



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 12:12 AM BST

PDB ID : 6A0T
Title : Homoserine dehydrogenase K99A mutant from *Thermus thermophilus* HB8 complexed with HSE and NADP+
Authors : Akai, S.; Ikushiro, H.; Sawai, T.; Yano, T.; Kamiya, N.; Miyahara, I.
Deposited on : 2018-06-06
Resolution : 1.87 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 : 2.13.1
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) : 2.13.1

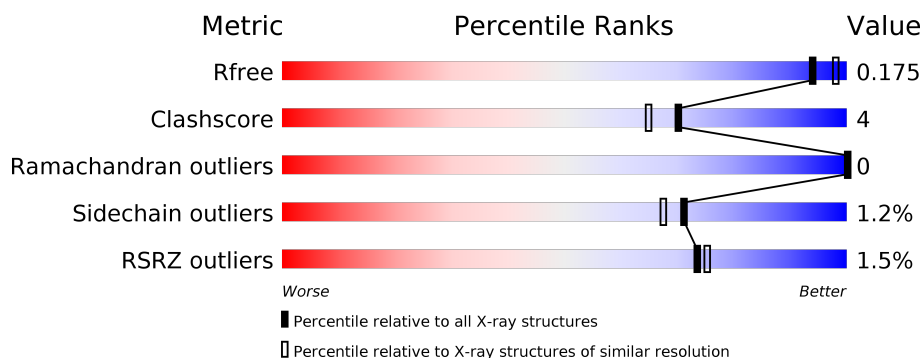
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	332	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div></div> </div> </div>
1	B	332	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div></div> </div> </div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6425 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.

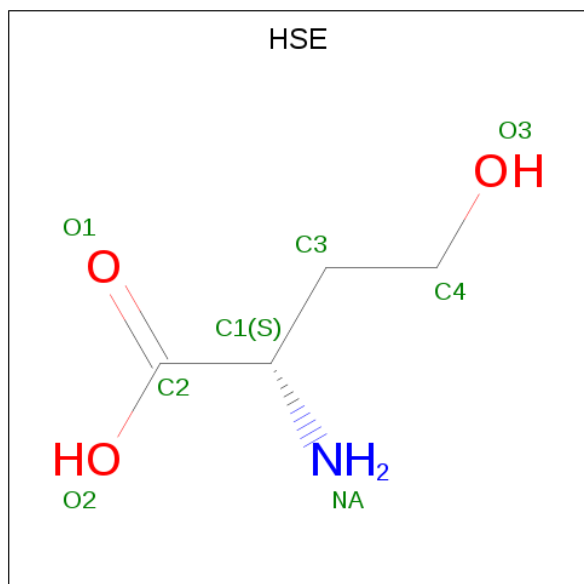
- Molecule 1 is a protein called Homoserine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	332	Total	C	N	O	S	0	18	0
			2657	1690	475	488	4			
1	A	331	Total	C	N	O	S	0	18	0
			2635	1683	471	477	4			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

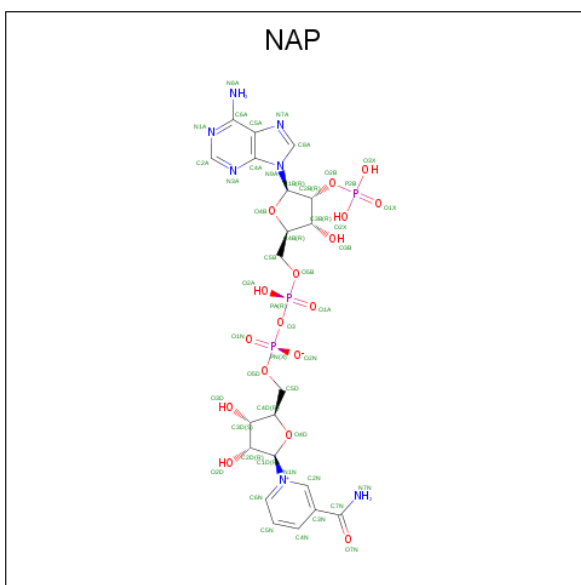
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is L-HOMOSERINE (three-letter code: HSE) (formula: C₄H₉NO₃).



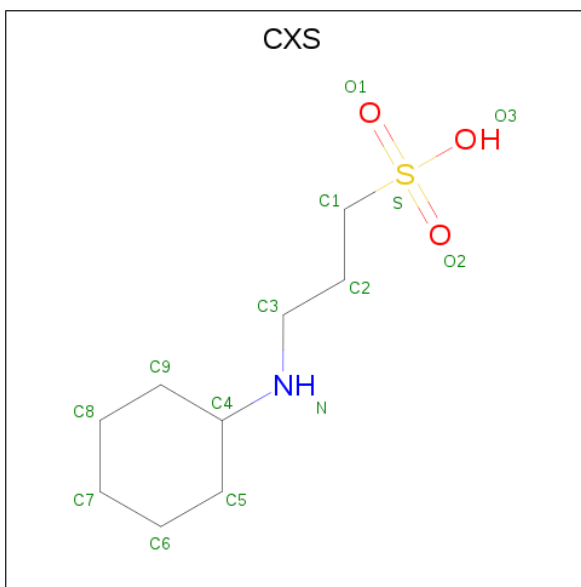
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 8	C 4	N 1	O 3	0	0
3	A	1	Total 8	C 4	N 1	O 3	0	0

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



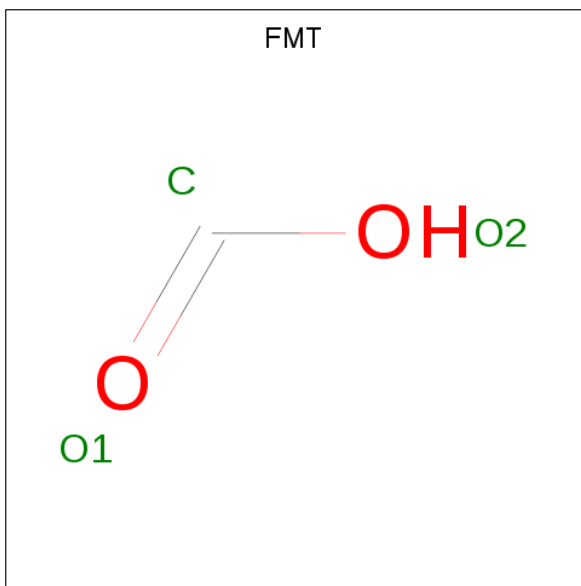
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	A	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 5 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula: $C_9H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

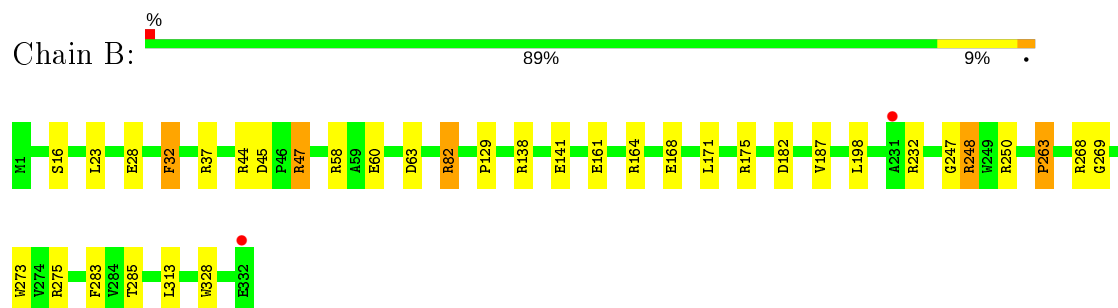
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	471	Total	O	0	35
			489	489		
8	A	439	Total	O	0	31
			456	456		

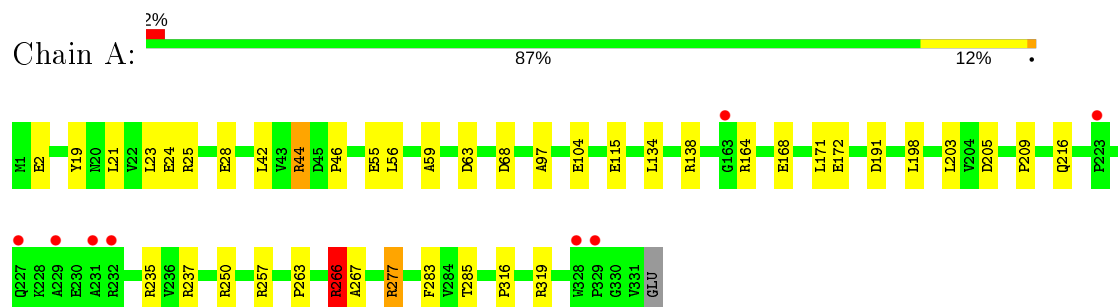
3 Residue-property plots [i](#)

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: Homoserine dehydrogenase



- Molecule 1: Homoserine dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.40Å 121.40Å 145.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.87 38.33 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.87) 99.9 (38.33-1.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.68 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.137 , 0.167 0.150 , 0.175	Depositor DCC
R_{free} test set	5175 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6425	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CXS, HSE, NA, FMT, NAP

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	1.34	13/2691 (0.5%)	1.29	25/3662 (0.7%)
1	B	1.41	12/2713 (0.4%)	1.41	22/3688 (0.6%)
All	All	1.38	25/5404 (0.5%)	1.35	47/7350 (0.6%)

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	2
1	B	0	1
All	All	0	3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	16	SER	CB-OG	-10.95	1.28	1.42
1	B	168[A]	GLU	CD-OE2	-8.22	1.16	1.25
1	B	168[B]	GLU	CD-OE2	-8.22	1.16	1.25
1	A	55	GLU	CD-OE1	7.41	1.33	1.25
1	A	28	GLU	CD-OE1	7.28	1.33	1.25
1	A	172	GLU	CG-CD	6.86	1.62	1.51
1	A	24	GLU	CB-CG	-6.67	1.39	1.52
1	B	273	TRP	CE3-CZ3	6.20	1.49	1.38
1	B	141	GLU	CG-CD	6.12	1.61	1.51
1	B	60	GLU	CD-OE1	5.88	1.32	1.25
1	A	172	GLU	CB-CG	5.88	1.63	1.52
1	A	28	GLU	CD-OE2	5.77	1.31	1.25
1	B	32	PHE	CG-CD1	-5.73	1.30	1.38
1	B	187	VAL	CB-CG2	-5.58	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	ARG	CD-NE	5.49	1.55	1.46
1	A	24	GLU	CD-OE1	5.49	1.31	1.25
1	B	28	GLU	CD-OE1	5.48	1.31	1.25
1	B	161	GLU	CB-CG	-5.36	1.42	1.52
1	A	168	GLU	CD-OE2	5.31	1.31	1.25
1	A	104	GLU	CG-CD	5.30	1.59	1.51
1	A	104	GLU	CD-OE2	5.21	1.31	1.25
1	A	266	ARG	CG-CD	5.12	1.64	1.51
1	B	45[A]	ASP	N-CA	-5.12	1.36	1.46
1	B	45[B]	ASP	N-CA	-5.12	1.36	1.46
1	A	115	GLU	CG-CD	5.07	1.59	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82[A]	ARG	NE-CZ-NH1	-16.86	111.87	120.30
1	B	82[B]	ARG	NE-CZ-NH1	-16.86	111.87	120.30
1	A	44	ARG	NE-CZ-NH2	-13.55	113.52	120.30
1	A	44	ARG	NE-CZ-NH1	12.39	126.50	120.30
1	B	63	ASP	CB-CG-OD1	11.99	129.09	118.30
1	B	82[A]	ARG	NE-CZ-NH2	10.68	125.64	120.30
1	B	82[B]	ARG	NE-CZ-NH2	10.68	125.64	120.30
1	A	138	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	B	37	ARG	NE-CZ-NH2	9.47	125.04	120.30
1	B	63	ASP	CB-CG-OD2	-8.97	110.23	118.30
1	A	164	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	A	266	ARG	CG-CD-NE	8.37	129.38	111.80
1	B	248	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	B	182	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	B	45[A]	ASP	CB-CG-OD1	-7.97	111.13	118.30
1	B	45[B]	ASP	CB-CG-OD1	-7.97	111.13	118.30
1	B	250	ARG	NE-CZ-NH2	7.73	124.17	120.30
1	A	266	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	58	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	277[A]	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	277[B]	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	198	LEU	CB-CG-CD1	6.65	122.30	111.00
1	B	138	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	266	ARG	CA-CB-CG	6.57	127.86	113.40
1	A	138	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	63	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	172	GLU	OE1-CD-OE2	-6.37	115.66	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269[A]	GLY	N-CA-C	-6.11	97.83	113.10
1	B	269[B]	GLY	N-CA-C	-6.11	97.83	113.10
1	A	68	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	A	56	LEU	CB-CG-CD1	-5.82	101.11	111.00
1	B	23	LEU	CB-CG-CD2	5.77	120.81	111.00
1	A	235	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	28	GLU	OE1-CD-OE2	5.55	129.96	123.30
1	B	250	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	198	LEU	CB-CG-CD2	5.48	120.32	111.00
1	A	257	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	A	44	ARG	CG-CD-NE	-5.34	100.59	111.80
1	A	257	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	B	268[A]	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	268[B]	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	205	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	191	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	A	25	ARG	CB-CG-CD	5.06	124.75	111.60
1	A	237	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	2	GLU	CA-CB-CG	5.01	124.41	113.40
1	B	164	ARG	CA-CB-CG	-5.00	102.40	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	ARG	Mainchain
1	A	44	ARG	Sidechain
1	B	129	PRO	Mainchain

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	2635	0	2663	16	0
1	B	2657	0	2669	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	8	1	0
3	B	8	0	8	1	0
4	A	48	0	25	3	0
4	B	48	0	25	1	0
5	B	14	0	18	0	0
6	A	18	0	7	0	0
6	B	12	0	4	0	0
7	A	18	0	24	0	0
7	B	12	0	16	2	0
8	A	456	0	0	4	1
8	B	489	0	0	9	1
All	All	6425	0	5467	40	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (40) 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:B:283[A]:PHE:CE2	1:B:285[A]:THR:CG2	2.53	0.91
1:A:171[A]:LEU:HD12	8:A:860[A]:HOH:O	1.78	0.81
1:A:277[A]:ARG:HH11	1:A:277[A]:ARG:HG3	1.43	0.80
1:B:283[A]:PHE:CE2	1:B:285[A]:THR:HG23	2.17	0.79
1:B:283[A]:PHE:CZ	1:B:285[A]:THR:CG2	2.72	0.72
1:B:171:LEU:HD21	1:B:175[A]:ARG:CZ	2.27	0.64
1:B:171:LEU:CD2	1:B:175[A]:ARG:CZ	2.77	0.63
1:B:283[A]:PHE:CE2	1:B:285[A]:THR:HG21	2.34	0.61
1:A:21[B]:LEU:HD23	1:A:21[B]:LEU:C	2.21	0.61
1:A:285[A]:THR:HG21	8:A:747[A]:HOH:O	1.99	0.61
1:A:277[A]:ARG:HH11	1:A:277[A]:ARG:CG	2.14	0.61
1:B:283[A]:PHE:CZ	1:B:285[A]:THR:HG22	2.41	0.55
1:A:171[A]:LEU:CD1	8:A:860[A]:HOH:O	2.46	0.55
1:B:232:ARG:NH2	8:B:510:HOH:O	2.37	0.54
1:B:171:LEU:HD22	1:B:175[A]:ARG:NH2	2.23	0.54
3:B:402:HSE:H42	4:B:403:NAP:C4N	2.40	0.51
1:A:19:TYR:CE2	1:A:23[B]:LEU:HD11	2.46	0.51
1:B:47:ARG:NH1	8:B:519:HOH:O	2.44	0.51
1:B:82[B]:ARG:NH2	8:B:878[B]:HOH:O	2.44	0.50
8:B:512:HOH:O	1:A:266:ARG:NH2	2.46	0.48
1:A:216[B]:GLN:HG3	1:A:216[B]:GLN:O	2.08	0.46
1:B:247:GLY:HA2	8:B:711:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275[A]:ARG:NH2	8:B:520:HOH:O	2.46	0.46
1:B:32:PHE:CE1	1:A:316:PRO:HG3	2.51	0.46
1:A:134:LEU:HD22	1:A:203:LEU:HD11	1.99	0.45
1:B:82[A]:ARG:HD3	8:B:857:HOH:O	2.17	0.45
1:B:44:ARG:HD3	8:B:663:HOH:O	2.17	0.44
1:A:97:ALA:O	4:A:403:NAP:H6N	2.17	0.44
1:B:328:TRP:CZ2	7:B:410:GOL:H31	2.52	0.43
1:A:42:LEU:HG	4:A:403:NAP:H2A	2.01	0.43
1:B:171:LEU:HD23	1:B:171:LEU:C	2.39	0.43
1:B:263:PRO:HB3	1:B:283[B]:PHE:CZ	2.54	0.43
1:B:171:LEU:HD22	1:B:175[A]:ARG:CZ	2.49	0.42
1:B:82[A]:ARG:CD	8:B:857:HOH:O	2.68	0.42
1:A:267[A]:ALA:HB2	1:A:283[A]:PHE:HZ	1.85	0.42
3:A:402:HSE:H42	4:A:403:NAP:C4N	2.50	0.41
1:A:46:PRO:HG3	1:A:59:ALA:HB2	2.01	0.41
1:B:328:TRP:CE2	7:B:410:GOL:H31	2.56	0.41
1:B:313:LEU:HD12	8:A:806:HOH:O	2.20	0.41
1:A:263:PRO:HB3	1:A:283[B]:PHE:CZ	2.56	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:830:HOH:O	8:A:674:HOH:O[4_455]	2.18	0.02

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	347/332 (104%)	340 (98%)	7 (2%)	0	100	100
1	B	348/332 (105%)	338 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	695/664 (105%)	678 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	260/248 (105%)	256 (98%)	4 (2%)	65	59
1	B	262/248 (106%)	259 (99%)	3 (1%)	73	70
All	All	522/496 (105%)	515 (99%)	7 (1%)	71	64

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	ARG
1	B	248	ARG
1	B	263	PRO
1	A	209	PRO
1	A	250[A]	ARG
1	A	250[B]	ARG
1	A	319	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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
6	FMT	A	406	-	0,2,2	0.00	-	0,1,1	0.00	-
7	GOL	B	409	-	5,5,5	0.86	0	5,5,5	1.39	1 (20%)
6	FMT	A	405	-	0,2,2	0.00	-	0,1,1	0.00	-
4	NAP	B	403	-	45,52,52	1.55	6 (13%)	56,80,80	1.65	12 (21%)
3	HSE	A	402	-	3,7,7	1.22	0	1,8,8	1.46	0
5	CXS	B	404	-	14,14,14	2.33	3 (21%)	18,18,18	2.10	6 (33%)
6	FMT	A	408	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	408	-	0,2,2	0.00	-	0,1,1	0.00	-
7	GOL	A	410	-	5,5,5	0.56	0	5,5,5	1.59	1 (20%)
7	GOL	B	410	-	5,5,5	0.73	0	5,5,5	0.97	0
6	FMT	B	407	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	407	-	0,2,2	0.00	-	0,1,1	0.00	-
4	NAP	A	403	-	45,52,52	1.56	9 (20%)	56,80,80	1.53	11 (19%)
6	FMT	B	405	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	409	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	404	-	0,2,2	0.00	-	0,1,1	0.00	-
7	GOL	A	411	-	5,5,5	0.32	0	5,5,5	0.98	0
3	HSE	B	402	-	3,7,7	0.80	0	1,8,8	0.54	0
6	FMT	B	406	-	0,2,2	0.00	-	0,1,1	0.00	-
7	GOL	A	412	-	5,5,5	0.95	0	5,5,5	0.99	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
7	GOL	B	409	-	-	0/4/4/4	-
4	NAP	B	403	-	-	7/31/67/67	0/5/5/5
3	HSE	A	402	-	-	0/3/7/7	-
5	CXS	B	404	-	-	4/8/16/16	0/1/1/1
7	GOL	A	410	-	-	3/4/4/4	-
7	GOL	B	410	-	-	3/4/4/4	-
4	NAP	A	403	-	-	7/31/67/67	0/5/5/5
7	GOL	A	411	-	-	0/4/4/4	-
3	HSE	B	402	-	-	0/3/7/7	-
7	GOL	A	412	-	-	0/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	404	CXS	C1-S	-6.15	1.68	1.77
5	B	404	CXS	O2-S	5.21	1.60	1.45
4	B	403	NAP	O4B-C1B	4.90	1.47	1.41
4	B	403	NAP	C2D-C1D	3.64	1.59	1.53
4	A	403	NAP	O4B-C1B	3.60	1.46	1.41
4	A	403	NAP	P2B-O2B	3.58	1.66	1.59
4	A	403	NAP	PA-O2A	-3.40	1.39	1.55
4	B	403	NAP	C2A-N3A	3.18	1.37	1.32
4	A	403	NAP	O4B-C4B	-3.02	1.38	1.45
4	B	403	NAP	PA-O2A	-2.96	1.41	1.55
5	B	404	CXS	C3-N	2.70	1.52	1.47
4	B	403	NAP	C2N-C3N	-2.49	1.35	1.39
4	A	403	NAP	P2B-O3X	-2.43	1.45	1.54
4	A	403	NAP	PN-O2N	-2.20	1.45	1.55
4	B	403	NAP	C4A-N3A	2.20	1.38	1.35
4	A	403	NAP	C4N-C3N	2.15	1.43	1.39
4	A	403	NAP	C2A-N1A	2.13	1.37	1.33
4	A	403	NAP	O4D-C1D	2.03	1.43	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	404	CXS	C3-N-C4	4.25	122.47	114.14
4	A	403	NAP	N3A-C2A-N1A	-4.23	122.06	128.68
4	B	403	NAP	N3A-C2A-N1A	-3.96	122.49	128.68
5	B	404	CXS	O3-S-O1	-3.74	102.13	111.27
5	B	404	CXS	C2-C1-S	3.46	118.56	113.25
4	B	403	NAP	O2B-P2B-O1X	-3.42	96.20	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	NAP	O3D-C3D-C4D	-3.31	101.48	111.05
4	B	403	NAP	PN-O3-PA	-3.22	121.78	132.83
4	B	403	NAP	O4B-C1B-C2B	3.17	112.08	106.59
4	B	403	NAP	O3X-P2B-O1X	3.11	122.86	110.68
4	A	403	NAP	PN-O3-PA	-2.94	122.73	132.83
4	A	403	NAP	O3D-C3D-C4D	-2.92	102.60	111.05
4	A	403	NAP	C6N-N1N-C2N	-2.89	119.34	121.97
4	B	403	NAP	C6N-C5N-C4N	2.83	123.56	119.44
7	B	409	GOL	C3-C2-C1	-2.69	101.25	111.70
4	A	403	NAP	C3N-C2N-N1N	2.68	123.05	120.43
5	B	404	CXS	O2-S-C1	2.60	110.04	106.92
4	B	403	NAP	C3N-C2N-N1N	2.54	122.91	120.43
4	A	403	NAP	C3D-C2D-C1D	-2.49	97.23	100.98
4	B	403	NAP	C6N-N1N-C2N	-2.47	119.72	121.97
5	B	404	CXS	O2-S-O1	2.47	122.50	113.95
7	A	410	GOL	O3-C3-C2	-2.44	98.50	110.20
4	B	403	NAP	O3X-P2B-O2B	2.42	116.81	105.99
4	A	403	NAP	C4A-C5A-N7A	2.36	111.86	109.40
4	A	403	NAP	C2A-N1A-C6A	2.35	122.78	118.75
4	B	403	NAP	C5N-C4N-C3N	-2.20	117.75	120.34
4	B	403	NAP	C2A-N1A-C6A	2.16	122.45	118.75
4	A	403	NAP	C2N-N1N-C1D	2.16	123.95	119.14
4	A	403	NAP	O2X-P2B-O2B	-2.15	96.34	105.99
4	A	403	NAP	C3N-C7N-N7N	2.08	120.25	117.75
5	B	404	CXS	C9-C4-C5	-2.05	107.26	110.82

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	NAP	O4D-C1D-N1N-C2N
4	B	403	NAP	O4D-C1D-N1N-C6N
4	B	403	NAP	C2D-C1D-N1N-C2N
4	B	403	NAP	C2D-C1D-N1N-C6N
4	A	403	NAP	O4D-C1D-N1N-C2N
4	A	403	NAP	O4D-C1D-N1N-C6N
4	A	403	NAP	C2D-C1D-N1N-C2N
4	A	403	NAP	C2D-C1D-N1N-C6N
7	A	410	GOL	O1-C1-C2-C3
7	B	410	GOL	C1-C2-C3-O3
4	B	403	NAP	C3B-C2B-O2B-P2B
5	B	404	CXS	C2-C1-S-O3

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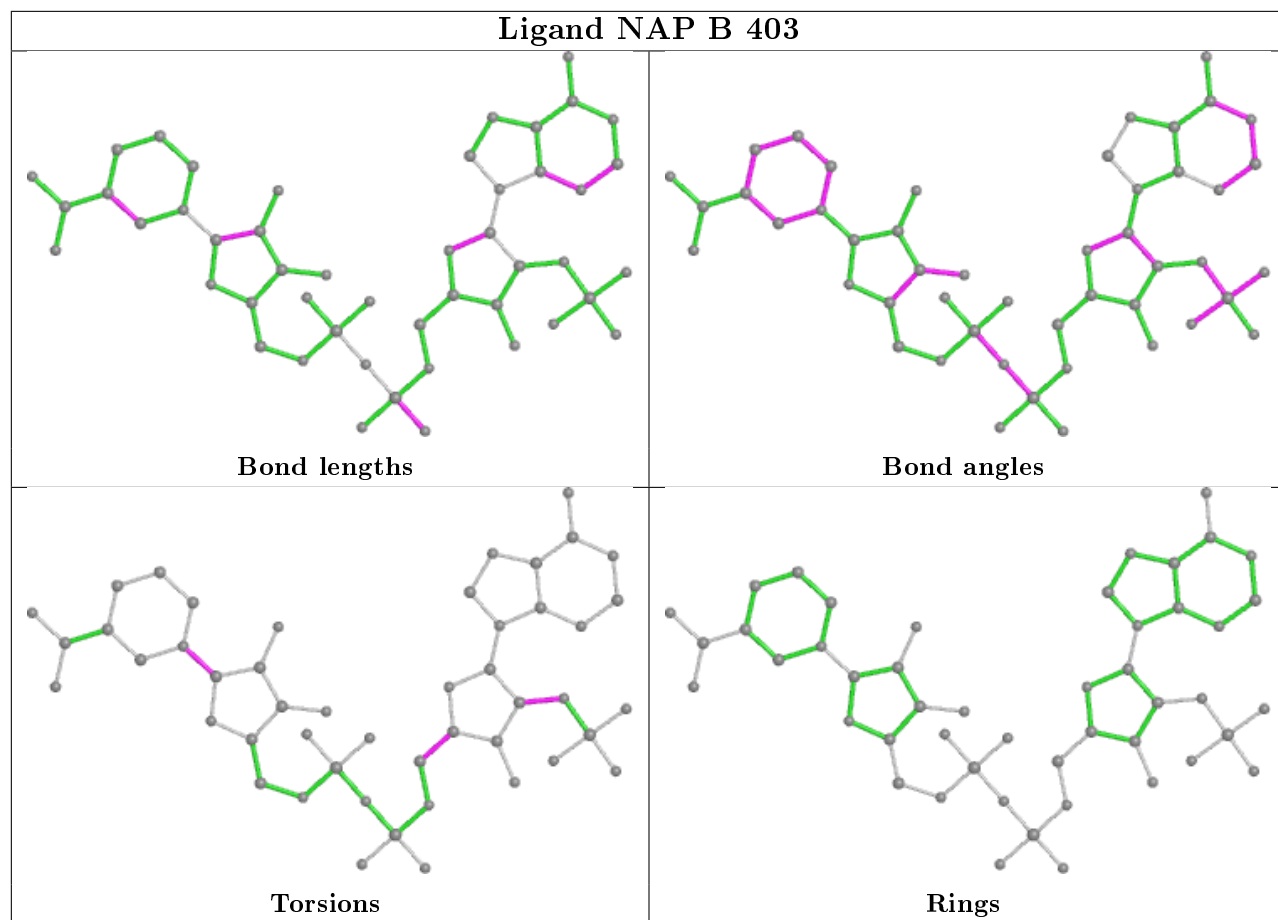
Mol	Chain	Res	Type	Atoms
4	A	403	NAP	C3B-C2B-O2B-P2B
4	A	403	NAP	C1B-C2B-O2B-P2B
7	B	410	GOL	O2-C2-C3-O3
7	A	410	GOL	O1-C1-C2-O2
4	B	403	NAP	C1B-C2B-O2B-P2B
5	B	404	CXS	C2-C1-S-O1
5	B	404	CXS	C2-C1-S-O2
5	B	404	CXS	C1-C2-C3-N
7	A	410	GOL	C1-C2-C3-O3
7	B	410	GOL	O1-C1-C2-O2
4	A	403	NAP	O4B-C4B-C5B-O5B
4	B	403	NAP	O4B-C4B-C5B-O5B

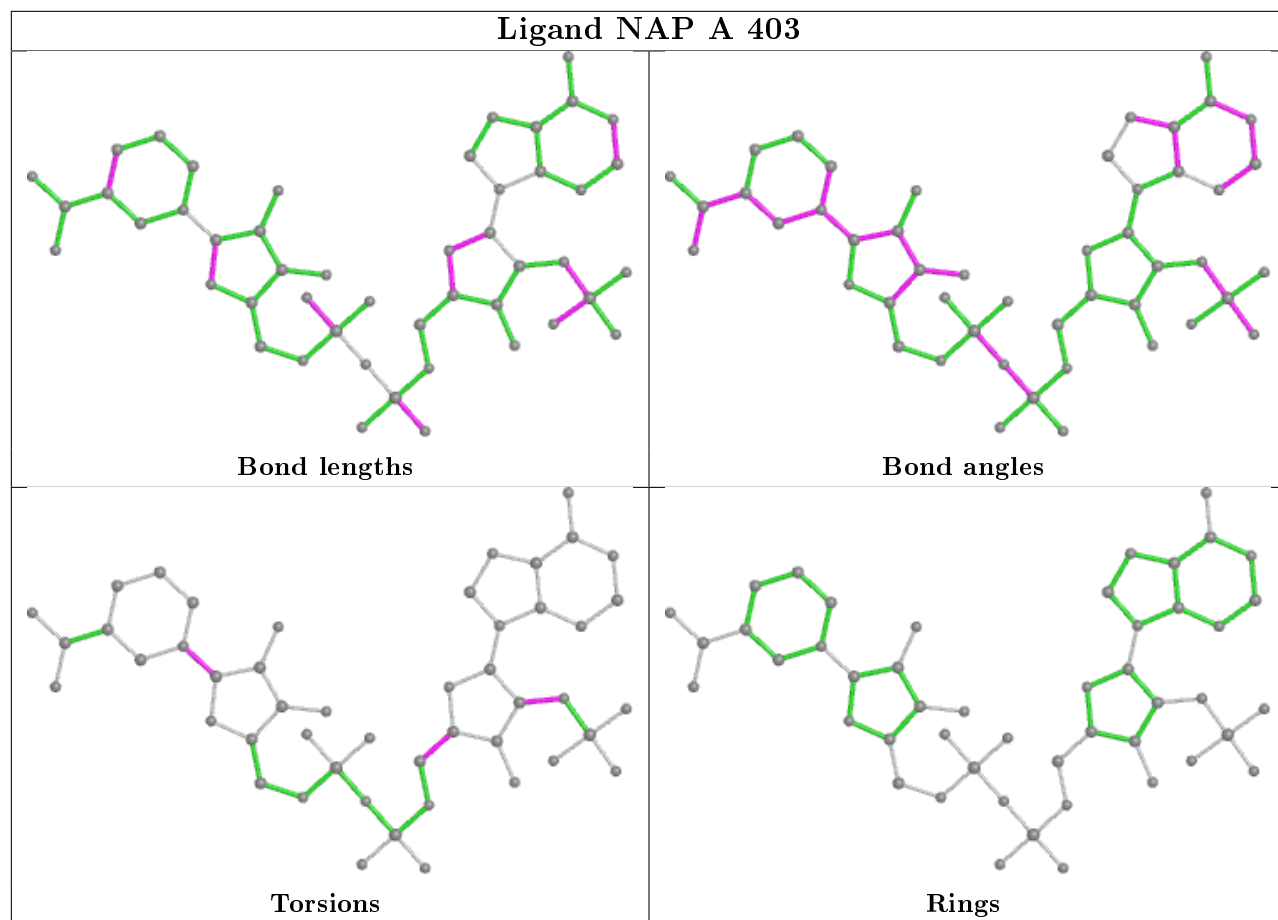
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	NAP	1	0
3	A	402	HSE	1	0
7	B	410	GOL	2	0
4	A	403	NAP	3	0
3	B	402	HSE	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 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	331/332 (99%)	-0.44	8 (2%) 59 60	12, 19, 43, 69	0
1	B	332/332 (100%)	-0.51	2 (0%) 89 90	12, 18, 38, 71	0
All	All	663/664 (99%)	-0.48	10 (1%) 73 75	12, 19, 41, 71	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	GLY	3.5
1	A	227	GLN	3.3
1	B	332	GLU	3.3
1	A	231	ALA	3.2
1	A	229	ALA	3.1
1	A	223	PRO	2.7
1	A	328	TRP	2.1
1	A	232	ARG	2.1
1	A	329	PRO	2.1
1	B	231	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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 ⓘ

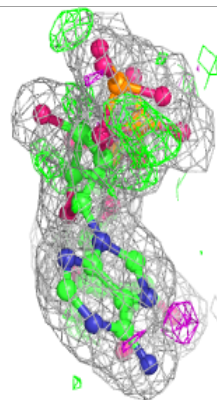
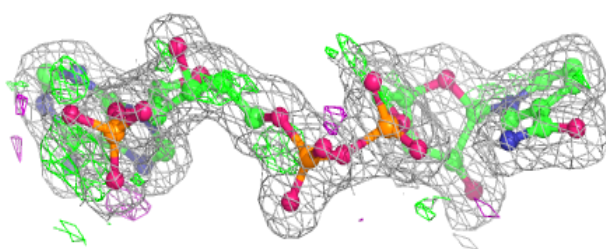
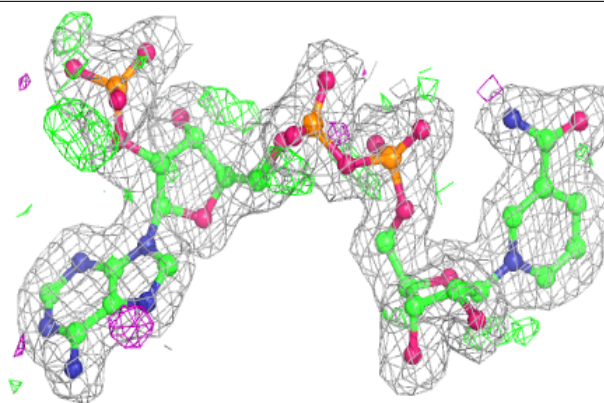
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	A	412	6/6	0.82	0.24	36,45,52,55	6
5	CXS	B	404	14/14	0.86	0.15	22,33,51,59	14
7	GOL	B	410	6/6	0.88	0.13	39,40,44,45	6
7	GOL	A	411	6/6	0.88	0.12	37,40,44,47	6
6	FMT	B	406	3/3	0.91	0.21	31,31,48,52	0
6	FMT	A	409	3/3	0.94	0.17	39,39,41,44	0
7	GOL	B	409	6/6	0.95	0.08	27,32,38,40	0
7	GOL	A	410	6/6	0.95	0.10	23,31,39,41	0
6	FMT	A	405	3/3	0.95	0.09	35,35,41,48	0
6	FMT	B	408	3/3	0.96	0.11	30,30,34,34	0
6	FMT	B	407	3/3	0.96	0.16	35,35,44,62	0
6	FMT	A	408	3/3	0.97	0.07	27,27,43,44	0
6	FMT	B	405	3/3	0.98	0.08	19,19,21,22	0
4	NAP	B	403	48/48	0.98	0.06	13,16,23,27	0
3	HSE	B	402	8/8	0.98	0.09	12,13,14,15	0
6	FMT	A	406	3/3	0.98	0.07	22,22,33,33	0
6	FMT	A	407	3/3	0.98	0.10	26,26,29,35	0
2	NA	B	401	1/1	0.99	0.05	12,12,12,12	0
4	NAP	A	403	48/48	0.99	0.05	12,16,23,26	0
3	HSE	A	402	8/8	0.99	0.08	12,13,14,15	0
6	FMT	A	404	3/3	0.99	0.04	15,15,17,18	0
2	NA	A	401	1/1	1.00	0.07	12,12,12,12	0

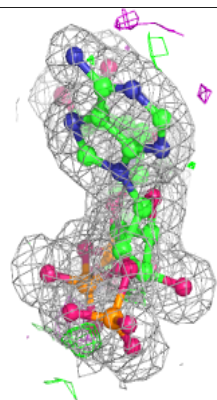
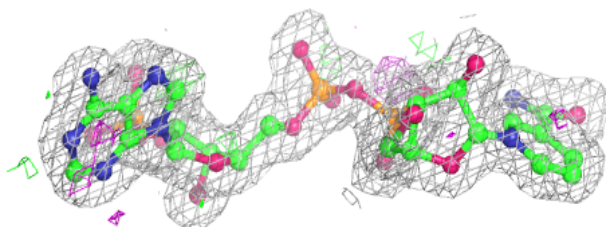
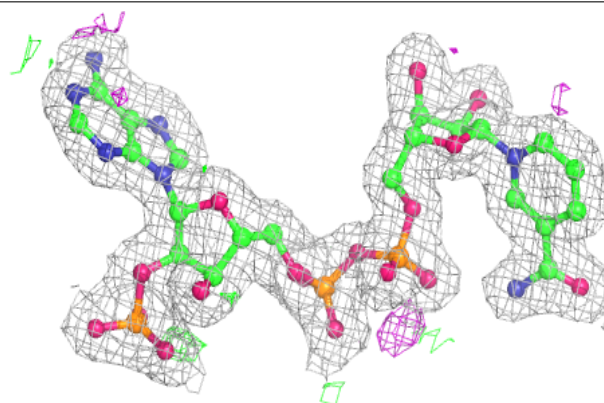
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP B 403:

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

**Electron density around NAP A 403:**

$2mF_o-DF_c$ (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.