1:A:288:LEU:N	1.89	0.54
1:B:7[B]:CYS:HG	5:B:327:BME:C2	2.15	0.54
1:A:270:LYS:HD3	1:A:270:LYS:C	2.28	0.54
5:A:326:BME:H11	5:B:327:BME:O1	2.08	0.54
1:A:77:GLU:H	1:A:77:GLU:CD	2.11	0.53
1:B:273:ASN:OD1	1:B:275:GLN:HB3	2.08	0.53
1:B:77:GLU:CD	1:B:77:GLU:H	2.12	0.53
1:A:5:TYR:O	5:A:326:BME:H12	2.08	0.53
1:A:3:SER:N	7:A:645:HOH:O	2.42	0.53
1:B:290:SER:O	1:B:294:LYS:HG3	2.08	0.53
1:B:270:LYS:C	1:B:270:LYS:HD3	2.28	0.53
1:A:192:GLU:OE2	1:A:194:HIS:HE1	1.91	0.52
1:A:289:THR:OG1	1:A:292:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:PRO:HB2	1:B:48:HIS:HB2	1.91	0.52
1:B:301:ARG:HG3	1:B:303:VAL:CG2	2.38	0.52
1:B:192:GLU:OE2	1:B:194:HIS:HE1	1.93	0.51
1:A:17:PRO:HB2	1:A:48:HIS:HB2	1.92	0.51
1:A:194:HIS:HD2	1:A:196:TYR:H	1.59	0.51
1:A:4:LYS:HD3	5:B:327:BME:S2	2.50	0.51
1:A:207:LYS:HG2	1:B:287:GLN:NE2	2.25	0.50
1:A:262:GLN:NE2	1:A:288:LEU:H	1.90	0.50
1:B:19:LEU:HB3	6:B:330:EDO:H22	1.93	0.49
5:A:326:BME:C1	5:B:327:BME:O1	2.60	0.49
1:A:242[B]:CYS:SG	5:A:327:BME:S2	3.03	0.49
1:B:22:GLY:HA3	3:B:2:NAP:H4D	1.95	0.48
1:B:200:ARG:C	1:B:200:ARG:HD2	2.35	0.47
1:B:7[B]:CYS:SG	5:B:327:BME:H22	2.53	0.47
1:B:274:GLU:O	1:B:278:ARG:HD3	2.14	0.47
1:A:291:GLU:HG3	7:B:380:HOH:O	2.15	0.47
1:B:133:GLU:HG2	7:B:404:HOH:O	2.15	0.46
1:B:270:LYS:O	3:B:2:NAP:H8A	2.15	0.46
1:A:9:LYS:H	1:B:6:GLN:NE2	2.14	0.46
1:A:22:GLY:HA3	3:A:1:NAP:H4D	1.97	0.46
1:B:190:GLN:OE1	3:B:2:NAP:H2N	2.15	0.46
1:B:273:ASN:ND2	1:B:276:ARG:NH2	2.64	0.45
1:B:262:GLN:NE2	1:B:288:LEU:H	1.88	0.45
1:B:201:LYS:HG3	7:B:564:HOH:O	2.16	0.44
1:A:248:HIS:O	1:A:249:LYS:HB2	2.18	0.44
1:B:240:VAL:HG21	1:B:299:LEU:HD21	1.99	0.44
1:A:193:CYS:HB3	1:A:215:ALA:CB	2.47	0.44
1:A:74:VAL:HG22	1:A:75:LYS:N	2.33	0.44
1:A:96:ARG:HB3	1:A:97:PRO:HD3	1.99	0.44
1:A:6:GLN:HG2	1:B:7[A]:CYS:O	2.17	0.43
1:B:86:TRP:CG	1:B:87:SER:N	2.86	0.43
1:A:9:LYS:H	1:B:6:GLN:HE21	1.67	0.43
1:B:270:LYS:HB2	3:B:2:NAP:H52N	2.01	0.43
1:B:21:PHE:HB3	1:B:49[A]:ILE:HD13	2.00	0.43
1:A:123:LYS:HA	1:A:124:PRO:HD3	1.89	0.43
1:A:190:GLN:OE1	3:A:1:NAP:H2N	2.19	0.42
1:B:91:ARG:NH2	2:B:325:SO4:O2	2.45	0.42
3:B:2:NAP:H4N	4:B:326:FFA:H17	2.00	0.42
1:A:7[B]:CYS:O	1:B:6:GLN:HG2	2.19	0.42
1:A:273:ASN:ND2	1:A:275:GLN:HB3	2.33	0.42
1:A:258:ARG:HE	1:A:262:GLN:NE2	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ARG:NH1	7:A:612:HOH:O	2.53	0.42
1:B:74:VAL:HG22	1:B:75:LYS:N	2.35	0.41
1:A:118:PHE:CE1	1:A:308:LEU:HD12	2.55	0.41
1:B:129:ILE:HG22	1:B:129:ILE:O	2.20	0.41
1:B:31:LYS:HE3	1:B:56:ASN:ND2	2.36	0.41
1:B:35:LEU:HD12	1:B:64:ALA:HB2	2.03	0.41
1:A:7[A]:CYS:O	1:B:6:GLN:HG2	2.20	0.40
1:B:314:PRO:HA	1:B:315:PRO:HD3	1.95	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	323/321 (101%)	315 (98%)	8 (2%)	0	100	100
1	B	323/321 (101%)	313 (97%)	10 (3%)	0	100	100
All	All	646/642 (101%)	628 (97%)	18 (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	286/282 (101%)	285 (100%)	1 (0%)	92	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	286/282 (101%)	283 (99%)	3 (1%)	76	71
All	All	572/564 (101%)	568 (99%)	4 (1%)	84	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	B	199	GLN
1	B	278	ARG
1	B	285	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	53	HIS
1	A	105	ASN
1	A	167	ASN
1	A	178	ASN
1	A	194	HIS
1	A	199	GLN
1	A	231	ASN
1	A	262	GLN
1	A	273	ASN
1	A	279	GLN
1	A	287	GLN
1	B	6	GLN
1	B	53	HIS
1	B	56	ASN
1	B	105	ASN
1	B	167	ASN
1	B	178	ASN
1	B	194	HIS
1	B	199	GLN
1	B	262	GLN
1	B	279	GLN
1	B	287	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

17 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
4	FFA	A	325	-	24,24,24	1.55	4 (16%)	39,39,39	1.26	4 (10%)
5	BME	B	327	-	3,3,3	0.27	0	1,2,2	0.19	0
6	EDO	B	330	-	3,3,3	2.31	1 (33%)	2,2,2	0.29	0
3	NAP	A	1	-	45,52,52	1.47	6 (13%)	56,80,80	0.92	2 (3%)
6	EDO	B	331	-	3,3,3	2.46	1 (33%)	2,2,2	0.31	0
6	EDO	A	328	-	3,3,3	2.44	1 (33%)	2,2,2	0.28	0
6	EDO	B	328	-	3,3,3	2.45	1 (33%)	2,2,2	0.31	0
6	EDO	A	329	-	3,3,3	2.44	1 (33%)	2,2,2	0.32	0
5	BME	A	326	-	3,3,3	0.18	0	1,2,2	0.49	0
3	NAP	B	2	-	45,52,52	1.50	6 (13%)	56,80,80	0.92	0
2	SO4	B	325	-	4,4,4	6.18	4 (100%)	6,6,6	3.15	2 (33%)
5	BME	A	327	-	3,3,3	0.31	0	1,2,2	0.35	0
6	EDO	A	330	-	3,3,3	2.36	1 (33%)	2,2,2	0.28	0
4	FFA	B	326	-	24,24,24	1.54	4 (16%)	39,39,39	1.24	4 (10%)
2	SO4	A	324	-	4,4,4	1.02	0	6,6,6	1.56	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	324	-	4,4,4	1.02	0	6,6,6	1.57	1 (16%)
6	EDO	B	329	-	3,3,3	2.47	1 (33%)	2,2,2	0.33	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
4	FFA	A	325	-	-	-	0/4/4/4
5	BME	B	327	-	-	0/1/1/1	-
6	EDO	B	330	-	-	0/1/1/1	-
3	NAP	A	1	-	-	5/31/67/67	0/5/5/5
6	EDO	B	331	-	-	1/1/1/1	-
6	EDO	A	328	-	-	0/1/1/1	-
6	EDO	B	328	-	-	0/1/1/1	-
6	EDO	A	329	-	-	1/1/1/1	-
5	BME	A	326	-	-	0/1/1/1	-
3	NAP	B	2	-	-	7/31/67/67	0/5/5/5
5	BME	A	327	-	-	0/1/1/1	-
6	EDO	A	330	-	-	0/1/1/1	-
4	FFA	B	326	-	-	-	0/4/4/4
6	EDO	B	329	-	-	0/1/1/1	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	325	SO4	O1-S	7.94	1.89	1.46
2	B	325	SO4	O2-S	7.71	1.87	1.46
3	A	1	NAP	C4N-C3N	4.14	1.46	1.39
3	B	2	NAP	C2N-N1N	4.06	1.39	1.35
6	B	331	EDO	O2-C2	-3.96	1.21	1.42
6	B	329	EDO	O2-C2	-3.96	1.21	1.42
3	A	1	NAP	C6N-N1N	3.95	1.45	1.35
6	B	328	EDO	O2-C2	-3.95	1.21	1.42
6	A	328	EDO	O2-C2	-3.91	1.21	1.42
6	A	329	EDO	O2-C2	-3.90	1.21	1.42
2	B	325	SO4	O3-S	3.90	1.80	1.47
3	B	2	NAP	C6N-N1N	3.88	1.44	1.35
2	B	325	SO4	O4-S	3.88	1.79	1.47
3	B	2	NAP	C4N-C3N	3.84	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	330	EDO	O2-C2	-3.80	1.22	1.42
3	B	2	NAP	C2A-N3A	3.68	1.38	1.32
6	B	330	EDO	O2-C2	-3.66	1.23	1.42
3	A	1	NAP	C2N-N1N	3.54	1.39	1.35
3	B	2	NAP	C4A-N3A	3.53	1.40	1.35
3	A	1	NAP	C2A-N3A	3.44	1.37	1.32
3	A	1	NAP	C4A-N3A	3.43	1.40	1.35
4	B	326	FFA	C11-C7	2.98	1.58	1.53
4	A	325	FFA	C11-C7	2.91	1.58	1.53
4	A	325	FFA	C1-C6	2.48	1.58	1.54
4	B	326	FFA	C1-C6	2.47	1.58	1.54
4	B	326	FFA	C8-C7	2.41	1.58	1.53
4	A	325	FFA	C8-C7	2.39	1.58	1.53
3	A	1	NAP	C2A-N1A	2.27	1.38	1.33
3	B	2	NAP	C2A-N1A	2.26	1.38	1.33
4	A	325	FFA	C6-C7	2.16	1.59	1.56
4	B	326	FFA	C6-C7	2.03	1.59	1.56

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	325	SO4	O4-S-O3	6.47	136.69	109.06
2	B	325	SO4	O2-S-O1	-3.90	80.66	109.43
2	B	324	SO4	O4-S-O3	3.61	124.46	109.06
2	A	324	SO4	O4-S-O3	3.59	124.40	109.06
4	A	325	FFA	C14-C13-C17	3.52	102.99	99.27
4	B	326	FFA	C14-C13-C17	3.36	102.82	99.27
4	A	325	FFA	C18-C13-C17	-2.47	105.61	109.54
4	B	326	FFA	C18-C13-C14	2.47	116.32	111.71
4	A	325	FFA	C18-C13-C14	2.43	116.25	111.71
4	B	326	FFA	C18-C13-C17	-2.42	105.69	109.54
4	B	326	FFA	C2-C1-C6	2.42	117.99	113.45
4	A	325	FFA	C2-C1-C6	2.27	117.72	113.45
3	A	1	NAP	PN-O3-PA	2.04	139.81	132.83
3	A	1	NAP	N3A-C2A-N1A	-2.00	125.55	128.68

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	329	EDO	O1-C1-C2-O2
3	A	1	NAP	PA-O3-PN-O1N

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Mol	Chain	Res	Type	Atoms
3	B	2	NAP	PA-O3-PN-O1N
3	B	2	NAP	PA-O3-PN-O5D
3	B	2	NAP	C5B-O5B-PA-O3
3	A	1	NAP	O4B-C4B-C5B-O5B
6	B	331	EDO	O1-C1-C2-O2
3	B	2	NAP	O4B-C4B-C5B-O5B
3	A	1	NAP	C4D-C5D-O5D-PN
3	A	1	NAP	PA-O3-PN-O5D
3	A	1	NAP	C3B-C4B-C5B-O5B
3	B	2	NAP	C5B-O5B-PA-O1A
3	B	2	NAP	C3B-C4B-C5B-O5B
3	B	2	NAP	C4D-C5D-O5D-PN

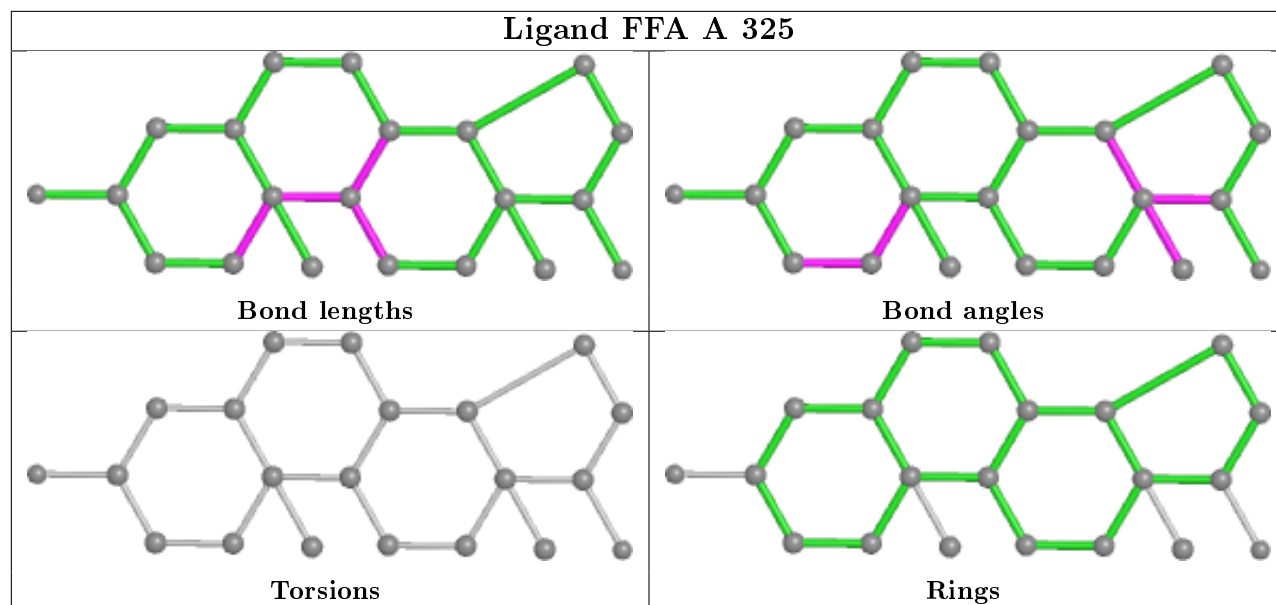
There are no ring outliers.

9 monomers are involved in 39 short contacts:

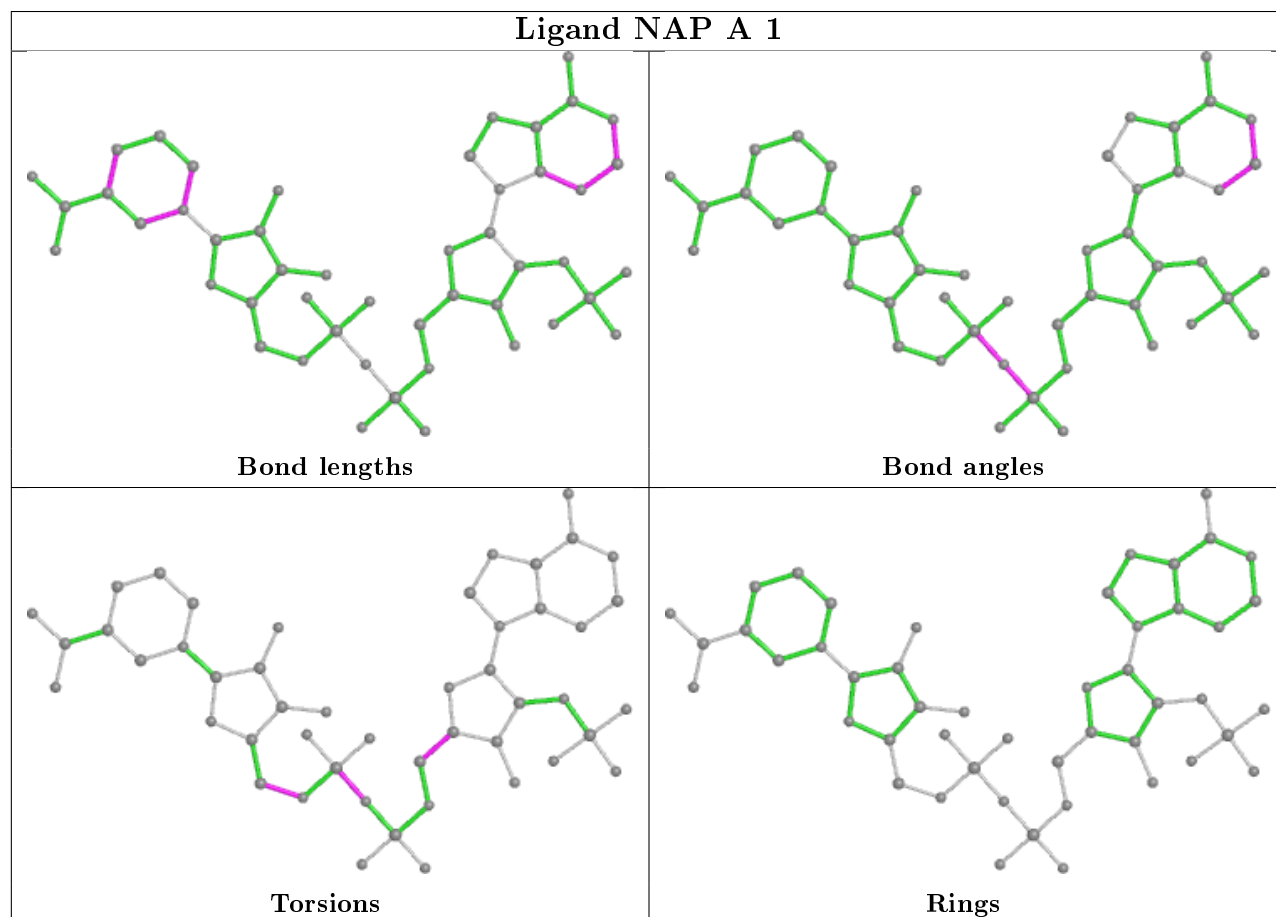
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	325	FFA	3	0
5	B	327	BME	13	0
6	B	330	EDO	1	0
3	A	1	NAP	5	0
5	A	326	BME	6	0
3	B	2	NAP	7	0
2	B	325	SO4	1	0
5	A	327	BME	4	0
4	B	326	FFA	4	0

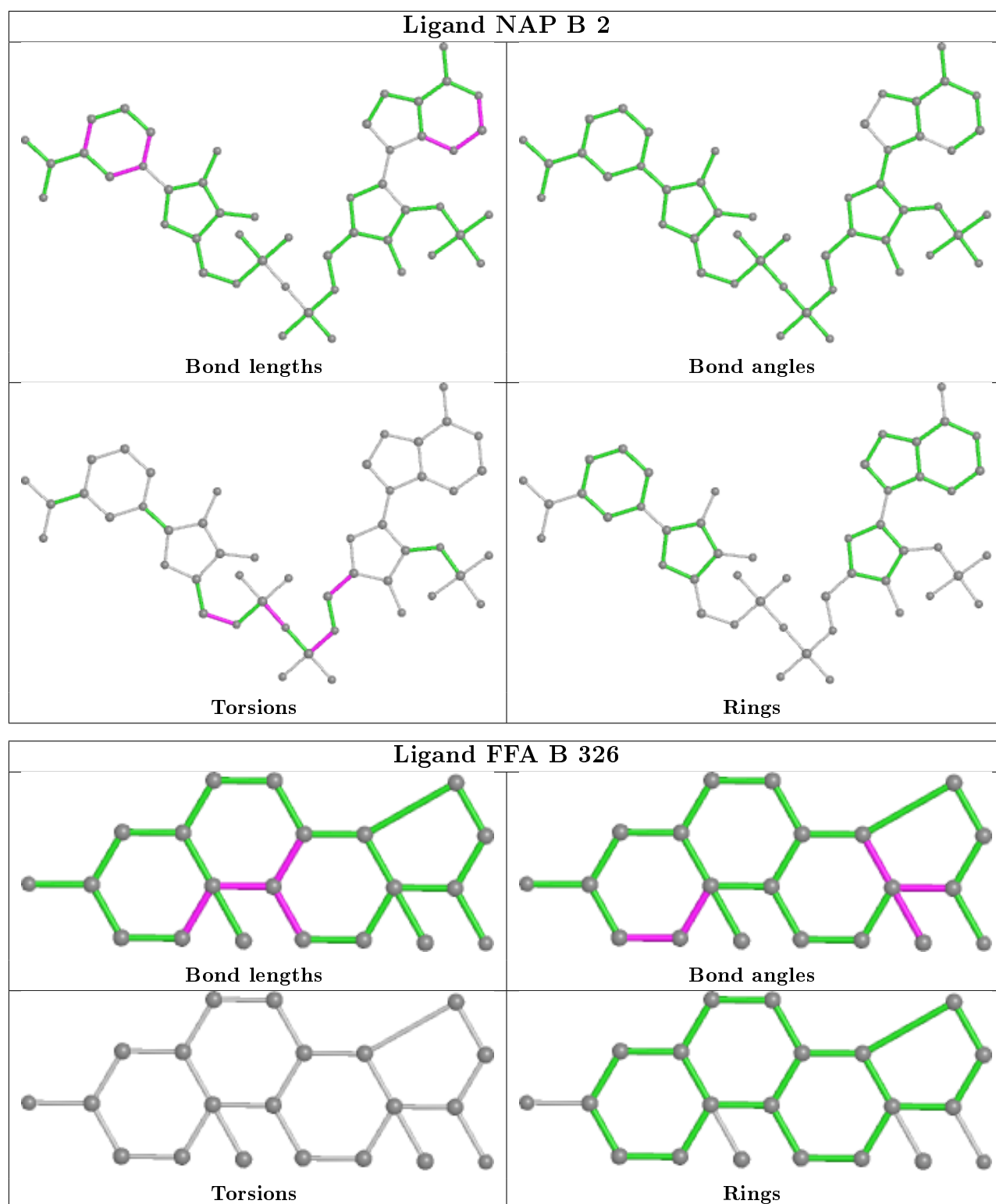
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 FFA A 325



Ligand NAP A 1





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	321/321 (100%)	-0.07	9 (2%)	53	47	17, 25, 41, 61	22 (6%)
1	B	321/321 (100%)	0.04	19 (5%)	22	17	10, 24, 50, 56	22 (6%)
All	All	642/642 (100%)	-0.01	28 (4%)	34	28	10, 25, 47, 61	44 (6%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	ASN	4.6
1	B	29	VAL	4.3
1	A	226	PRO	4.1
1	B	230	PRO	4.1
1	B	27	ALA	3.9
1	B	231	ASN	3.4
1	B	28	GLU	3.0
1	B	224	GLU	2.8
1	B	70	ALA	2.8
1	A	3	SER	2.8
1	B	249	LYS	2.8
1	A	229	ASP	2.8
1	B	246	LYS	2.7
1	A	225	GLU	2.7
1	B	226	PRO	2.7
1	B	275	GLN	2.4
1	A	28	GLU	2.4
1	B	32	SER	2.3
1	B	30	PRO	2.3
1	A	230	PRO	2.3
1	B	237	GLU	2.2
1	A	224	GLU	2.2
1	B	33	LYS	2.2
1	B	26	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	233	PRO	2.1
1	A	27	ALA	2.1
1	B	242[A]	CYS	2.1
1	B	49[A]	ILE	2.0

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

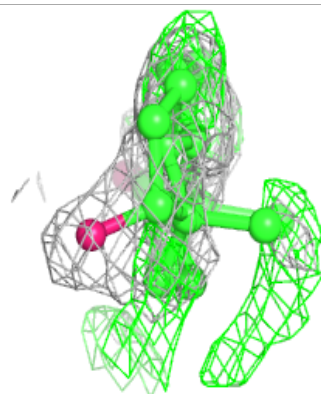
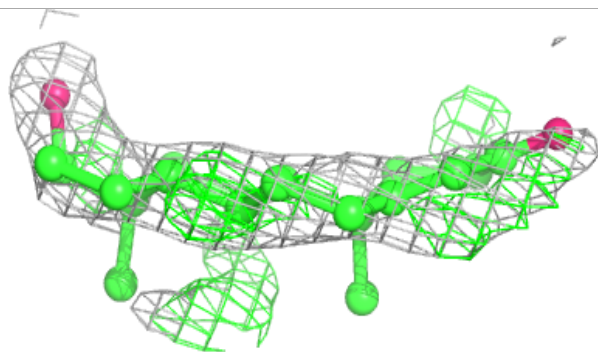
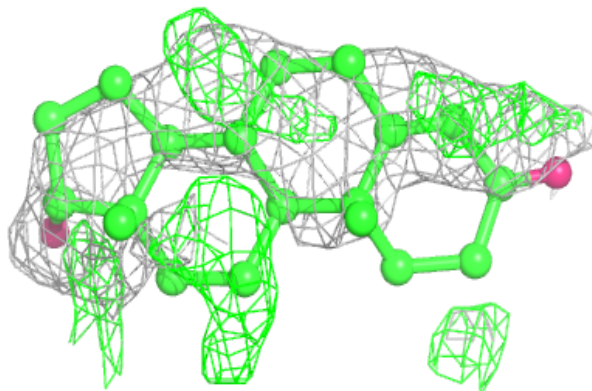
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FFA	A	325	21/21	0.56	0.51	38,42,43,43	21
5	BME	A	327	4/4	0.63	0.30	51,51,52,52	4
4	FFA	B	326	21/21	0.65	0.42	36,42,43,43	21
5	BME	B	327	4/4	0.70	0.63	37,38,39,40	4
2	SO4	A	324	5/5	0.74	0.26	51,51,52,52	5
2	SO4	B	324	5/5	0.77	0.23	50,51,51,51	5
5	BME	A	326	4/4	0.84	0.59	34,36,37,38	4
6	EDO	B	328	4/4	0.88	0.13	30,32,33,35	0
6	EDO	B	330	4/4	0.88	0.12	23,25,26,29	0
6	EDO	B	331	4/4	0.89	0.09	55,57,58,58	0
6	EDO	A	329	4/4	0.91	0.18	46,48,49,49	0
6	EDO	B	329	4/4	0.92	0.16	48,50,50,50	0
3	NAP	B	2	48/48	0.93	0.11	21,37,48,50	0
6	EDO	A	328	4/4	0.94	0.16	31,35,36,36	0
3	NAP	A	1	48/48	0.96	0.09	20,26,32,36	0
6	EDO	A	330	4/4	0.96	0.08	17,19,23,24	0
2	SO4	B	325	5/5	0.97	0.30	43,44,45,45	5

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.

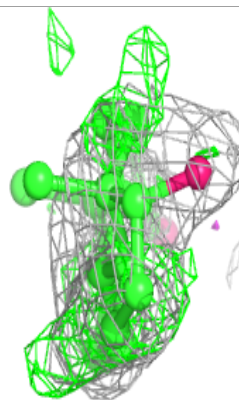
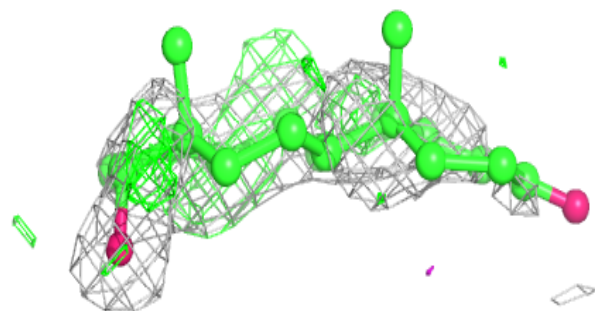
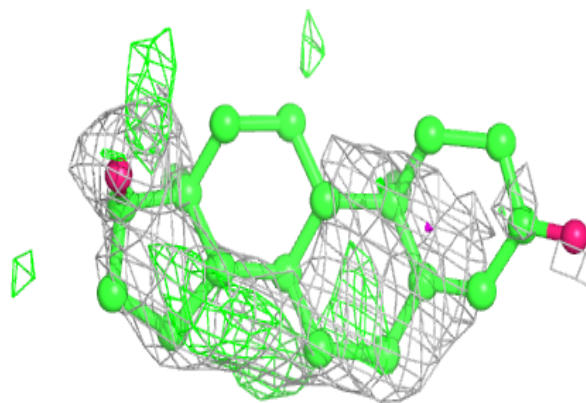
Electron density around FFA A 325:

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

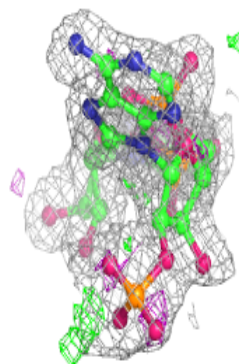
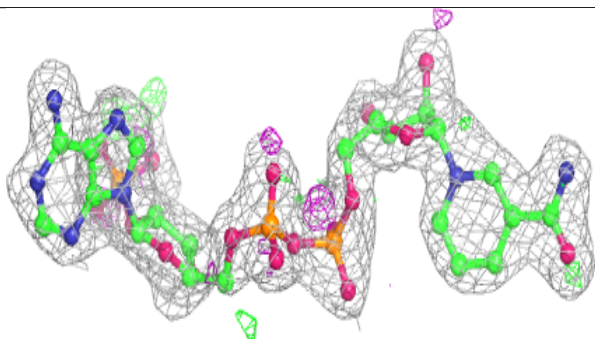
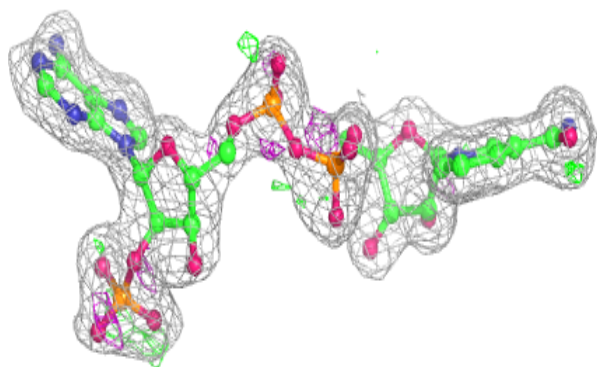


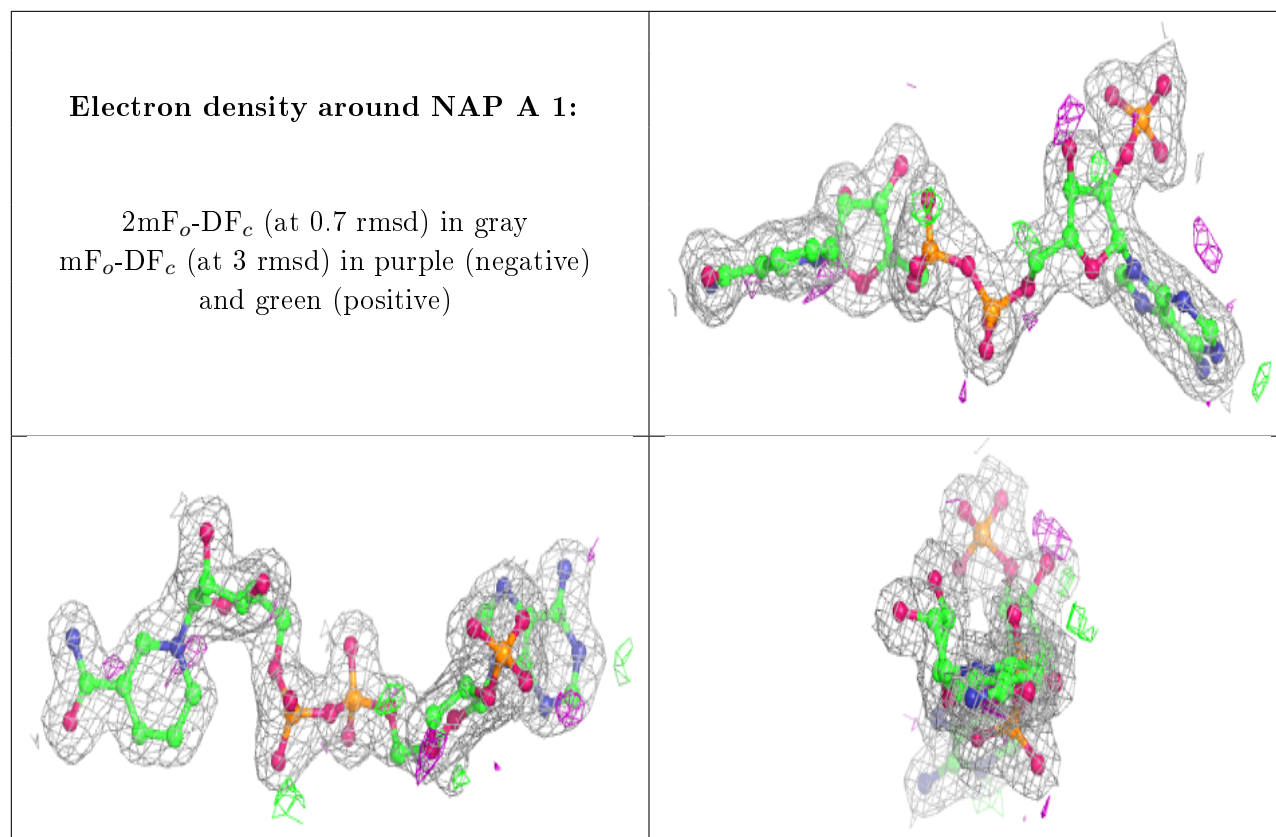
Electron density around FFA B 326:

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

**Electron density around NAP B 2:**

$2mF_o-DF_c$ (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.