



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:42 AM UTC

PDB ID : 8K32 / pdb_00008k32
Title : The complex structure of SLKARI with NADH at 2.12-angstrom resolution
Authors : Chen, C.Y.; Huang, C.H.
Deposited on : 2023-07-14
Resolution : 2.12 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

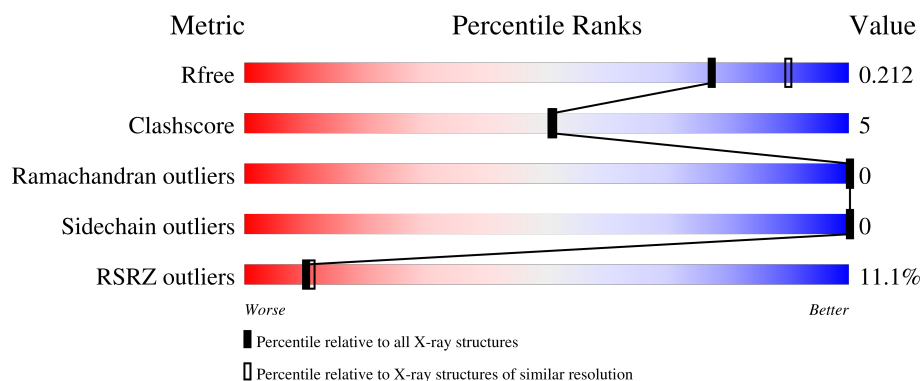
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	334	3% 91% 8%
1	B	334	33% 85% 15%
1	C	334	7% 88% 12%
1	D	334	2% 93% 7%

2 Entry composition ⓘ

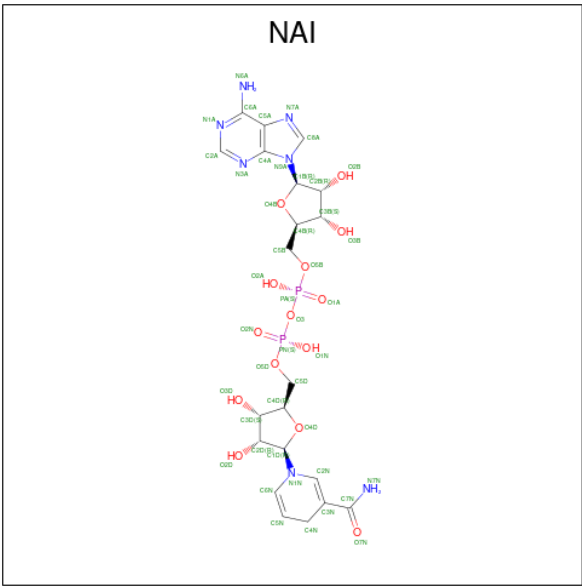
There are 7 unique types of molecules in this entry. The entry contains 11652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ketol-acid reductoisomerase (NADP(+)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2561	1631	438	481	11			
1	B	332	Total	C	N	O	S	0	0	0
			2561	1631	438	481	11			
1	C	333	Total	C	N	O	S	0	0	0
			2570	1637	440	482	11			
1	D	332	Total	C	N	O	S	0	0	0
			2561	1631	438	481	11			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



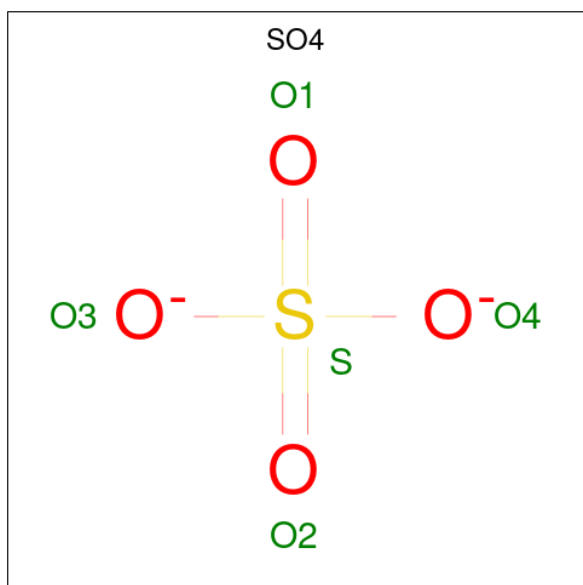
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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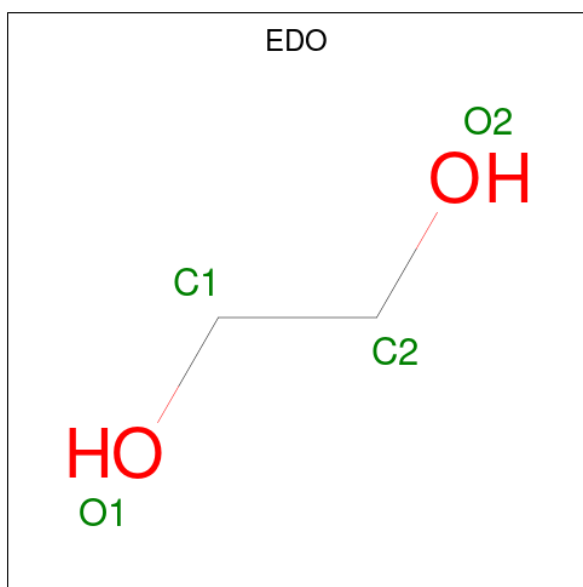
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

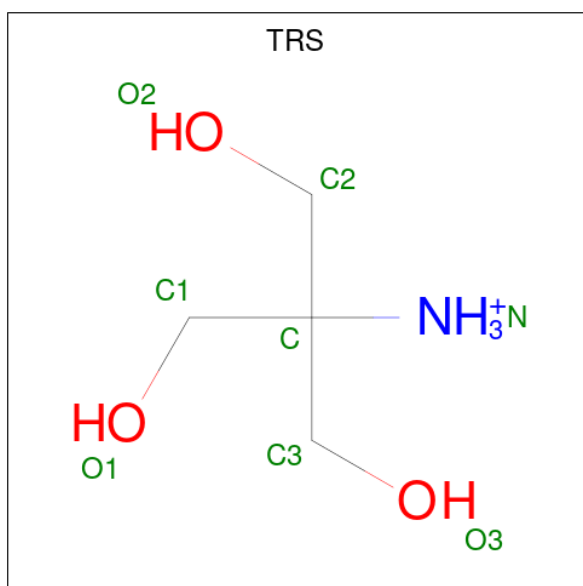
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

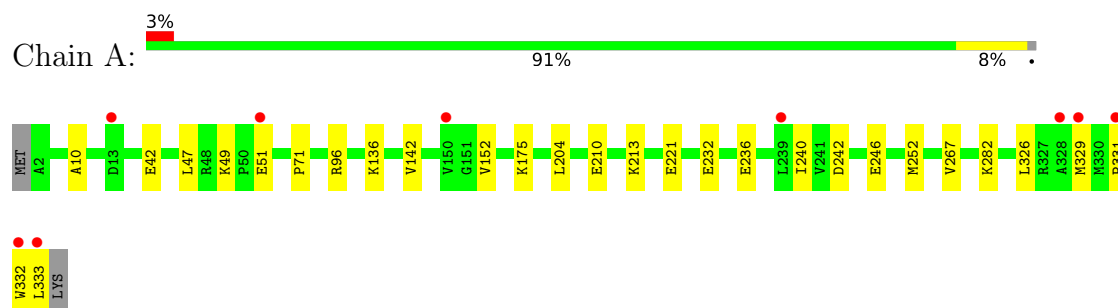
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	371	Total	O	0	0
			371	371		
7	B	179	Total	O	0	0
			179	179		
7	C	221	Total	O	0	0
			221	221		
7	D	311	Total	O	0	0
			311	311		

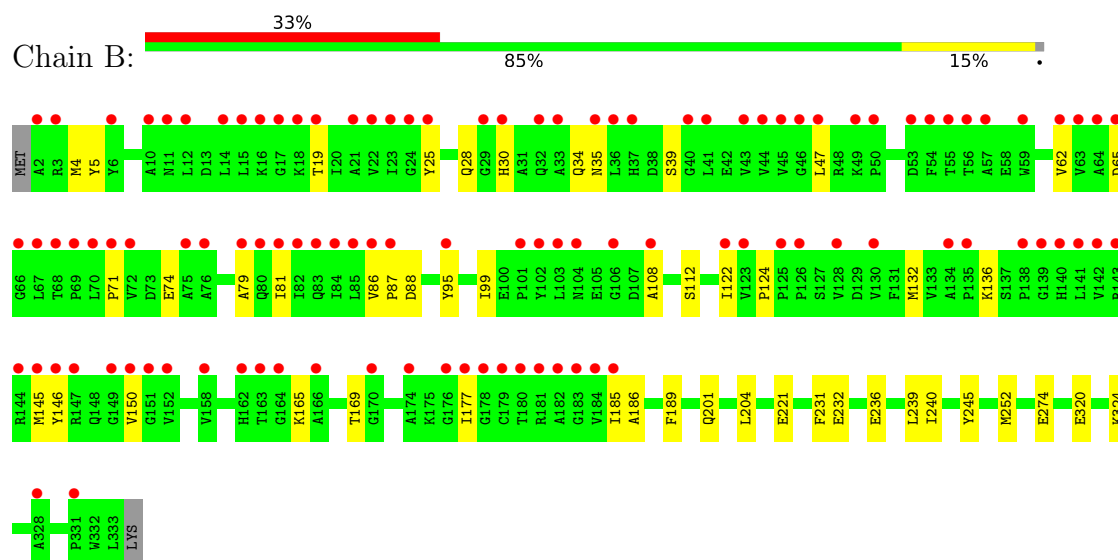
3 Residue-property plots [i](#)

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.

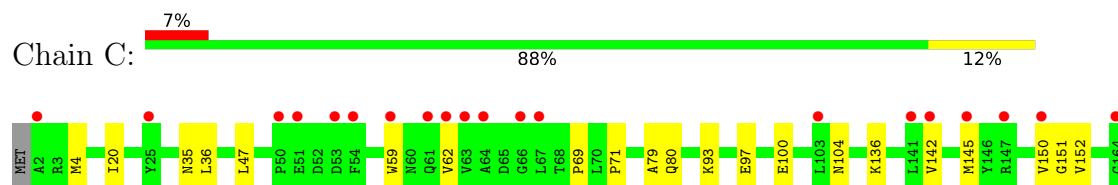
- Molecule 1: Ketol-acid reductoisomerase (NADP(+))

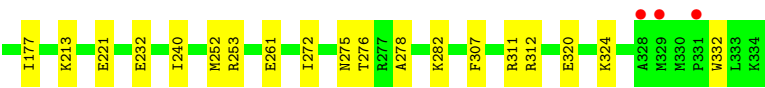


- Molecule 1: Ketol-acid reductoisomerase (NADP(+))

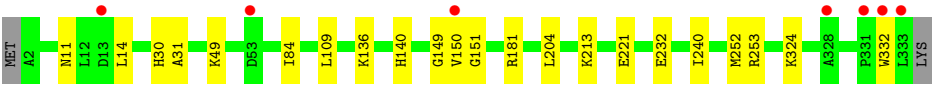
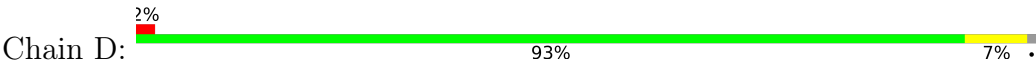


- Molecule 1: Ketol-acid reductoisomerase (NADP(+))





● Molecule 1: Ketol-acid reductoisomerase (NADP(+))



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	131.56Å 131.56Å 297.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.09 – 2.12 29.09 – 2.12	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.09-2.12) 97.4 (29.09-2.12)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 2.12Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.179 , 0.212 0.179 , 0.212	Depositor DCC
R_{free} test set	5081 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11652	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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, EDO, NAI, MG, TRS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/2612	0.60	2/3540 (0.1%)
1	B	0.31	0/2612	0.48	0/3540
1	C	0.32	0/2621	0.50	0/3551
1	D	0.35	0/2612	0.54	1/3540 (0.0%)
All	All	0.35	0/10457	0.53	3/14171 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	GLU	CA-CB-CG	5.92	125.94	114.10
1	D	49	LYS	N-CA-C	-5.31	102.89	109.64
1	A	42	GLU	N-CA-CB	-5.04	102.20	110.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2561	0	2556	23	0
1	B	2561	0	2556	34	0
1	C	2570	0	2569	34	0
1	D	2561	0	2556	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	26	1	0
2	B	44	0	26	7	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
3	A	30	0	0	2	0
3	B	20	0	0	1	0
3	C	25	0	0	0	0
3	D	30	0	0	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	4	0	6	0	0
5	C	8	0	12	3	0
6	A	8	0	12	0	0
6	B	8	0	12	0	0
7	A	371	0	0	7	1
7	B	179	0	0	4	0
7	C	221	0	0	6	0
7	D	311	0	0	6	0
All	All	11652	0	10383	108	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 5.

All (108) 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:282:LYS:NZ	7:A:501:HOH:O	2.02	0.91
1:D:253:ARG:NH2	7:D:503:HOH:O	2.16	0.77
1:C:312:ARG:NH1	7:C:503:HOH:O	2.19	0.76
1:B:221:GLU:OE1	7:B:501:HOH:O	2.06	0.74
1:C:100:GLU:OE1	7:C:501:HOH:O	2.04	0.74
1:D:149:GLY:O	1:D:181:ARG:NH1	2.24	0.71
1:D:221:GLU:OE1	7:D:501:HOH:O	2.09	0.70
1:C:307:PHE:HE2	1:C:311:ARG:NH1	1.90	0.70
1:C:213:LYS:NZ	7:D:503:HOH:O	2.22	0.69
1:B:274:GLU:OE2	7:B:502:HOH:O	2.13	0.66
3:D:406:SO4:O1	7:D:502:HOH:O	2.14	0.65
1:C:307:PHE:HE2	1:C:311:ARG:HH11	1.45	0.65
1:B:39:SER:OG	1:B:146:TYR:OH	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:404:SO4:O4	7:A:502:HOH:O	2.11	0.65
1:C:282:LYS:N	1:C:282:LYS:HD2	2.11	0.64
1:B:4:MET:HE1	1:B:185:ILE:HG12	1.81	0.63
1:B:87:PRO:HD3	2:B:401:NAI:H51A	1.80	0.61
3:B:404:SO4:O2	7:B:503:HOH:O	2.16	0.61
1:A:136:LYS:NZ	1:B:232:GLU:OE2	2.33	0.61
1:C:282:LYS:NZ	7:C:507:HOH:O	2.33	0.60
1:A:142:VAL:HG22	1:A:152:VAL:HG21	1.82	0.60
1:D:11:ASN:HB3	1:D:14:LEU:HD13	1.85	0.59
1:C:145:MET:HE2	1:D:332:TRP:CD1	2.38	0.58
1:C:232:GLU:OE2	1:D:136:LYS:NZ	2.35	0.58
1:D:332:TRP:CD1	1:D:332:TRP:H	2.22	0.58
1:B:231:PHE:O	1:B:236:GLU:HG3	2.03	0.58
1:C:145:MET:HE3	1:C:150:VAL:HB	1.85	0.58
3:A:406:SO4:O2	7:A:503:HOH:O	2.17	0.57
3:D:404:SO4:O4	7:D:504:HOH:O	2.16	0.57
1:A:221:GLU:OE2	7:A:504:HOH:O	2.18	0.56
1:A:232:GLU:OE2	1:B:136:LYS:NZ	2.36	0.56
1:C:320:GLU:O	1:C:324:LYS:HG3	2.06	0.56
1:A:96:ARG:NH1	7:A:505:HOH:O	2.18	0.56
1:B:239:LEU:HD12	7:B:599:HOH:O	2.05	0.56
1:C:278:ALA:O	1:C:282:LYS:HD3	2.09	0.53
1:A:332:TRP:H	1:A:332:TRP:CD1	2.25	0.53
1:D:213:LYS:NZ	7:D:509:HOH:O	2.40	0.53
1:B:35:ASN:HB3	1:B:177:ILE:HA	1.91	0.52
1:B:47:LEU:HD11	1:B:62:VAL:HG21	1.90	0.52
1:C:100:GLU:HG2	7:C:659:HOH:O	2.09	0.52
1:C:35:ASN:HB3	1:C:177:ILE:HA	1.92	0.52
1:A:240:ILE:HG21	1:B:204:LEU:O	2.10	0.51
1:B:28:GLN:HE21	2:B:401:NAI:C7N	2.23	0.51
1:C:136:LYS:NZ	1:D:232:GLU:OE1	2.43	0.51
1:C:80:GLN:HE21	5:C:410:EDO:H22	1.76	0.51
1:B:25:TYR:CE1	1:B:30:HIS:HA	2.48	0.48
1:C:253:ARG:HG2	1:C:261:GLU:HG3	1.95	0.48
1:B:71:PRO:HG2	1:B:74:GLU:HB2	1.95	0.48
1:B:320:GLU:O	1:B:324:LYS:HG3	2.13	0.48
1:B:88:ASP:OD1	2:B:401:NAI:O3D	2.32	0.48
1:A:236:GLU:HA	7:A:697:HOH:O	2.13	0.47
1:B:132:MET:HB2	1:B:189:PHE:CZ	2.49	0.47
1:C:240:ILE:HG23	1:C:252:MET:HG3	1.97	0.47
1:D:240:ILE:HG23	1:D:252:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LEU:CD2	1:A:329:MET:HE2	2.44	0.47
1:D:136:LYS:HE2	1:D:136:LYS:HA	1.95	0.47
1:C:142:VAL:HG22	1:C:152:VAL:HG21	1.97	0.46
1:A:136:LYS:HA	1:A:136:LYS:HE2	1.97	0.46
1:B:165:LYS:O	1:B:169:THR:OG1	2.14	0.46
1:A:10:ALA:HB3	1:A:175:LYS:HD2	1.98	0.45
1:C:104:ASN:OD1	5:C:410:EDO:H12	2.17	0.45
1:C:93:LYS:HE3	1:C:97:GLU:OE2	2.16	0.45
1:C:47:LEU:HD11	1:C:62:VAL:HG21	1.99	0.45
1:C:240:ILE:HG21	1:D:204:LEU:O	2.17	0.45
1:A:49:LYS:HG3	7:A:642:HOH:O	2.17	0.45
1:A:242:ASP:O	1:A:246:GLU:HG3	2.15	0.45
1:B:122:ILE:HG22	1:B:124:PRO:HD3	1.99	0.45
1:B:112:SER:HB3	2:B:401:NAI:H6N	1.99	0.45
1:B:47:LEU:O	1:B:71:PRO:HA	2.17	0.44
1:C:221:GLU:HG3	7:C:653:HOH:O	2.18	0.44
2:D:401:NAI:H8A	2:D:401:NAI:H2B	1.83	0.44
1:A:210:GLU:OE2	1:A:213:LYS:HE2	2.18	0.44
1:D:324:LYS:HG2	3:D:407:SO4:O4	2.18	0.44
1:B:5:TYR:HE2	1:B:186:ALA:HB2	1.83	0.44
2:B:401:NAI:H2N	2:B:401:NAI:H2D	1.78	0.44
1:B:81:ILE:HG12	1:B:108:ALA:HB3	2.00	0.43
1:B:240:ILE:HG23	1:B:252:MET:HG3	1.99	0.43
1:C:20:ILE:HG21	1:C:36:LEU:HD13	2.00	0.43
1:C:275:ASN:ND2	7:C:520:HOH:O	2.51	0.43
1:A:204:LEU:O	1:B:240:ILE:HG21	2.19	0.43
1:A:49:LYS:O	1:A:51:GLU:HG2	2.19	0.43
1:A:331:PRO:C	1:A:333:LEU:H	2.26	0.43
1:A:47:LEU:O	1:A:71:PRO:HA	2.18	0.43
1:A:267:VAL:HG11	1:B:201:GLN:HB3	2.00	0.43
1:A:326:LEU:HD23	1:A:329:MET:HE2	2.01	0.43
1:B:86:VAL:HB	1:B:87:PRO:HD2	2.01	0.42
2:B:401:NAI:H8A	2:B:401:NAI:H2B	1.81	0.42
1:D:140:HIS:N	3:D:402:SO4:O1	2.53	0.42
1:C:272:ILE:HG23	1:C:276:THR:HG21	2.02	0.42
1:B:19:THR:HB	1:B:79:ALA:HA	2.01	0.42
1:C:332:TRP:CD1	1:C:332:TRP:H	2.36	0.42
1:A:332:TRP:HZ3	1:B:245:TYR:HH	1.63	0.41
1:B:95:TYR:HA	1:B:99:ILE:HB	2.02	0.41
2:C:401:NAI:H2N	2:C:401:NAI:H2D	1.79	0.41
1:D:30:HIS:CG	1:D:31:ALA:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:MET:HG3	1:B:150:VAL:O	2.21	0.41
1:C:4:MET:HE3	1:C:4:MET:HB3	1.83	0.41
1:B:34:GLN:NE2	1:B:65:ASP:OD2	2.53	0.41
1:D:84:ILE:HD11	1:D:109:LEU:HD11	2.02	0.41
1:C:59:TRP:CE2	1:C:69:PRO:HG2	2.56	0.41
1:C:79:ALA:O	5:C:410:EDO:H21	2.21	0.41
1:C:136:LYS:HA	1:C:136:LYS:HE2	2.01	0.41
1:C:47:LEU:O	1:C:71:PRO:HA	2.21	0.40
1:C:150:VAL:HG12	1:C:151:GLY:H	1.86	0.40
1:A:240:ILE:HG23	1:A:252:MET:HG3	2.02	0.40
2:A:401:NAI:H8A	2:A:401:NAI:H2B	1.77	0.40
1:B:28:GLN:NE2	2:B:401:NAI:O7N	2.53	0.40
1:D:150:VAL:HG12	1:D:151:GLY:O	2.22	0.40

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)
7:A:727:HOH:O	7:A:806:HOH:O[3_555]	2.13	0.07

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	330/334 (99%)	319 (97%)	11 (3%)	0	100	100
1	B	330/334 (99%)	316 (96%)	14 (4%)	0	100	100
1	C	331/334 (99%)	318 (96%)	13 (4%)	0	100	100
1	D	330/334 (99%)	316 (96%)	14 (4%)	0	100	100
All	All	1321/1336 (99%)	1269 (96%)	52 (4%)	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	267/269 (99%)	267 (100%)	0	100	100
1	B	267/269 (99%)	267 (100%)	0	100	100
1	C	268/269 (100%)	268 (100%)	0	100	100
1	D	267/269 (99%)	267 (100%)	0	100	100
All	All	1069/1076 (99%)	1069 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	116	ASN
1	B	34	GLN
1	B	60	ASN
1	B	118	HIS
1	B	162	HIS
1	B	288	GLN
1	D	104	ASN
1	D	140	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 8 are monoatomic - leaving 30 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
3	SO4	C	406	-	4,4,4	0.26	0	6,6,6	0.12	0
3	SO4	B	404	-	4,4,4	0.24	0	6,6,6	0.09	0
2	NAI	A	401	-	47,48,48	3.57	20 (42%)	64,73,73	1.91	14 (21%)
3	SO4	D	404	-	4,4,4	0.38	0	6,6,6	0.21	0
6	TRS	A	411	-	7,7,7	0.36	0	9,9,9	0.12	0
3	SO4	C	403	-	4,4,4	0.28	0	6,6,6	0.43	0
3	SO4	A	406	-	4,4,4	0.30	0	6,6,6	0.12	0
3	SO4	A	402	-	4,4,4	0.32	0	6,6,6	0.26	0
5	EDO	C	410	-	3,3,3	0.42	0	2,2,2	0.26	0
5	EDO	C	409	-	3,3,3	0.46	0	2,2,2	0.37	0
3	SO4	B	405	-	4,4,4	0.24	0	6,6,6	0.08	0
2	NAI	B	401	-	47,48,48	4.01	23 (48%)	64,73,73	1.72	10 (15%)
3	SO4	C	404	-	4,4,4	0.25	0	6,6,6	0.15	0
3	SO4	C	402	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	D	407	-	4,4,4	0.28	0	6,6,6	0.14	0
6	TRS	B	408	-	7,7,7	0.36	0	9,9,9	0.34	0
3	SO4	B	403	-	4,4,4	0.23	0	6,6,6	0.21	0
3	SO4	D	403	-	4,4,4	0.32	0	6,6,6	0.21	0
3	SO4	A	407	-	4,4,4	0.27	0	6,6,6	0.17	0
3	SO4	D	405	-	4,4,4	0.28	0	6,6,6	0.15	0
2	NAI	D	401	-	47,48,48	3.63	20 (42%)	64,73,73	1.82	13 (20%)
3	SO4	A	404	-	4,4,4	0.35	0	6,6,6	0.23	0
3	SO4	B	402	-	4,4,4	0.26	0	6,6,6	0.07	0
3	SO4	A	405	-	4,4,4	0.24	0	6,6,6	0.12	0
2	NAI	C	401	-	47,48,48	3.70	23 (48%)	64,73,73	1.86	10 (15%)
3	SO4	C	405	-	4,4,4	0.26	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	402	-	4,4,4	0.22	0	6,6,6	0.12	0
3	SO4	A	403	-	4,4,4	0.27	0	6,6,6	0.19	0
5	EDO	A	410	-	3,3,3	0.41	0	2,2,2	0.45	0
3	SO4	D	406	-	4,4,4	0.26	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	D	401	-	-	8/29/72/72	0/5/5/5
2	NAI	B	401	-	-	12/29/72/72	0/5/5/5
2	NAI	C	401	-	-	6/29/72/72	0/5/5/5
6	TRS	B	408	-	-	5/9/9/9	-
2	NAI	A	401	-	-	6/29/72/72	0/5/5/5
5	EDO	A	410	-	-	1/1/1/1	-
5	EDO	C	410	-	-	1/1/1/1	-
5	EDO	C	409	-	-	0/1/1/1	-
6	TRS	A	411	-	-	7/9/9/9	-

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAI	O4D-C1D	9.18	1.63	1.42
2	B	401	NAI	PA-O3	8.97	1.69	1.59
2	B	401	NAI	O4B-C1B	8.92	1.62	1.42
2	B	401	NAI	PN-O3	8.90	1.69	1.59
2	C	401	NAI	O4B-C1B	8.74	1.62	1.42
2	A	401	NAI	O4D-C1D	8.25	1.61	1.42
2	C	401	NAI	O4D-C1D	8.10	1.60	1.42
2	D	401	NAI	O4B-C1B	7.89	1.60	1.42
2	D	401	NAI	O4D-C1D	7.79	1.60	1.42
2	A	401	NAI	O4B-C1B	7.63	1.59	1.42
2	B	401	NAI	C2B-C1B	-7.60	1.29	1.53
2	C	401	NAI	C2B-C1B	-7.43	1.30	1.53
2	D	401	NAI	C2N-C3N	7.33	1.55	1.35
2	A	401	NAI	C2N-C3N	7.30	1.55	1.35
2	A	401	NAI	PA-O3	7.28	1.67	1.59
2	D	401	NAI	C2B-C1B	-7.25	1.30	1.53
2	B	401	NAI	C2N-C3N	7.15	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAI	PN-O3	7.12	1.67	1.59
2	C	401	NAI	PA-O3	7.07	1.67	1.59
2	A	401	NAI	C2B-C1B	-7.06	1.31	1.53
2	C	401	NAI	C2N-C3N	7.01	1.54	1.35
2	B	401	NAI	C6N-C5N	6.89	1.54	1.33
2	C	401	NAI	C6N-C5N	6.85	1.54	1.33
2	D	401	NAI	PA-O3	6.85	1.66	1.59
2	D	401	NAI	C6N-C5N	6.67	1.53	1.33
2	C	401	NAI	C2D-C1D	-6.62	1.32	1.53
2	D	401	NAI	C2D-C1D	-6.56	1.32	1.53
2	B	401	NAI	C2D-C1D	-6.55	1.32	1.53
2	A	401	NAI	C2D-C1D	-6.50	1.33	1.53
2	A	401	NAI	C6N-C5N	6.48	1.53	1.33
2	C	401	NAI	PN-O3	6.44	1.66	1.59
2	B	401	NAI	O4D-C4D	-6.35	1.30	1.45
2	C	401	NAI	O4D-C4D	-6.23	1.31	1.45
2	A	401	NAI	O4D-C4D	-6.10	1.31	1.45
2	D	401	NAI	O4D-C4D	-6.08	1.31	1.45
2	D	401	NAI	O4B-C4B	-5.59	1.32	1.45
2	B	401	NAI	O4B-C4B	-5.55	1.32	1.45
2	A	401	NAI	PN-O3	5.43	1.65	1.59
2	C	401	NAI	O4B-C4B	-5.40	1.33	1.45
2	A	401	NAI	O4B-C4B	-5.31	1.33	1.45
2	C	401	NAI	C7N-N7N	3.99	1.44	1.33
2	B	401	NAI	C7N-N7N	3.97	1.44	1.33
2	B	401	NAI	C6N-N1N	3.89	1.46	1.37
2	A	401	NAI	C7N-N7N	3.83	1.44	1.33
2	C	401	NAI	C6N-N1N	3.82	1.46	1.37
2	D	401	NAI	C5A-C4A	-3.79	1.32	1.39
2	D	401	NAI	C7N-N7N	3.75	1.44	1.33
2	A	401	NAI	C5A-C4A	-3.66	1.32	1.39
2	B	401	NAI	C7N-C3N	3.62	1.56	1.48
2	C	401	NAI	C5A-C4A	-3.58	1.32	1.39
2	C	401	NAI	C7N-C3N	3.45	1.56	1.48
2	B	401	NAI	C5A-C4A	-3.44	1.33	1.39
2	C	401	NAI	O3D-C3D	-3.43	1.34	1.43
2	D	401	NAI	C6N-N1N	3.43	1.45	1.37
2	A	401	NAI	C6A-N6A	3.35	1.42	1.34
2	A	401	NAI	C6N-N1N	3.32	1.45	1.37
2	B	401	NAI	C6A-N6A	3.28	1.42	1.34
2	D	401	NAI	C7N-C3N	3.23	1.55	1.48
2	B	401	NAI	O3D-C3D	-3.20	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAI	C7N-C3N	3.20	1.55	1.48
2	D	401	NAI	C5A-N7A	-3.17	1.33	1.39
2	C	401	NAI	C6A-N6A	3.10	1.42	1.34
2	D	401	NAI	C6A-N6A	3.01	1.41	1.34
2	B	401	NAI	C8A-N9A	-2.91	1.32	1.37
2	B	401	NAI	C5A-N7A	-2.86	1.33	1.39
2	A	401	NAI	C8A-N9A	-2.83	1.32	1.37
2	B	401	NAI	O2D-C2D	2.77	1.49	1.43
2	A	401	NAI	O3D-C3D	-2.76	1.36	1.43
2	A	401	NAI	C5A-N7A	-2.68	1.34	1.39
2	D	401	NAI	O3D-C3D	-2.52	1.36	1.43
2	D	401	NAI	C8A-N9A	-2.48	1.33	1.37
2	C	401	NAI	C8A-N9A	-2.43	1.33	1.37
2	A	401	NAI	O5D-C5D	-2.25	1.36	1.44
2	C	401	NAI	C6A-N1A	-2.24	1.29	1.35
2	B	401	NAI	C4N-C5N	2.23	1.54	1.49
2	C	401	NAI	C5A-N7A	-2.21	1.35	1.39
2	B	401	NAI	O3B-C3B	-2.12	1.37	1.43
2	C	401	NAI	PN-O5D	2.10	1.67	1.59
2	D	401	NAI	O2D-C2D	2.10	1.48	1.43
2	C	401	NAI	O2D-C2D	2.10	1.48	1.43
2	B	401	NAI	PN-O5D	2.05	1.67	1.59
2	A	401	NAI	O2D-C2D	2.05	1.48	1.43
2	C	401	NAI	O2B-C2B	2.03	1.48	1.43
2	B	401	NAI	O5D-C5D	-2.01	1.37	1.44
2	D	401	NAI	O5D-C5D	-2.01	1.37	1.44
2	C	401	NAI	C4N-C5N	2.01	1.54	1.49

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAI	N3A-C2A-N1A	-6.61	118.58	128.58
2	C	401	NAI	N3A-C2A-N1A	-6.24	119.13	128.58
2	C	401	NAI	N6A-C6A-N1A	-6.18	104.61	118.38
2	D	401	NAI	N3A-C2A-N1A	-6.14	119.30	128.58
2	B	401	NAI	N3A-C2A-N1A	-5.71	119.94	128.58
2	B	401	NAI	N6A-C6A-N1A	-5.17	106.86	118.38
2	C	401	NAI	C5A-C6A-N6A	4.87	135.35	123.29
2	C	401	NAI	N9A-C8A-N7A	-4.79	107.14	113.94
2	D	401	NAI	C5A-C4A-N3A	-4.71	120.23	126.72
2	A	401	NAI	C5A-C4A-N3A	-4.54	120.47	126.72
2	A	401	NAI	N9A-C8A-N7A	-4.54	107.50	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAI	N6A-C6A-N1A	-4.42	108.52	118.38
2	B	401	NAI	C5A-C4A-N3A	-4.40	120.65	126.72
2	D	401	NAI	N9A-C8A-N7A	-4.37	107.73	113.94
2	B	401	NAI	N9A-C8A-N7A	-4.12	108.09	113.94
2	B	401	NAI	C5A-C6A-N6A	4.09	133.42	123.29
2	A	401	NAI	N6A-C6A-N1A	-4.04	109.39	118.38
2	C	401	NAI	C5A-C4A-N3A	-3.72	121.59	126.72
2	A	401	NAI	N3A-C4A-N9A	3.47	133.06	127.17
2	D	401	NAI	C2A-N3A-C4A	3.39	120.11	111.83
2	A	401	NAI	C4A-N9A-C8A	3.35	109.26	105.74
2	A	401	NAI	C2A-N3A-C4A	3.33	119.97	111.83
2	D	401	NAI	C5A-C6A-N6A	3.29	131.43	123.29
2	D	401	NAI	N3A-C4A-N9A	3.24	132.68	127.17
2	B	401	NAI	C2A-N3A-C4A	3.20	119.66	111.83
2	C	401	NAI	C2A-N3A-C4A	3.10	119.40	111.83
2	A	401	NAI	C5A-C6A-N6A	3.04	130.82	123.29
2	C	401	NAI	C4A-N9A-C8A	2.97	108.86	105.74
2	C	401	NAI	C5A-N7A-C8A	2.93	108.06	103.45
2	B	401	NAI	C5A-N7A-C8A	2.79	107.83	103.45
2	A	401	NAI	C5A-N7A-C8A	2.72	107.72	103.45
2	A	401	NAI	O3-PA-O1A	-2.70	102.59	110.70
2	D	401	NAI	C5A-N7A-C8A	2.62	107.57	103.45
2	D	401	NAI	C4A-N9A-C8A	2.57	108.44	105.74
2	A	401	NAI	C1B-N9A-C8A	-2.55	121.43	127.09
2	D	401	NAI	C1B-N9A-C8A	-2.54	121.46	127.09
2	A	401	NAI	O3B-C3B-C2B	-2.54	103.68	111.82
2	A	401	NAI	O4D-C1D-C2D	-2.51	101.25	106.62
2	B	401	NAI	N3A-C4A-N9A	2.47	131.36	127.17
2	C	401	NAI	C4A-C5A-N7A	-2.32	107.93	110.58
2	D	401	NAI	O4B-C1B-C2B	-2.20	101.90	106.62
2	B	401	NAI	C4A-C5A-N7A	-2.20	108.06	110.58
2	B	401	NAI	C4A-N9A-C8A	2.18	108.03	105.74
2	D	401	NAI	C6A-C5A-C4A	2.05	119.98	117.18
2	A	401	NAI	O4B-C1B-C2B	-2.03	102.27	106.62
2	D	401	NAI	O4D-C1D-N1N	-2.03	104.22	108.08
2	C	401	NAI	C5A-C4A-N9A	2.01	108.01	105.81

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	NAI	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
2	D	401	NAI	C2N-C3N-C7N-N7N
2	B	401	NAI	O4B-C4B-C5B-O5B
2	C	401	NAI	C2D-C1D-N1N-C6N
5	C	410	EDO	O1-C1-C2-O2
2	B	401	NAI	C2D-C1D-N1N-C2N
2	B	401	NAI	C2D-C1D-N1N-C6N
2	C	401	NAI	C2D-C1D-N1N-C2N
2	D	401	NAI	C2D-C1D-N1N-C6N
2	C	401	NAI	PN-O3-PA-O1A
2	B	401	NAI	C3B-C4B-C5B-O5B
6	A	411	TRS	C3-C-C1-O1
6	A	411	TRS	N-C-C1-O1
6	B	408	TRS	C1-C-C3-O3
6	B	408	TRS	N-C-C3-O3
2	D	401	NAI	C2D-C1D-N1N-C2N
2	A	401	NAI	PN-O3-PA-O1A
2	B	401	NAI	C2B-C1B-N9A-C8A
6	A	411	TRS	C2-C-C1-O1
6	A	411	TRS	C1-C-C2-O2
6	A	411	TRS	C3-C-C2-O2
2	B	401	NAI	O4D-C1D-N1N-C2N
2	B	401	NAI	C5B-O5B-PA-O1A
2	B	401	NAI	C5B-O5B-PA-O3
2	A	401	NAI	C2D-C1D-N1N-C6N
2	B	401	NAI	O4D-C1D-N1N-C6N
2	A	401	NAI	PN-O3-PA-O2A
2	D	401	NAI	PN-O3-PA-O2A
2	D	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C6N
6	A	411	TRS	N-C-C2-O2
5	A	410	EDO	O1-C1-C2-O2
2	A	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C2N
2	D	401	NAI	O4D-C1D-N1N-C2N
2	A	401	NAI	C2B-C1B-N9A-C8A
6	A	411	TRS	C2-C-C3-O3
6	B	408	TRS	C3-C-C2-O2
6	B	408	TRS	C2-C-C3-O3
2	A	401	NAI	C2D-C1D-N1N-C2N
2	B	401	NAI	O4B-C1B-N9A-C8A
2	B	401	NAI	PN-O3-PA-O2A
2	C	401	NAI	PN-O3-PA-O2A

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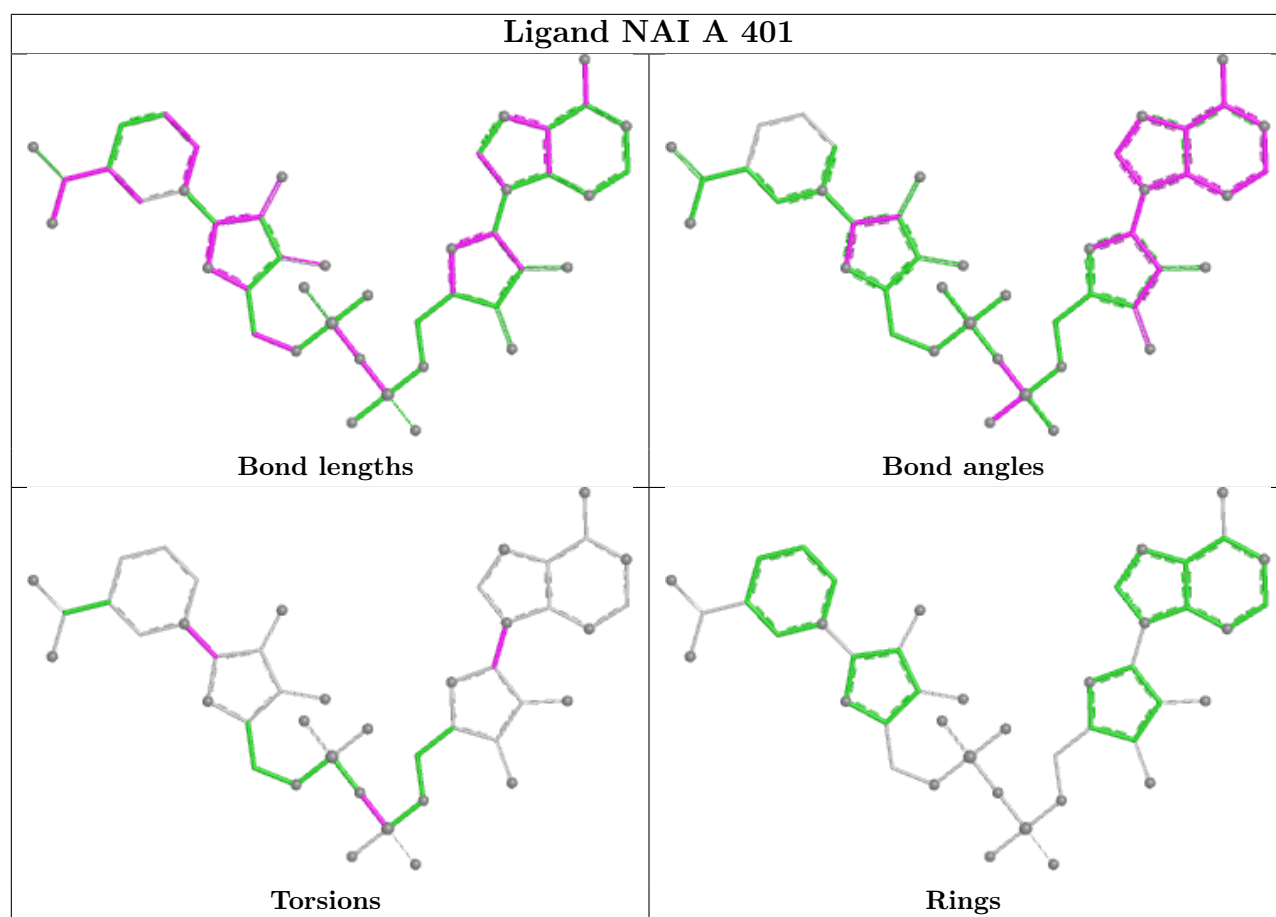
Mol	Chain	Res	Type	Atoms
2	D	401	NAI	PN-O3-PA-O1A
2	D	401	NAI	C2B-C1B-N9A-C8A
6	B	408	TRS	N-C-C2-O2

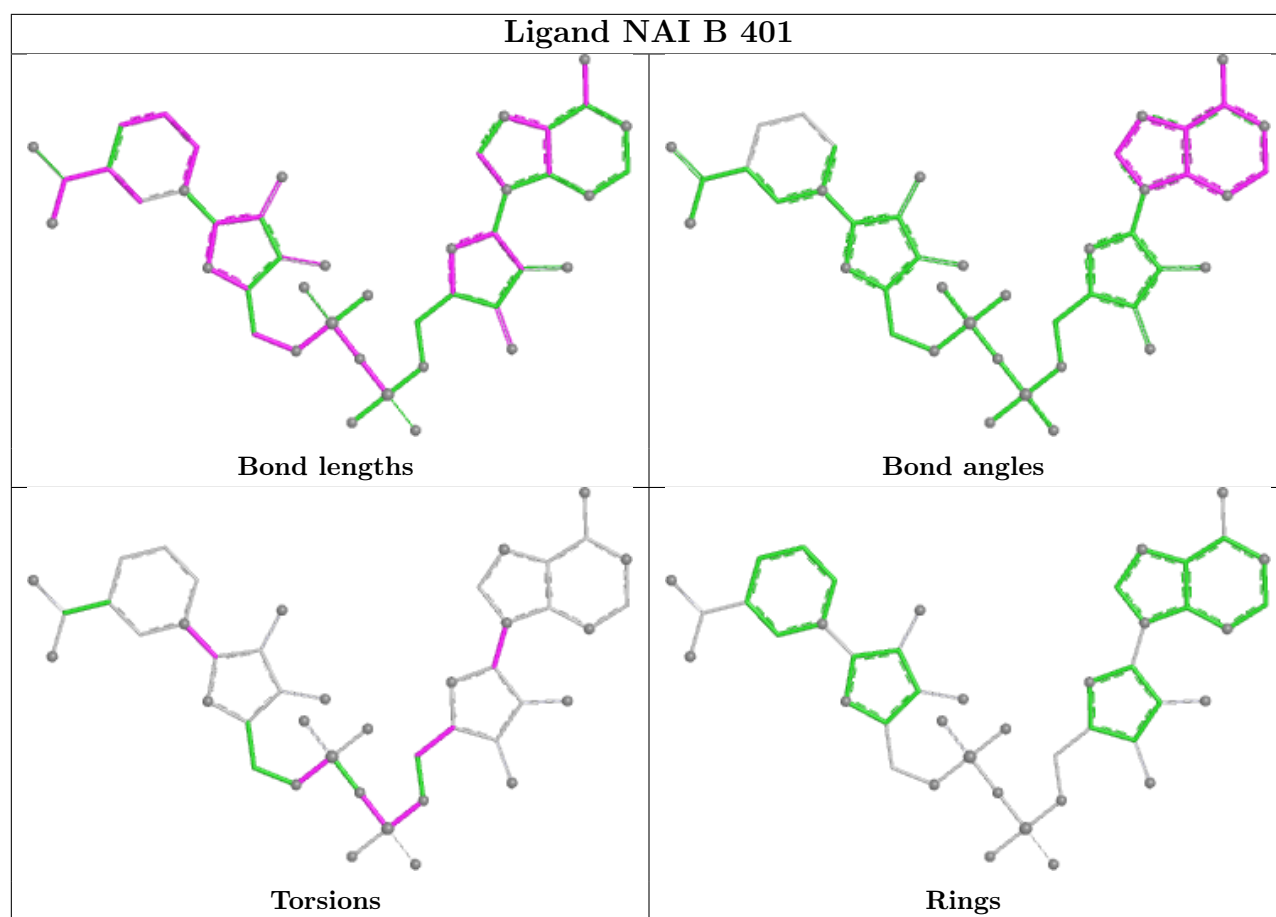
There are no ring outliers.

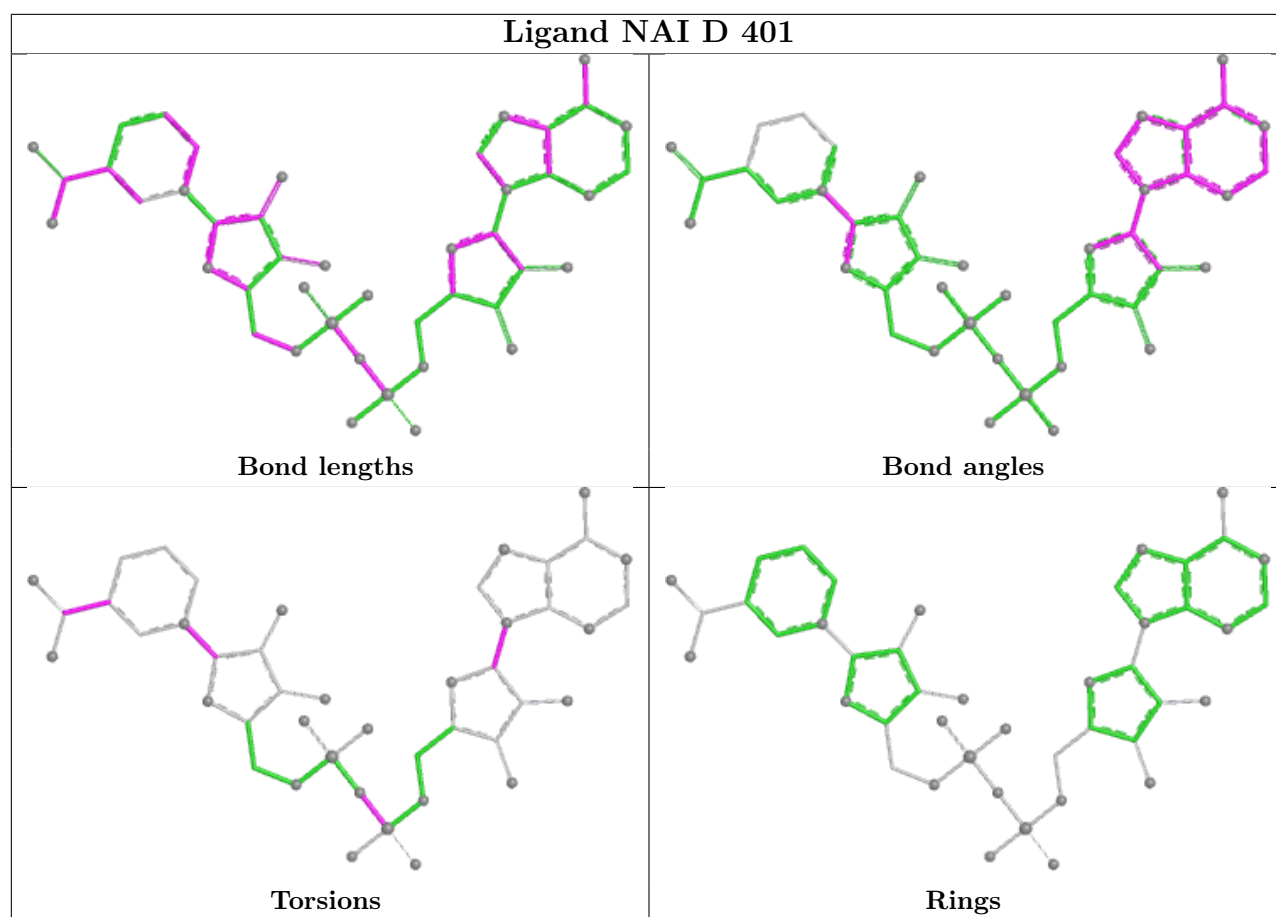
12 monomers are involved in 20 short contacts:

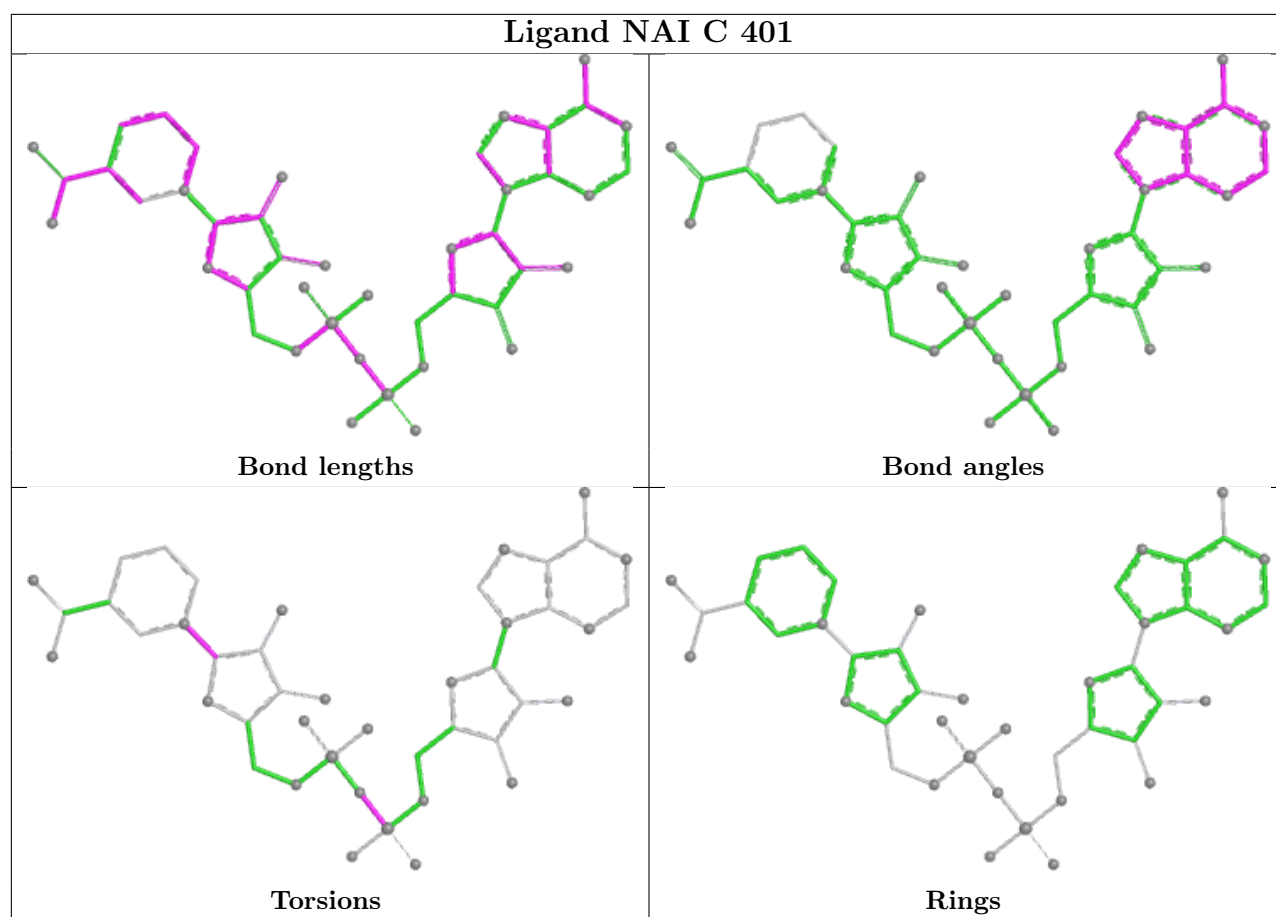
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	SO4	1	0
2	A	401	NAI	1	0
3	D	404	SO4	1	0
3	A	406	SO4	1	0
5	C	410	EDO	3	0
2	B	401	NAI	7	0
3	D	407	SO4	1	0
2	D	401	NAI	1	0
3	A	404	SO4	1	0
2	C	401	NAI	1	0
3	D	402	SO4	1	0
3	D	406	SO4	1	0

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

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	332/334 (99%)	-0.22	9 (2%) 56 59	12, 26, 44, 90	0
1	B	332/334 (99%)	1.18	109 (32%) 1 1	14, 57, 108, 125	0
1	C	333/334 (99%)	0.34	23 (6%) 23 25	18, 38, 69, 123	0
1	D	332/334 (99%)	-0.13	7 (2%) 63 66	17, 30, 49, 73	0
All	All	1329/1336 (99%)	0.29	148 (11%) 10 11	12, 31, 94, 125	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	GLY	6.0
1	B	23	ILE	5.4
1	B	103	LEU	5.1
1	B	54	PHE	5.0
1	B	128	VAL	5.0
1	B	47	LEU	4.8
1	B	142	VAL	4.8
1	B	25	TYR	4.5
1	B	44	VAL	4.3
1	B	67	LEU	4.2
1	B	68	THR	4.1
1	B	69	PRO	4.1
1	B	145	MET	4.1
1	B	180	THR	4.1
1	B	14	LEU	3.9
1	B	63	VAL	3.9
1	B	15	LEU	3.9
1	B	36	LEU	3.8
1	A	331	PRO	3.8
1	C	2	ALA	3.8
1	B	125	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	59	TRP	3.7
1	C	54	PHE	3.7
1	B	181	ARG	3.7
1	B	33	ALA	3.7
1	B	177	ILE	3.7
1	C	328	ALA	3.7
1	B	166	ALA	3.6
1	B	183	GLY	3.6
1	B	179	CYS	3.5
1	B	45	VAL	3.5
1	B	141	LEU	3.5
1	B	62	VAL	3.4
1	B	84	ILE	3.4
1	B	24	GLY	3.4
1	B	30	HIS	3.4
1	B	178	GLY	3.4
1	B	21	ALA	3.4
1	B	82	ILE	3.4
1	B	2	ALA	3.3
1	B	55	THR	3.2
1	B	163	THR	3.2
1	B	12	LEU	3.2
1	C	145	MET	3.2
1	B	29	GLY	3.2
1	C	66	GLY	3.2
1	A	13	ASP	3.2
1	C	50	PRO	3.1
1	B	72	VAL	3.1
1	B	102	TYR	3.1
1	B	328	ALA	3.1
1	B	71	PRO	3.1
1	B	22	VAL	3.1
1	D	332	TRP	3.0
1	C	329	MET	3.0
1	A	51	GLU	3.0
1	B	135	PRO	3.0
1	D	331	PRO	3.0
1	B	146	TYR	3.0
1	B	185	ILE	3.0
1	B	57	ALA	2.8
1	B	75	ALA	2.8
1	B	151	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	170	GLY	2.8
1	C	63	VAL	2.8
1	B	86	VAL	2.8
1	B	184	VAL	2.8
1	B	176	GLY	2.8
1	B	122	ILE	2.8
1	B	80	GLN	2.7
1	B	79	ALA	2.7
1	B	41	LEU	2.7
1	C	331	PRO	2.7
1	B	140	HIS	2.7
1	B	150	VAL	2.7
1	D	53	ASP	2.7
1	B	182	ALA	2.7
1	B	158	VAL	2.6
1	B	56	THR	2.6
1	B	50	PRO	2.6
1	B	10	ALA	2.6
1	B	123	VAL	2.6
1	B	17	GLY	2.6
1	B	331	PRO	2.6
1	B	70	LEU	2.6
1	C	51	GLU	2.5
1	A	332	TRP	2.5
1	C	150	VAL	2.5
1	B	37	HIS	2.5
1	B	81	ILE	2.5
1	C	53	ASP	2.5
1	B	143	ARG	2.5
1	B	162	HIS	2.4
1	B	83	GLN	2.4
1	B	149	GLY	2.4
1	A	329	MET	2.4
1	B	49	LYS	2.4
1	B	6	TYR	2.3
1	B	64	ALA	2.3
1	B	164	GLY	2.3
1	B	19	THR	2.3
1	A	328	ALA	2.3
1	B	35	ASN	2.3
1	B	104	ASN	2.3
1	B	66	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	150	VAL	2.3
1	B	152	VAL	2.3
1	B	32	GLN	2.3
1	B	87	PRO	2.3
1	B	126	PRO	2.3
1	B	85	LEU	2.3
1	B	139	GLY	2.3
1	B	147	ARG	2.3
1	C	61	GLN	2.3
1	D	150	VAL	2.3
1	B	76	ALA	2.3
1	B	106	GLY	2.3
1	B	138	PRO	2.2
1	B	65	ASP	2.2
1	C	62	VAL	2.2
1	C	25	TYR	2.2
1	B	53	ASP	2.2
1	D	328	ALA	2.2
1	A	333	LEU	2.2
1	B	3	ARG	2.2
1	C	59	TRP	2.2
1	B	101	PRO	2.1
1	C	164	GLY	2.1
1	D	333	LEU	2.1
1	B	40	GLY	2.1
1	B	43	VAL	2.1
1	B	130	VAL	2.1
1	B	11	ASN	2.1
1	C	142	VAL	2.1
1	B	18	LYS	2.1
1	B	108	ALA	2.1
1	B	134	ALA	2.1
1	C	64	ALA	2.1
1	A	239	LEU	2.1
1	C	147	ARG	2.1
1	C	67	LEU	2.0
1	C	103	LEU	2.0
1	C	141	LEU	2.0
1	B	144	ARG	2.0
1	B	174	ALA	2.0
1	D	13	ASP	2.0
1	B	16	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	95	TYR	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(Å ²)	Q<0.9
3	SO4	C	402	5/5	0.57	0.17	127,127,128,128	0
3	SO4	D	406	5/5	0.63	0.22	125,126,126,126	0
3	SO4	C	405	5/5	0.64	0.14	78,78,81,93	0
3	SO4	B	402	5/5	0.72	0.15	99,99,102,106	0
3	SO4	D	402	5/5	0.75	0.19	90,90,90,95	0
3	SO4	A	402	5/5	0.75	0.17	74,75,76,83	0
3	SO4	A	406	5/5	0.80	0.11	61,61,68,78	0
2	NAI	B	401	44/44	0.83	0.12	54,72,82,87	0
3	SO4	B	404	5/5	0.84	0.12	77,77,80,92	0
3	SO4	A	405	5/5	0.84	0.10	62,67,73,82	0
3	SO4	C	403	5/5	0.84	0.21	53,54,62,66	0
6	TRS	A	411	8/8	0.84	0.14	45,52,57,58	8
3	SO4	C	404	5/5	0.85	0.10	62,62,69,77	0
6	TRS	B	408	8/8	0.85	0.11	46,49,50,52	0
3	SO4	A	407	5/5	0.86	0.12	82,82,82,91	0
3	SO4	A	404	5/5	0.87	0.24	58,58,59,64	0
3	SO4	B	403	5/5	0.88	0.21	53,57,64,71	0
4	MG	B	407	1/1	0.88	0.08	51,51,51,51	0
3	SO4	D	407	5/5	0.89	0.11	73,73,79,81	0
3	SO4	D	404	5/5	0.89	0.25	35,45,54,57	0
5	EDO	A	410	4/4	0.90	0.18	35,37,37,44	0
5	EDO	C	409	4/4	0.90	0.12	43,43,50,50	0

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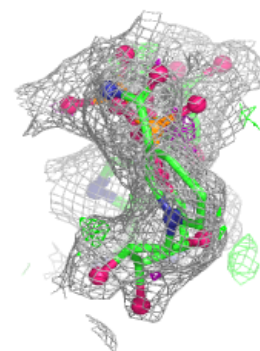
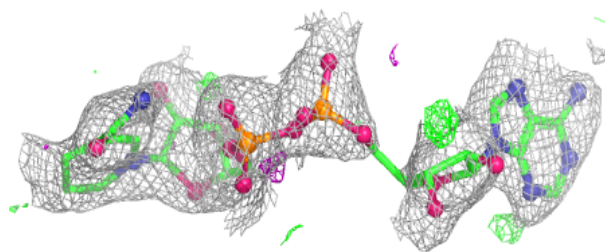
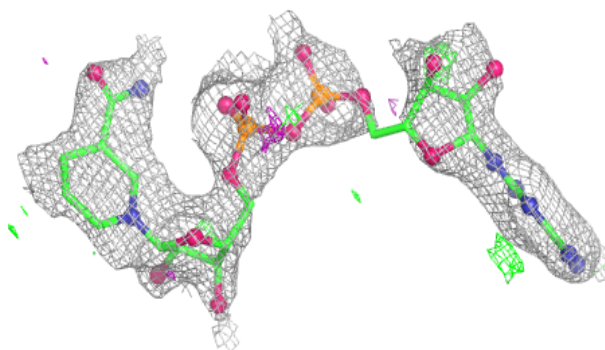
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	405	5/5	0.90	0.07	61,62,70,78	0
4	MG	D	408	1/1	0.90	0.16	51,51,51,51	0
5	EDO	C	410	4/4	0.91	0.22	48,48,48,50	0
3	SO4	C	406	5/5	0.92	0.14	55,56,66,67	0
3	SO4	B	405	5/5	0.93	0.11	75,75,80,82	0
3	SO4	A	403	5/5	0.93	0.13	51,56,64,68	0
3	SO4	D	403	5/5	0.94	0.16	49,54,57,64	0
4	MG	A	409	1/1	0.95	0.09	50,50,50,50	0
2	NAI	C	401	44/44	0.95	0.09	30,41,46,51	0
4	MG	A	408	1/1	0.96	0.15	41,41,41,41	0
4	MG	C	407	1/1	0.96	0.11	38,38,38,38	0
2	NAI	D	401	44/44	0.96	0.07	21,27,34,38	0
4	MG	B	406	1/1	0.96	0.10	43,43,43,43	0
4	MG	D	409	1/1	0.97	0.12	39,39,39,39	0
4	MG	C	408	1/1	0.97	0.09	51,51,51,51	0
2	NAI	A	401	44/44	0.97	0.06	15,22,28,34	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.

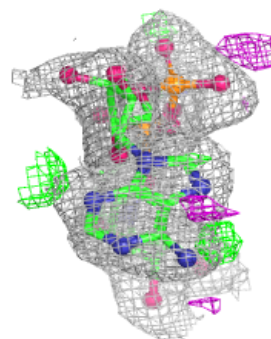
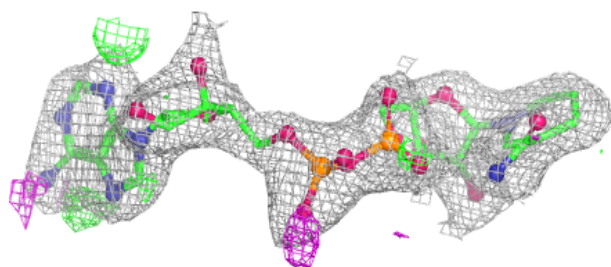
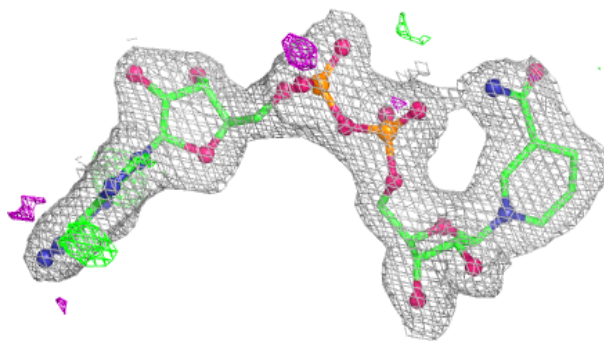
Electron density around NAI B 401:

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

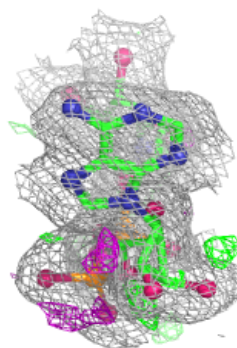
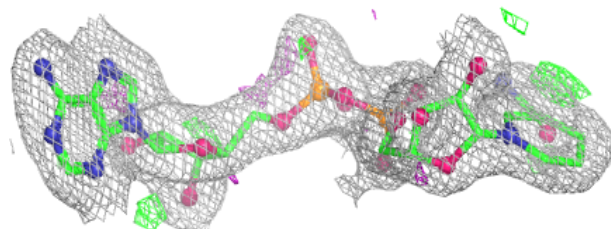
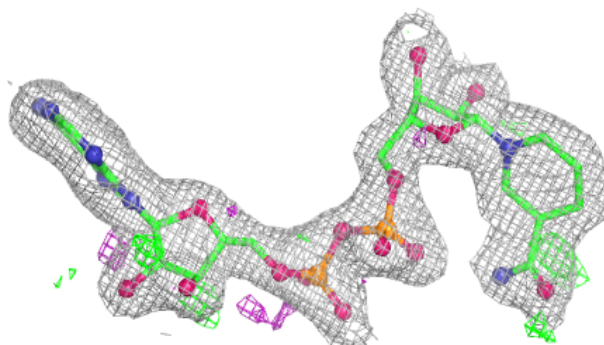


Electron density around NAI C 401:

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

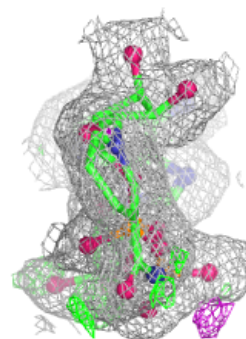
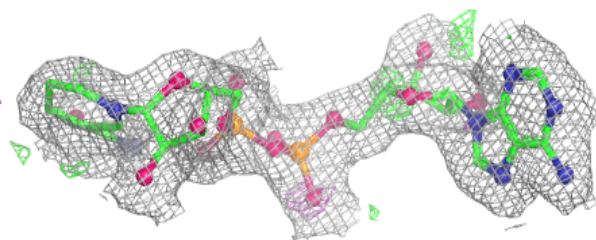
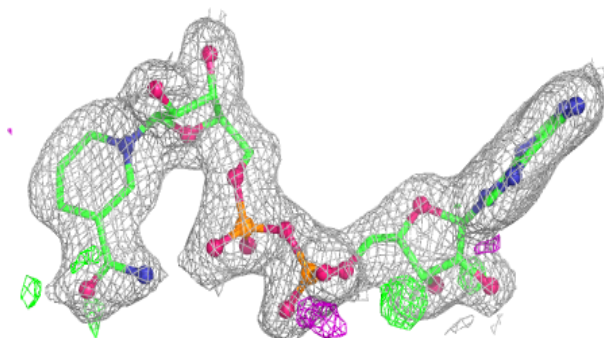
**Electron density around NAI D 401:**

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



Electron density around NAI A 401:

$2mF_o-DF_c$ (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.