



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:25 PM EDT

PDB ID : 6A0T / pdb_00006a0t
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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

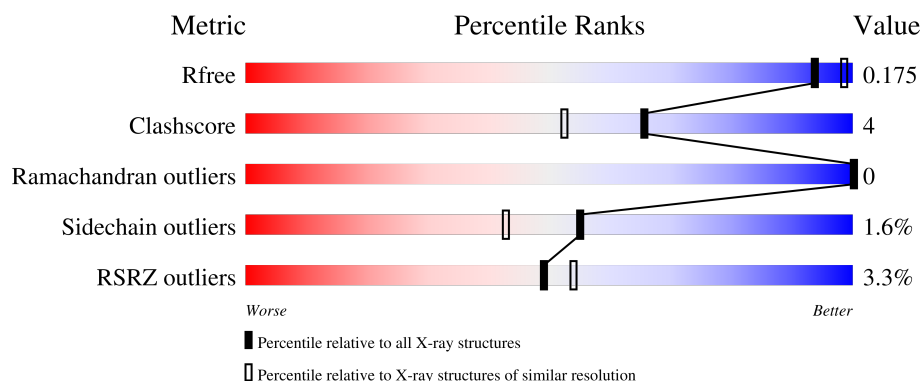
1 Overall quality at a glance

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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 $\leq 5\%$. 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	
1	B	332	

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.

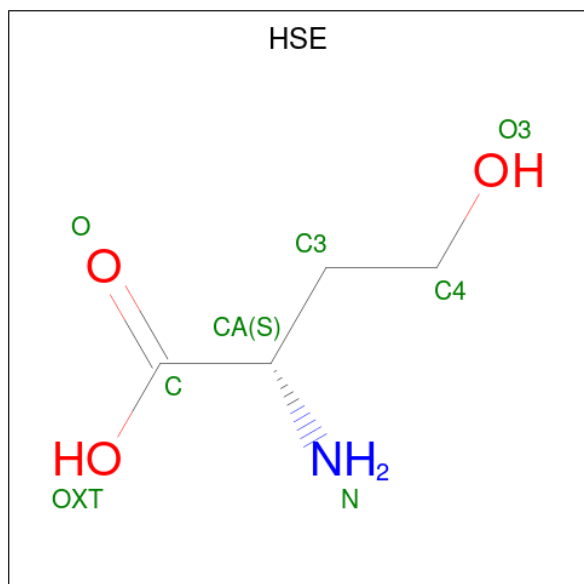
- Molecule 1 is a protein called Homoserine dehydrogenase.

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 (CCD ID: NA) (formula: Na).

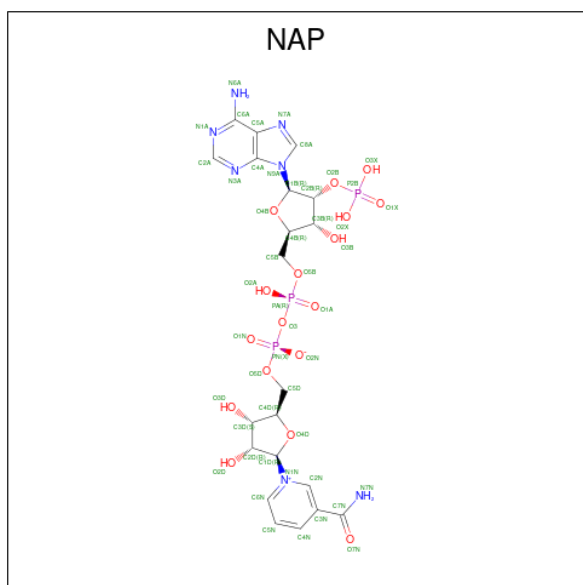
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is L-HOMOSERINE (CCD ID: HSE) (formula: C₄H₉NO₃).



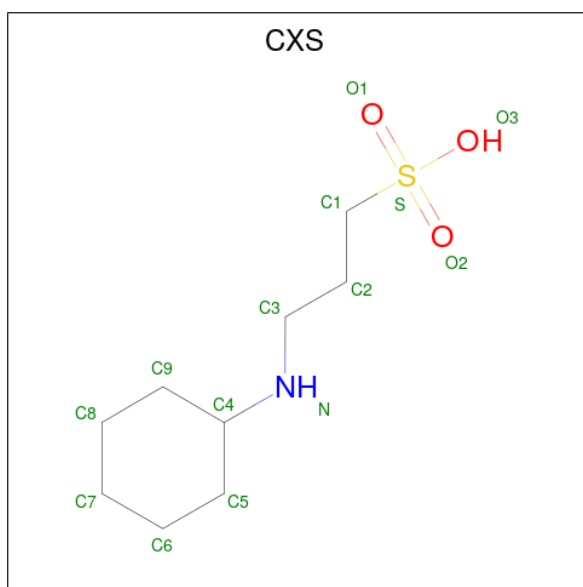
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			8	4	1	3		
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

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



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

- Molecule 5 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (CCD ID: 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 (CCD ID: 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 (CCD ID: 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		

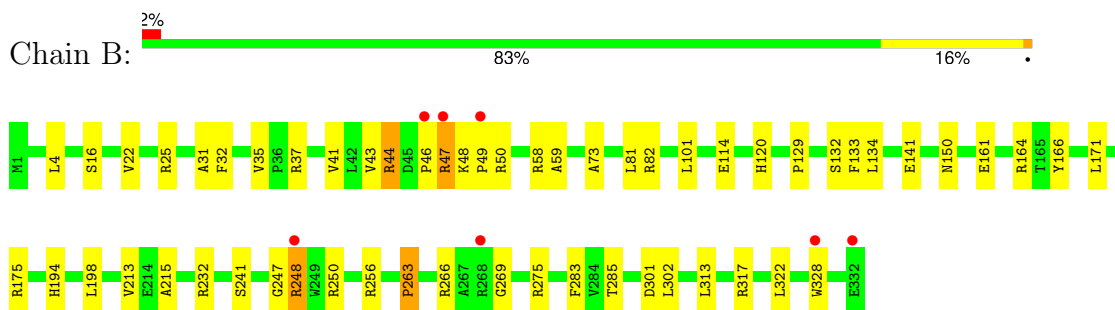
- Molecule 8 is water.

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

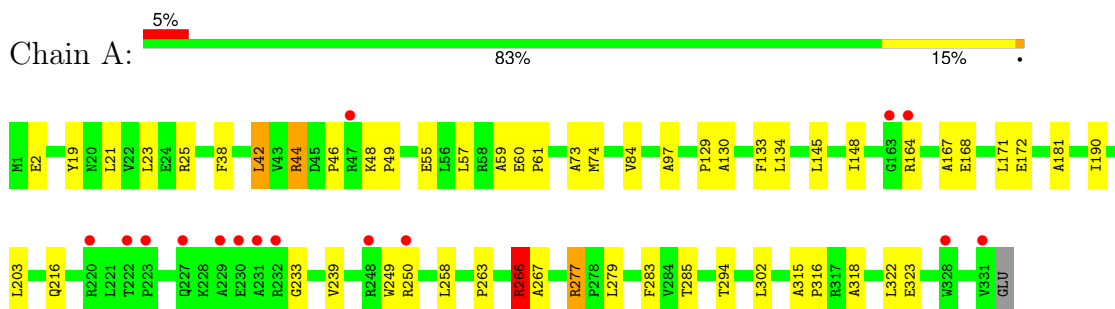
3 Residue-property plots [i](#)

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 50.00 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.87) 99.9 (50.00-1.87)	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 (5.05%)	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 , 54.1	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

5.1 Standard geometry

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

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	1.67	23/2691 (0.9%)	1.40	19/3662 (0.5%)
1	B	1.74	33/2713 (1.2%)	1.44	15/3688 (0.4%)
All	All	1.71	56/5404 (1.0%)	1.42	34/7350 (0.5%)

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 (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	GLU	CA-C	-8.37	1.42	1.52
1	B	73	ALA	CA-CB	-8.20	1.47	1.53
1	B	81	LEU	N-CA	-7.81	1.36	1.46
1	B	101	LEU	N-CA	-7.70	1.37	1.46
1	A	239	VAL	C-O	7.33	1.31	1.24
1	B	16	SER	CB-OG	-7.07	1.28	1.42
1	B	302	LEU	CA-C	7.00	1.61	1.52
1	A	266	ARG	CD-NE	6.81	1.55	1.46
1	B	150	ASN	N-CA	6.75	1.54	1.46
1	B	256	ARG	CA-C	-6.71	1.44	1.52
1	A	181	ALA	N-CA	6.65	1.54	1.46
1	B	44	ARG	C-O	-6.60	1.16	1.23
1	B	50	ARG	CA-CB	-6.55	1.43	1.53
1	A	133	PHE	N-CA	-6.39	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	31	ALA	N-CA	6.32	1.54	1.46
1	B	132	SER	N-CA	6.30	1.53	1.46
1	A	190	ILE	CA-C	6.29	1.60	1.52
1	A	168	GLU	CA-C	6.21	1.60	1.52
1	A	233	GLY	CA-C	6.19	1.57	1.51
1	A	42	LEU	N-CA	6.16	1.53	1.46
1	B	59	ALA	N-CA	6.14	1.53	1.45
1	B	161	GLU	CA-C	-6.14	1.44	1.52
1	B	4	LEU	C-O	-6.10	1.16	1.24
1	B	194	HIS	CA-C	6.03	1.60	1.52
1	B	49	PRO	CA-C	6.03	1.59	1.52
1	A	249	TRP	N-CA	5.90	1.53	1.46
1	B	134	LEU	CA-C	-5.89	1.44	1.52
1	B	301	ASP	N-CA	-5.87	1.39	1.46
1	A	48	LYS	CA-C	5.83	1.59	1.53
1	B	241	SER	CA-C	-5.80	1.45	1.52
1	A	57	LEU	CA-C	-5.76	1.45	1.52
1	A	302	LEU	CA-C	5.70	1.60	1.52
1	B	322	LEU	CA-C	-5.63	1.45	1.52
1	B	215	ALA	CA-C	-5.61	1.45	1.52
1	B	44	ARG	N-CA	5.60	1.53	1.46
1	B	48	LYS	CA-C	5.56	1.59	1.53
1	A	60	GLU	N-CA	-5.51	1.40	1.45
1	B	266	ARG	CD-NE	5.50	1.53	1.46
1	B	44	ARG	CA-C	-5.50	1.46	1.53
1	B	41	VAL	CA-CB	-5.50	1.46	1.54
1	A	129	PRO	C-N	-5.47	1.26	1.33
1	B	248	ARG	CA-C	5.47	1.59	1.52
1	A	164	ARG	NE-CZ	5.46	1.39	1.33
1	A	73	ALA	CA-CB	-5.42	1.49	1.53
1	A	294	THR	N-CA	-5.34	1.39	1.46
1	B	22	VAL	CA-CB	-5.34	1.48	1.54
1	A	74	MET	N-CA	5.30	1.53	1.46
1	B	58	ARG	CA-C	5.26	1.58	1.52
1	A	38	PHE	N-CA	5.26	1.52	1.46
1	A	129	PRO	CA-CB	5.24	1.60	1.53
1	A	315	ALA	CA-C	-5.23	1.48	1.53
1	B	43	VAL	CA-C	5.17	1.58	1.52
1	A	318	ALA	CA-C	-5.10	1.46	1.52
1	A	61	PRO	C-O	-5.05	1.17	1.23
1	B	35	VAL	N-CA	-5.05	1.41	1.46
1	B	213	VAL	CA-CB	5.03	1.59	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ARG	CG-CD-NE	7.90	129.38	112.00
1	A	172	GLU	CB-CG-CD	7.46	125.27	112.60
1	A	258	LEU	CA-C-N	-7.10	112.66	119.90
1	A	258	LEU	C-N-CA	-7.10	112.66	119.90
1	A	266	ARG	CA-CB-CG	6.88	127.86	114.10
1	B	35	VAL	CA-C-N	-6.57	112.90	119.99
1	B	35	VAL	C-N-CA	-6.57	112.90	119.99
1	B	37	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	B	269[A]	GLY	N-CA-C	-6.48	97.83	113.18
1	B	269[B]	GLY	N-CA-C	-6.48	97.83	113.18
1	A	44	ARG	NE-CZ-NH2	-6.31	113.52	119.20
1	A	130	ALA	N-CA-C	6.03	117.65	111.14
1	B	164	ARG	CA-CB-CG	-5.85	102.40	114.10
1	A	25	ARG	CB-CG-CD	5.85	124.75	111.30
1	A	49	PRO	CB-CA-C	-5.73	104.42	111.64
1	A	84	VAL	N-CA-C	5.73	119.11	111.44
1	B	317	ARG	CB-CG-CD	5.63	124.24	111.30
1	B	59	ALA	O-C-N	-5.53	116.20	123.16
1	B	250	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	B	120	HIS	N-CA-C	5.47	117.45	110.61
1	A	167	ALA	N-CA-C	5.39	117.24	111.36
1	B	132	SER	CA-CB-OG	-5.38	100.34	111.10
1	A	279	LEU	N-CA-C	5.36	117.56	111.02
1	A	168	GLU	CB-CA-C	-5.36	101.75	110.85
1	A	148	ILE	N-CA-C	-5.21	98.43	106.72
1	A	315	ALA	CA-C-N	-5.19	114.47	119.87
1	A	315	ALA	C-N-CA	-5.19	114.47	119.87
1	A	44	ARG	CG-CD-NE	-5.19	100.59	112.00
1	B	46	PRO	N-CA-C	5.18	120.66	113.98
1	B	25	ARG	CB-CG-CD	5.16	123.18	111.30
1	A	2	GLU	CA-CB-CG	5.16	124.41	114.10
1	A	322	LEU	CB-CA-C	-5.10	102.33	110.79
1	B	133	PHE	CA-CB-CG	5.01	118.81	113.80
1	B	114	GLU	CB-CG-CD	5.00	121.10	112.60

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

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Mol	Chain	Res	Type	Group
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	17	0
1	B	2657	0	2669	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	3	1	0
3	B	8	0	3	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	5457	42	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 (42) 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:A:21[B]:LEU:HD23	1:A:21[B]:LEU:C	2.21	0.66
1:B:171:LEU:HD21	1:B:175[A]:ARG:CZ	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:171:LEU:HD23	1:B:171:LEU:C	2.39	0.47
1:B:247:GLY:HA2	8:B:711:HOH:O	2.14	0.46
1:A:216[B]:GLN:O	1:A:216[B]:GLN:HG3	2.08	0.46
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:A:145:LEU:C	1:A:145:LEU:HD23	2.44	0.43
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:263:PRO:HB3	1:B:283[B]:PHE:CZ	2.54	0.43
1:B:166:TYR:CD2	1:B:166:TYR:C	2.98	0.42
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

5.3.1 Protein backbone

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
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%)	254 (98%)	6 (2%)	44	29
1	B	262/248 (106%)	258 (98%)	4 (2%)	57	46
All	All	522/496 (105%)	512 (98%)	10 (2%)	55	36

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	ARG
1	B	198	LEU
1	B	248	ARG
1	B	263	PRO
1	A	55	GLU
1	A	250[A]	ARG
1	A	250[B]	ARG
1	A	277[A]	ARG

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Mol	Chain	Res	Type
1	A	277[B]	ARG
1	A	323	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	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 oligosaccharides 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	$\# Z > 2$
7	GOL	A	411	-	5,5,5	0.34	0	5,5,5	1.04	0
6	FMT	B	406	-	2,2,2	1.05	0	1,1,1	0.94	0
5	CXS	B	404	-	14,14,14	2.40	3 (21%)	18,18,18	2.06	6 (33%)
3	HSE	B	402	-	6,7,7	1.33	1 (16%)	5,8,8	0.86	0
3	HSE	A	402	-	6,7,7	1.32	1 (16%)	5,8,8	1.78	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	B	403	-	50,52,52	2.03	10 (20%)	71,80,80	2.04	23 (32%)
6	FMT	A	407	-	2,2,2	1.18	0	1,1,1	0.02	0
7	GOL	A	410	-	5,5,5	0.56	0	5,5,5	1.70	2 (40%)
6	FMT	B	405	-	2,2,2	0.46	0	1,1,1	0.23	0
6	FMT	A	406	-	2,2,2	0.78	0	1,1,1	0.29	0
7	GOL	B	409	-	5,5,5	0.90	0	5,5,5	1.49	1 (20%)
6	FMT	A	408	-	2,2,2	0.33	0	1,1,1	0.91	0
6	FMT	A	404	-	2,2,2	0.69	0	1,1,1	0.13	0
4	NAP	A	403	-	50,52,52	2.06	14 (28%)	71,80,80	1.78	16 (22%)
6	FMT	A	409	-	2,2,2	0.54	0	1,1,1	2.34	1 (100%)
6	FMT	B	407	-	2,2,2	0.20	0	1,1,1	1.18	0
7	GOL	A	412	-	5,5,5	0.98	0	5,5,5	1.04	0
6	FMT	B	408	-	2,2,2	0.87	0	1,1,1	0.42	0
7	GOL	B	410	-	5,5,5	0.77	0	5,5,5	1.05	0
6	FMT	A	405	-	2,2,2	0.33	0	1,1,1	0.30	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
3	HSE	A	402	-	-	0/7/7/7	-
7	GOL	B	409	-	-	0/4/4/4	-
7	GOL	A	411	-	-	0/4/4/4	-
4	NAP	A	403	-	-	6/35/67/67	0/5/5/5
7	GOL	A	412	-	-	0/4/4/4	-
7	GOL	A	410	-	-	2/4/4/4	-
7	GOL	B	410	-	-	3/4/4/4	-
3	HSE	B	402	-	-	0/7/7/7	-
5	CXS	B	404	-	-	4/8/16/16	0/1/1/1
4	NAP	B	403	-	-	6/35/67/67	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	NAP	PN-O3	9.20	1.69	1.59
4	A	403	NAP	PN-O3	8.58	1.68	1.59
5	B	404	CXS	C1-S	-6.29	1.68	1.77
5	B	404	CXS	O2-S	5.42	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	NAP	P2B-O2B	3.73	1.66	1.59
4	A	403	NAP	C5A-C4A	3.54	1.45	1.39
4	A	403	NAP	PA-O2A	-3.45	1.39	1.55
4	A	403	NAP	PA-O3	-3.35	1.55	1.59
4	B	403	NAP	C8A-N9A	3.22	1.43	1.37
4	B	403	NAP	C5A-C4A	3.20	1.44	1.39
4	B	403	NAP	C4A-N9A	-3.16	1.31	1.37
4	A	403	NAP	O4B-C4B	-3.03	1.38	1.45
4	B	403	NAP	PA-O2A	-3.00	1.41	1.55
5	B	404	CXS	C3-N	2.78	1.52	1.47
4	B	403	NAP	C2B-C1B	-2.71	1.46	1.53
4	B	403	NAP	O4B-C1B	2.56	1.47	1.42
4	A	403	NAP	P2B-O3X	-2.51	1.45	1.54
3	B	402	HSE	O-C	2.46	1.29	1.22
4	B	403	NAP	C2N-C3N	-2.44	1.35	1.39
3	A	402	HSE	O-C	2.43	1.29	1.22
4	A	403	NAP	C4N-C3N	2.35	1.43	1.39
4	A	403	NAP	O4D-C1D	2.30	1.43	1.40
4	B	403	NAP	C4A-N3A	2.28	1.38	1.34
4	A	403	NAP	PN-O2N	-2.24	1.45	1.55
4	A	403	NAP	C2A-N1A	2.21	1.37	1.33
4	B	403	NAP	C1B-N9A	-2.16	1.40	1.46
4	A	403	NAP	C8A-N7A	2.14	1.35	1.31
4	A	403	NAP	C4A-N9A	-2.13	1.33	1.37
4	A	403	NAP	C2N-N1N	2.09	1.37	1.35

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	NAP	N3A-C4A-N9A	4.79	135.31	127.17
4	B	403	NAP	C5A-C4A-N3A	-4.61	120.37	126.72
5	B	404	CXS	C3-N-C4	4.31	122.47	114.18
4	A	403	NAP	N3A-C2A-N1A	-4.31	122.06	128.58
4	B	403	NAP	C4A-N9A-C8A	4.11	110.06	105.74
4	B	403	NAP	N3A-C4A-N9A	4.10	134.15	127.17
4	A	403	NAP	O2A-PA-O3	4.05	118.23	107.27
4	A	403	NAP	C4A-N9A-C8A	4.04	109.98	105.74
4	B	403	NAP	N3A-C2A-N1A	-4.02	122.49	128.58
4	B	403	NAP	O3-PA-O1A	-3.83	99.17	110.70
5	B	404	CXS	O3-S-O1	-3.70	102.13	111.40
4	B	403	NAP	O2B-P2B-O1X	-3.69	96.20	109.33
4	A	403	NAP	C5A-C4A-N3A	-3.67	121.67	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	404	CXS	C2-C1-S	3.46	118.56	113.25
4	A	403	NAP	O3-PA-O1A	-3.35	100.61	110.70
4	B	403	NAP	O3D-C3D-C4D	-3.34	101.48	111.08
4	B	403	NAP	C2B-C1B-N9A	3.31	119.20	113.75
4	B	403	NAP	O3-PN-O1N	-3.29	100.82	110.70
4	B	403	NAP	O2A-PA-O3	3.27	116.11	107.27
3	A	402	HSE	OXT-C-O	-3.20	116.82	124.08
4	B	403	NAP	O4B-C1B-C2B	3.19	112.08	106.59
4	B	403	NAP	N9A-C8A-N7A	-3.11	109.52	113.94
4	B	403	NAP	O3X-P2B-O1X	3.08	122.86	110.83
4	A	403	NAP	C6N-N1N-C2N	-2.98	119.34	121.88
4	A	403	NAP	P2B-O2B-C2B	-2.98	115.48	123.43
4	A	403	NAP	O3D-C3D-C4D	-2.95	102.60	111.08
4	B	403	NAP	C2A-N3A-C4A	2.90	118.90	111.83
7	B	409	GOL	C3-C2-C1	-2.88	101.25	111.80
4	B	403	NAP	C6N-C5N-C4N	2.85	123.56	119.45
4	B	403	NAP	O3X-P2B-O2B	2.81	116.81	105.85
4	B	403	NAP	O2N-PN-O3	2.73	114.66	107.27
4	B	403	NAP	C4B-O4B-C1B	-2.70	103.50	109.47
5	B	404	CXS	O2-S-O1	2.67	122.50	113.82
4	B	403	NAP	C5N-C4N-C3N	-2.67	117.75	120.36
7	A	410	GOL	O3-C3-C2	-2.64	98.50	110.38
4	A	403	NAP	C5A-C4A-N9A	-2.58	102.99	105.81
4	B	403	NAP	C6N-N1N-C2N	-2.54	119.72	121.88
4	A	403	NAP	C2A-N3A-C4A	2.48	117.88	111.83
4	A	403	NAP	C2A-N1A-C6A	2.46	122.78	118.73
4	A	403	NAP	O2X-P2B-O2B	-2.44	96.34	105.85
4	B	403	NAP	C1B-N9A-C8A	-2.41	121.74	127.09
6	A	409	FMT	O2-C-O1	-2.34	101.55	126.59
4	B	403	NAP	C2A-N1A-C6A	2.27	122.45	118.73
5	B	404	CXS	O2-S-C1	2.19	110.04	106.73
4	A	403	NAP	C2N-N1N-C1D	2.18	123.95	119.13
4	B	403	NAP	P2B-O2B-C2B	-2.17	117.63	123.43
4	A	403	NAP	C5N-C4N-C3N	-2.11	118.29	120.36
7	A	410	GOL	O2-C2-C1	2.10	117.86	109.18
5	B	404	CXS	C9-C4-C5	-2.05	107.26	110.80
4	A	403	NAP	C3N-C7N-N7N	2.03	120.25	117.74

There are no chirality outliers.

All (21) 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	B	410	GOL	C1-C2-C3-O3
7	A	410	GOL	O1-C1-C2-C3
5	B	404	CXS	C2-C1-S-O3
4	B	403	NAP	C3B-C2B-O2B-P2B
4	A	403	NAP	C3B-C2B-O2B-P2B
7	B	410	GOL	O2-C2-C3-O3
4	A	403	NAP	C1B-C2B-O2B-P2B
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	B	410	GOL	O1-C1-C2-O2

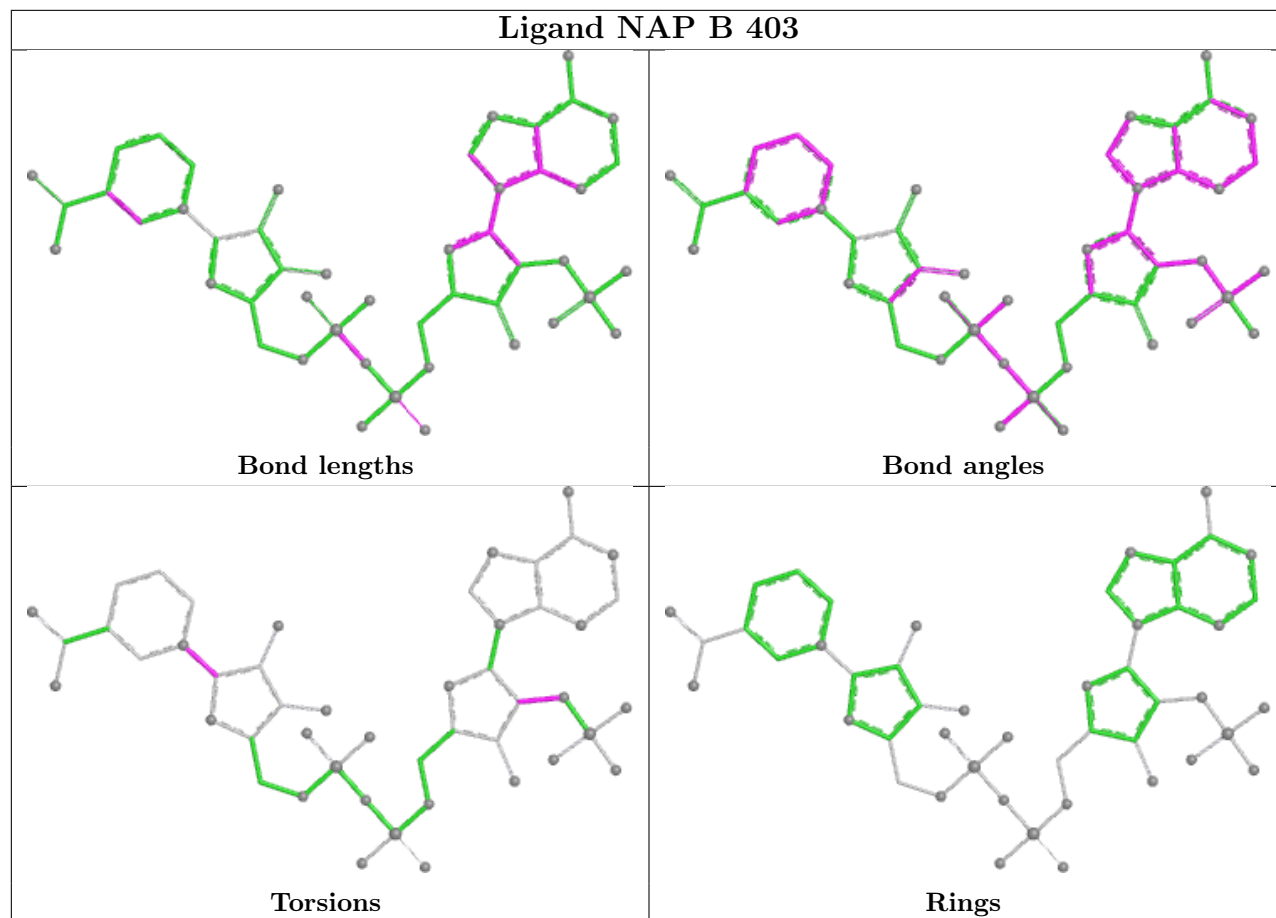
There are no ring outliers.

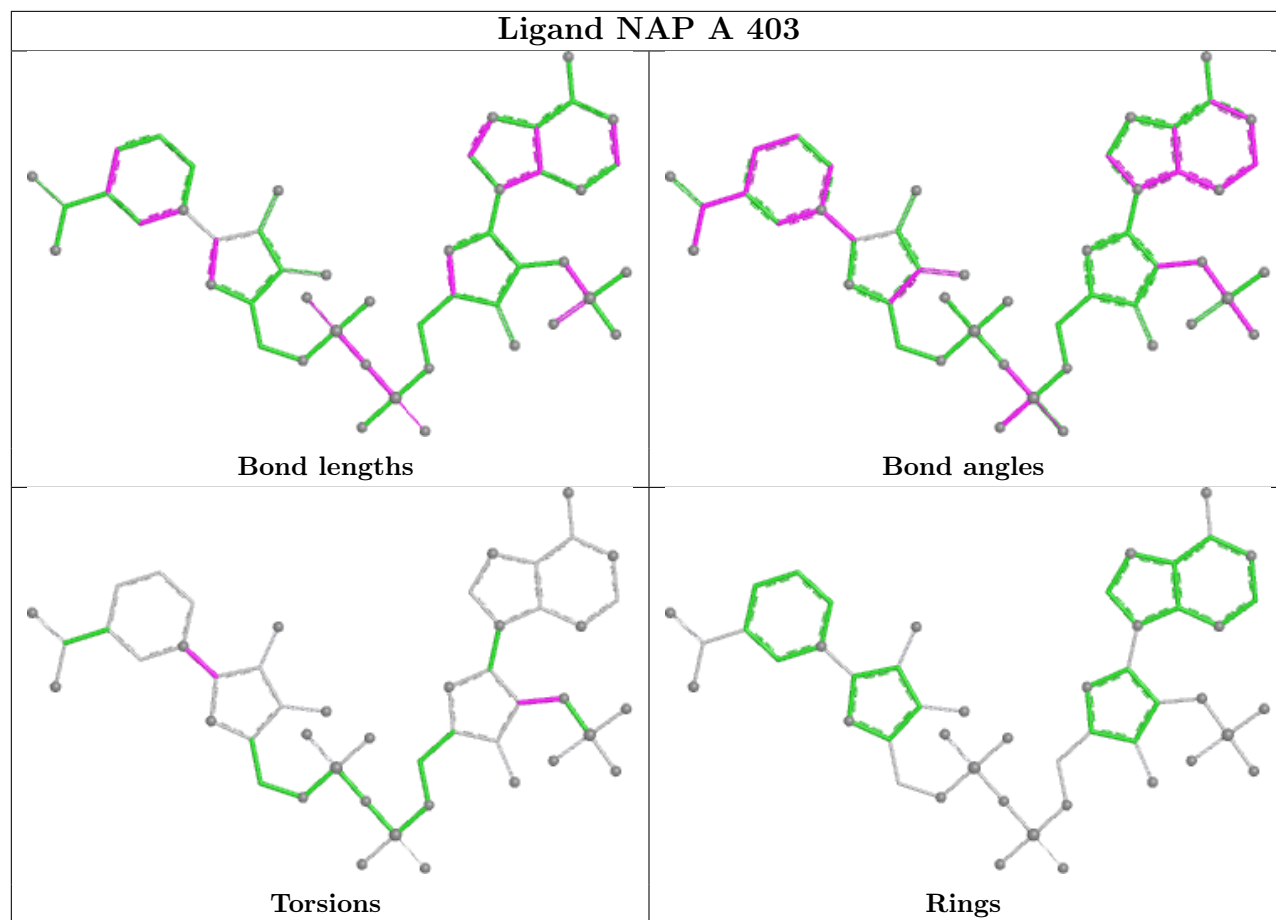
5 monomers are involved in 6 short contacts:

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

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	331/332 (99%)	-0.29	15 (4%) 38 41	6, 18, 43, 69	18 (5%)
1	B	332/332 (100%)	-0.31	7 (2%) 63 70	7, 18, 38, 71	18 (5%)
All	All	663/664 (99%)	-0.30	22 (3%) 49 54	6, 18, 41, 71	36 (5%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268[A]	ARG	10.6
1	A	331	VAL	4.9
1	B	47	ARG	3.9
1	A	163	GLY	3.4
1	B	46	PRO	3.3
1	A	47	ARG	3.3
1	B	332	GLU	3.2
1	B	49	PRO	2.9
1	A	227	GLN	2.9
1	A	164	ARG	2.6
1	A	250[A]	ARG	2.6
1	A	328	TRP	2.5
1	A	220	ARG	2.5
1	A	232	ARG	2.5
1	A	231	ALA	2.5
1	A	248	ARG	2.4
1	A	223	PRO	2.3
1	A	229	ALA	2.2
1	A	230	GLU	2.2
1	B	328	TRP	2.2
1	A	222	THR	2.0
1	B	248	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

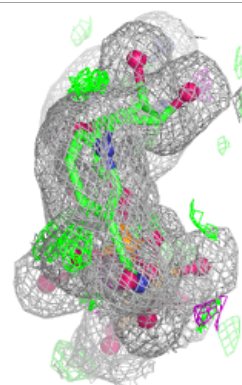
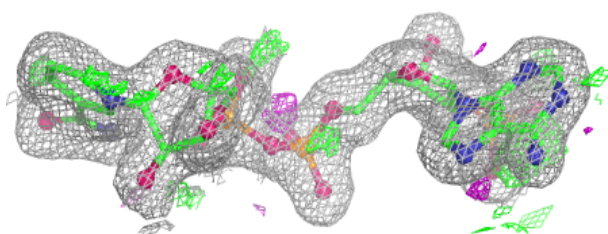
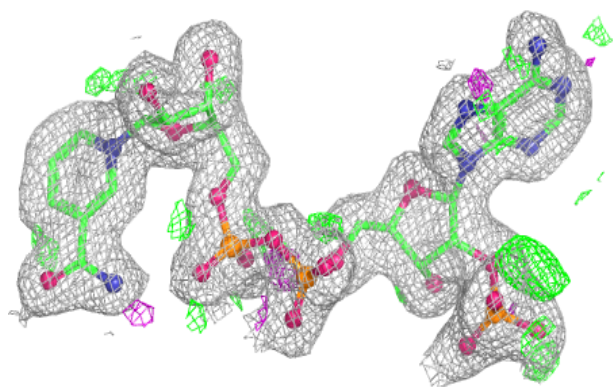
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	412	6/6	0.84	0.23	36,45,52,55	6
5	CXS	B	404	14/14	0.85	0.17	22,33,51,59	14
7	GOL	B	410	6/6	0.86	0.17	39,40,44,45	6
6	FMT	A	409	3/3	0.86	0.17	39,39,41,44	0
6	FMT	A	405	3/3	0.87	0.15	35,35,41,48	0
6	FMT	B	406	3/3	0.88	0.17	31,31,48,52	0
7	GOL	A	411	6/6	0.89	0.13	37,40,44,47	6
6	FMT	B	407	3/3	0.91	0.18	35,35,44,62	0
7	GOL	B	409	6/6	0.92	0.12	27,32,38,40	0
7	GOL	A	410	6/6	0.93	0.10	23,31,39,41	0
6	FMT	B	408	3/3	0.96	0.11	30,30,34,34	0
6	FMT	A	408	3/3	0.96	0.12	27,27,43,44	0
6	FMT	A	406	3/3	0.97	0.09	22,22,33,33	0
6	FMT	A	407	3/3	0.97	0.10	26,26,29,35	0
6	FMT	B	405	3/3	0.97	0.10	19,19,21,22	0
3	HSE	B	402	8/8	0.98	0.04	12,13,14,15	0
6	FMT	A	404	3/3	0.98	0.06	15,15,17,18	0
3	HSE	A	402	8/8	0.98	0.05	12,13,14,15	0
4	NAP	B	403	48/48	0.99	0.04	13,16,23,27	0
4	NAP	A	403	48/48	0.99	0.04	12,16,23,26	0
2	NA	B	401	1/1	0.99	0.04	12,12,12,12	0
2	NA	A	401	1/1	1.00	0.03	12,12,12,12	0

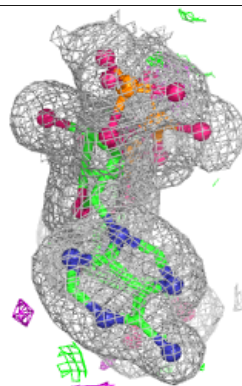
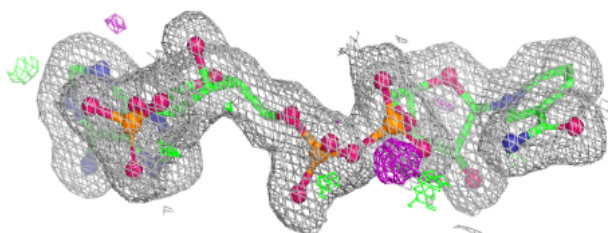
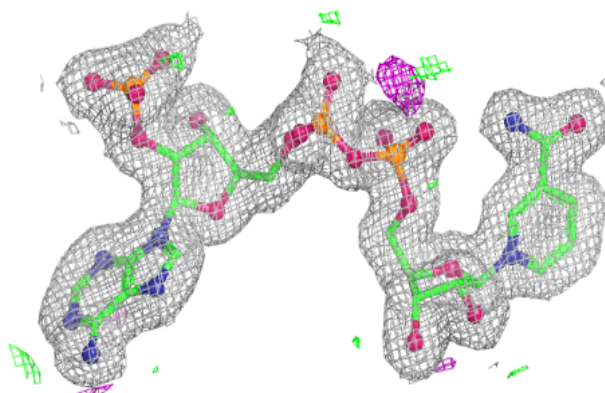
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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