



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:52 AM UTC

PDB ID : 8CFB / pdb_00008cfb
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *P. aeruginosa* in complex with F2X-Entry library fragment D02
Authors : Malecki, P.H.; Gawel, M.; Stepniewska, M.; Brzezinski, K.
Deposited on : 2023-02-03
Resolution : 2.07 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

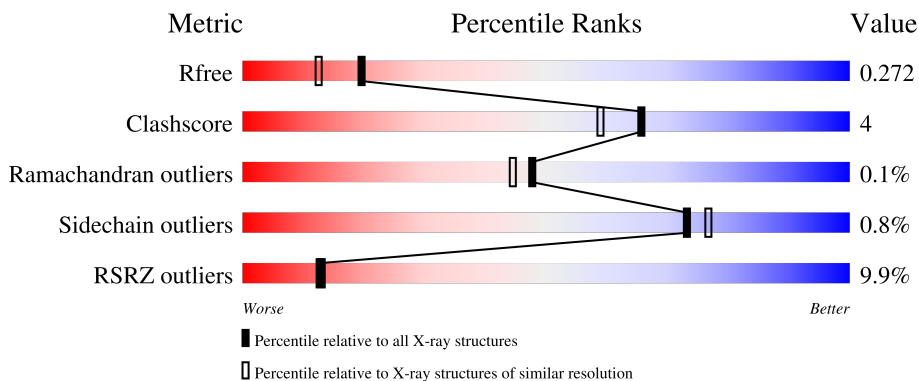
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	472	
1	B	472	
1	C	472	
1	D	472	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15122 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 Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	462	3570	2250	618	680	22	0	2	0
1	B	461	3577	2256	619	680	22	0	4	0
1	C	462	3576	2255	619	680	22	0	3	0
1	D	461	3565	2247	616	680	22	0	2	0

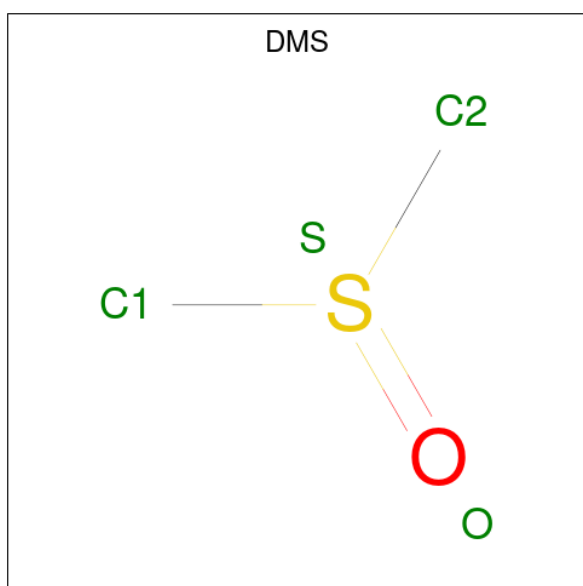
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9I685
A	-1	ASN	-	expression tag	UNP Q9I685
A	0	ALA	-	expression tag	UNP Q9I685
B	-2	SER	-	expression tag	UNP Q9I685
B	-1	ASN	-	expression tag	UNP Q9I685
B	0	ALA	-	expression tag	UNP Q9I685
C	-2	SER	-	expression tag	UNP Q9I685
C	-1	ASN	-	expression tag	UNP Q9I685
C	0	ALA	-	expression tag	UNP Q9I685
D	-2	SER	-	expression tag	UNP Q9I685
D	-1	ASN	-	expression tag	UNP Q9I685
D	0	ALA	-	expression tag	UNP Q9I685

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 10 5 5	0	0
3	B	1	Total C N 10 5 5	0	0
3	C	1	Total C N 10 5 5	0	0
3	D	1	Total C N 10 5 5	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).

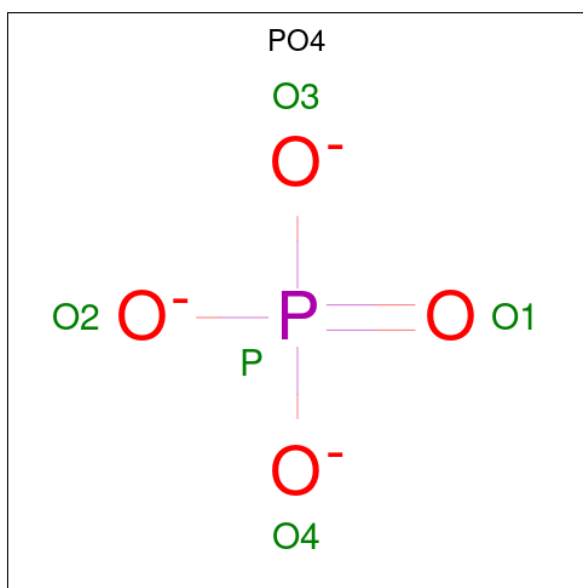


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



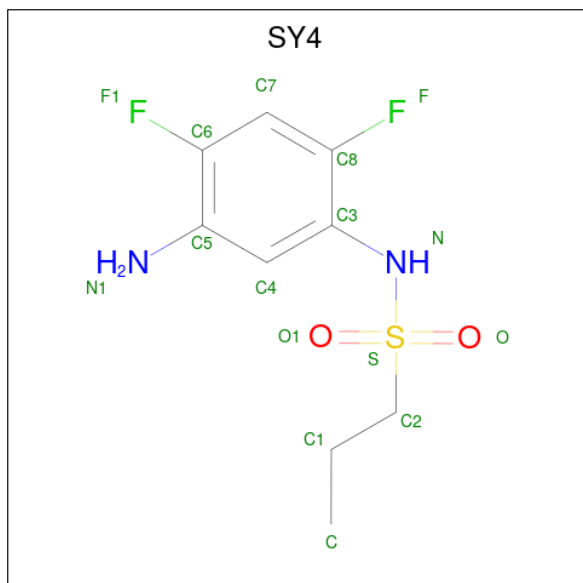
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	D	1	Total O P 5 4 1	0	0
6	D	1	Total O P 5 4 1	0	0
6	D	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is {N}-[5-azanyl-2,4-bis(fluoranyl)phenyl]propane-1-sulfonamide (CCD ID: SY4) (formula: C₉H₁₂F₂N₂O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
7	A	1	Total	C	F	N	O	S	0	0
			16	9	2	2	2	1		

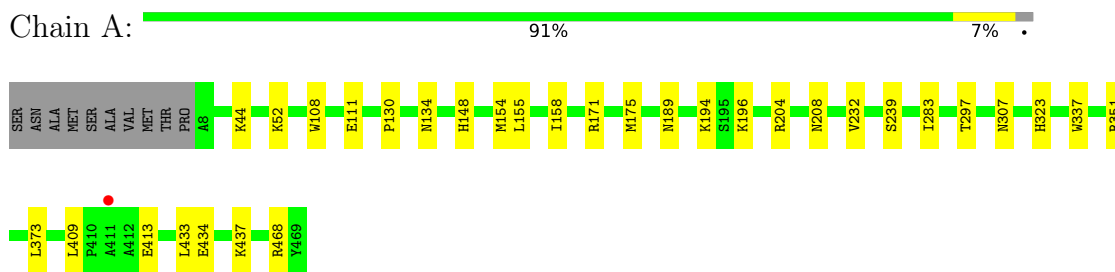
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	233	Total	O	0	2
			235	235		
8	B	118	Total	O	0	0
			118	118		
8	C	47	Total	O	0	0
			47	47		
8	D	118	Total	O	0	1
			119	119		

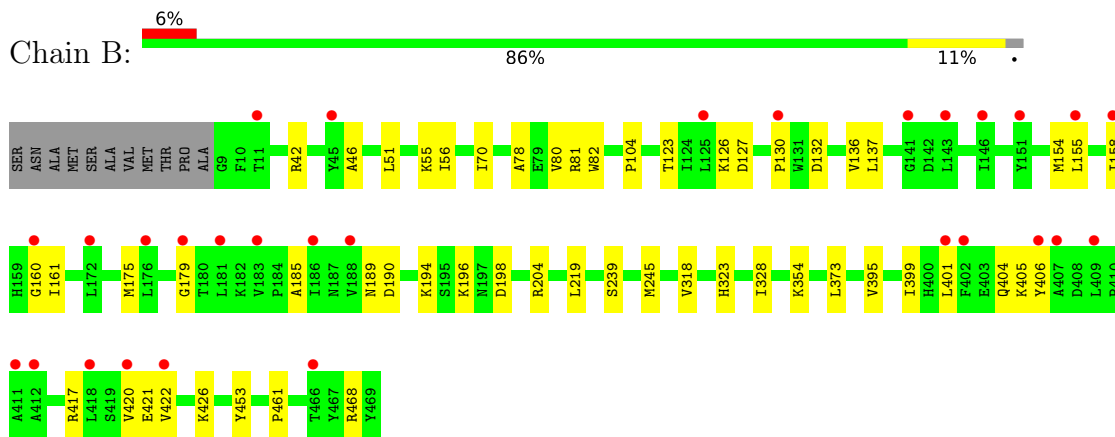
3 Residue-property plots [i](#)

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.

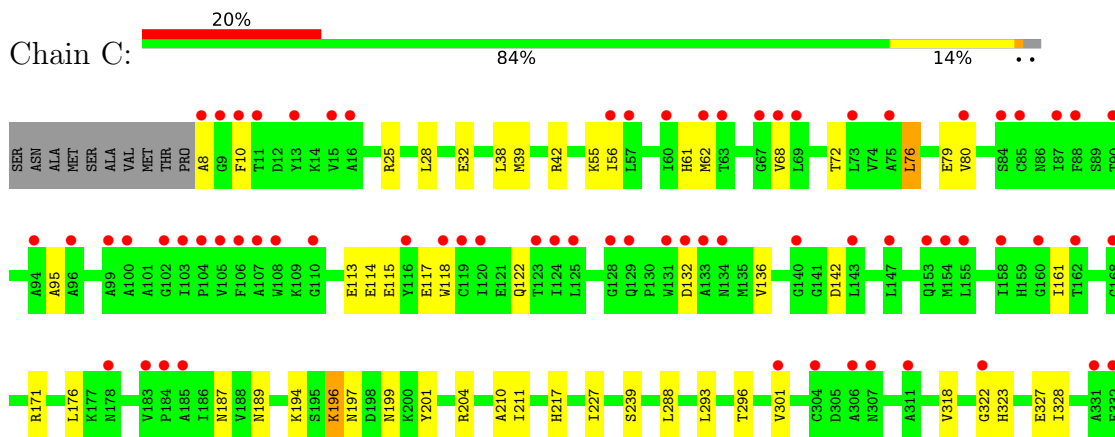
- Molecule 1: Adenosylhomocysteinase

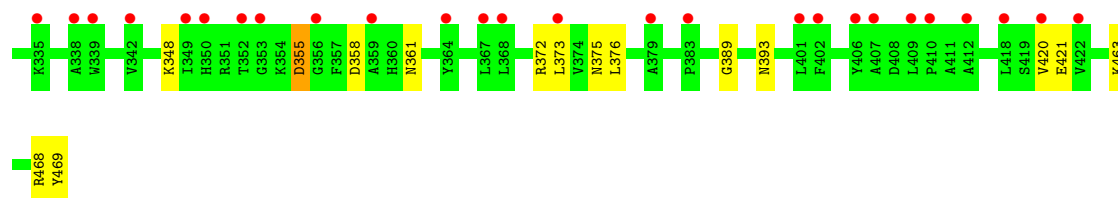


- Molecule 1: Adenosylhomocysteinase

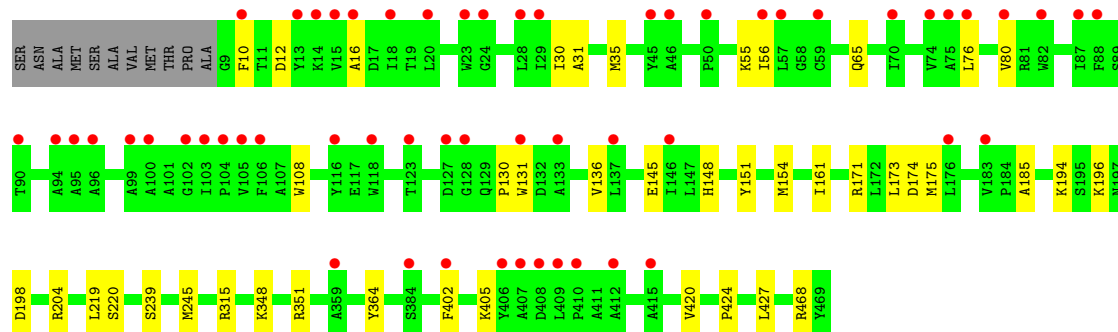
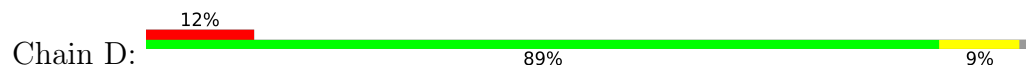


- Molecule 1: Adenosylhomocysteinase





- Molecule 1: Adenosylhomocysteinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.97Å 103.68Å 109.20Å 90.00° 99.99° 90.00°	Depositor
Resolution (Å)	32.64 – 2.07 32.64 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.64-2.07) 99.5 (32.64-2.07)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.07Å)	Xtrriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, R_{free}	0.235 , 0.271 0.236 , 0.272	Depositor DCC
R_{free} test set	2100 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtrriage
Anisotropy	0.407	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15122	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, PO4, NAD, SY4, K, ADE

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	0.11	0/3636	0.33	0/4916
1	B	0.12	0/3649	0.31	0/4932
1	C	0.11	0/3645	0.30	0/4927
1	D	0.11	0/3631	0.30	0/4909
All	All	0.11	0/14561	0.31	0/19684

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3570	0	3576	19	0
1	B	3577	0	3592	31	0
1	C	3576	0	3589	41	0
1	D	3565	0	3570	25	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	1	0
3	A	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	A	4	0	6	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	0	0	0
6	B	15	0	0	0	0
6	C	20	0	0	2	0
6	D	25	0	0	1	0
7	A	16	0	0	2	0
8	A	235	0	0	0	0
8	B	118	0	0	0	0
8	C	47	0	0	1	0
8	D	119	0	0	0	0
All	All	15122	0	14453	111	0

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

All (111) 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:C:204:ARG:HA	1:C:239:SER:HB2	1.71	0.71
1:A:189:ASN:HA	1:A:194:LYS:HD2	1.75	0.69
1:B:130:PRO:HB3	1:B:154:MET:HE3	1.75	0.68
1:C:211:ILE:HD13	1:C:293:LEU:HD11	1.77	0.65
1:D:130:PRO:HB3	1:D:154:MET:HE2	1.78	0.64
1:C:204:ARG:NH2	1:D:220:SER:OG	2.31	0.64
1:B:404:GLN:HB3	1:B:417:ARG:HH12	1.63	0.64
1:D:31:ALA:HB1	1:D:35:MET:HE3	1.79	0.64
1:B:404:GLN:HB3	1:B:417:ARG:NH1	2.14	0.63
1:B:204:ARG:HA	1:B:239:SER:HB2	1.81	0.63
1:D:145:GLU:OE1	1:D:171:ARG:NH2	2.33	0.62
1:B:51:LEU:HB3	1:B:78:ALA:HB2	1.82	0.62
1:D:204:ARG:HA	1:D:239:SER:HB2	1.84	0.59
1:B:160:GLY:HA3	1:B:401:LEU:HD13	1.83	0.59
1:B:56:ILE:HB	1:B:80:VAL:HG12	1.87	0.57
1:C:189:ASN:HA	1:C:194:LYS:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ARG:NH2	6:D:504:PO4:O2	2.38	0.57
1:B:196[B]:LYS:NZ	1:C:469:TYR:OXT	2.38	0.57
1:C:227:ILE:HD13	1:C:296:THR:HG22	1.87	0.56
1:B:323:HIS:HA	1:B:373:LEU:HD21	1.88	0.56
1:D:35:MET:HE1	1:D:65:GLN:HA	1.87	0.56
1:C:348:LYS:HD2	1:D:30:ILE:HD11	1.88	0.55
1:C:55:LYS:NZ	1:C:79:GLU:OE1	2.37	0.54
1:D:16:ALA:HB2	1:D:108:TRP:HB2	1.90	0.54
1:B:189:ASN:HA	1:B:194:LYS:HD2	1.88	0.54
1:A:204:ARG:HA	1:A:239:SER:HB2	1.89	0.53
1:C:323:HIS:HA	1:C:373:LEU:HD21	1.90	0.53
1:C:32:GLU:HG2	1:C:39:MET:HE3	1.91	0.53
1:C:25:ARG:NH1	6:C:504:PO4:O2	2.43	0.52
1:D:171:ARG:O	1:D:175:MET:HG3	2.10	0.52
1:B:426:LYS:HG2	1:B:461:PRO:HG3	1.91	0.52
1:A:44:LYS:HD2	7:A:508:SY4:O1	2.11	0.51
1:C:187:ASN:N	1:C:421:GLU:O	2.31	0.50
1:B:453:TYR:CE2	1:C:301:VAL:HB	2.48	0.49
1:A:283:ILE:HG13	1:A:307:ASN:HB3	1.94	0.49
1:B:453:TYR:HE2	1:C:301:VAL:HB	1.78	0.49
1:D:219:LEU:O	1:D:245:MET:HG2	2.13	0.49
1:C:136:VAL:HB	1:C:161:ILE:HG12	1.94	0.48
1:D:56:ILE:HB	1:D:80:VAL:HG12	1.95	0.48
1:C:114:GLU:HG2	1:C:115:GLU:N	2.29	0.48
1:D:148:HIS:CG	1:D:175:MET:HE1	2.48	0.48
1:B:81:ARG:NH1	1:B:123:THR:O	2.46	0.48
1:C:113:GLU:OE2	1:C:372:ARG:NH2	2.47	0.48
1:C:142:ASP:OD1	1:C:171:ARG:NH2	2.47	0.48
1:A:208[A]:ASN:ND2	1:A:239:SER:OG	2.46	0.48
1:C:389:GLY:O	1:C:393:ASN:ND2	2.40	0.48
1:A:148:HIS:CG	1:A:175:MET:HE1	2.49	0.47
1:C:197:ASN:HA	1:C:201:TYR:HD2	1.79	0.47
1:C:55:LYS:HD2	1:C:132:ASP:O	2.15	0.47
1:D:136:VAL:HB	1:D:161:ILE:HG12	1.97	0.47
1:D:185:ALA:HB3	1:D:420:VAL:HG22	1.97	0.47
1:B:136:VAL:HB	1:B:161:ILE:HG12	1.97	0.46
1:C:118:TRP:O	1:C:122:GLN:HG2	2.16	0.46
1:D:151:TYR:HB3	1:D:154:MET:HE3	1.97	0.46
1:C:56:ILE:HB	1:C:80:VAL:HG12	1.96	0.46
1:B:70:ILE:HG23	1:B:80:VAL:HG21	1.96	0.45
1:B:395:VAL:O	1:B:399:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:PHE:O	1:D:405:LYS:HD2	2.16	0.45
1:B:81:ARG:HG2	1:B:104:PRO:HG2	1.99	0.45
1:B:404:GLN:O	1:B:406:TYR:N	2.49	0.45
1:C:194:LYS:NZ	6:C:505:PO4:O1	2.37	0.45
1:B:155:LEU:HA	1:B:158:ILE:HD12	1.98	0.45
1:C:176:LEU:HD22	1:C:420:VAL:HG23	1.99	0.45
1:C:210:ALA:HB2	1:C:375:ASN:HA	1.99	0.45
1:A:468:ARG:HB2	1:D:196:LYS:HE3	1.98	0.45
1:B:194:LYS:O	1:B:198:ASP:N	2.49	0.45
1:C:199:ASN:OD1	2:C:501:NAD:H5N	2.17	0.44
1:D:194:LYS:HD2	1:D:198:ASP:HB3	1.99	0.44
1:D:10:PHE:CZ	1:D:12:ASP:HB3	2.52	0.44
1:A:409:LEU:HB3	1:A:413:GLU:HB2	2.00	0.44
1:B:42:ARG:O	1:B:46:ALA:HB2	2.17	0.44
1:A:232:VAL:HG12	1:A:297:THR:HB	2.00	0.44
1:A:434:GLU:HG3	7:A:508:SY4:N1	2.32	0.44
1:C:322:GLY:HA3	1:C:327:GLU:OE2	2.18	0.43
1:C:358:ASP:HB3	1:C:361:ASN:HB2	1.99	0.43
1:C:318:VAL:HG12	1:C:328:ILE:HD13	1.99	0.43
1:A:337:TRP:CD1	1:A:351:ARG:HA	2.54	0.43
1:B:82:TRP:HH2	1:B:137:LEU:HD13	1.83	0.43
1:C:61:HIS:CE1	1:C:376:LEU:HD13	2.54	0.43
1:B:55:LYS:NZ	1:B:132:ASP:OD2	2.48	0.43
1:B:190:ASP:O	1:C:468:ARG:NH1	2.44	0.43
1:D:315:ARG:HG2	1:D:364:TYR:CZ	2.54	0.43
1:D:348:LYS:HD2	1:D:364:TYR:CD1	2.54	0.43
1:C:72:THR:O	1:C:76:LEU:HD22	2.18	0.43
1:B:185:ALA:HB3	1:B:420:VAL:HG22	2.02	0.42
1:A:155:LEU:HA	1:A:158:ILE:HD12	2.01	0.42
1:C:38:LEU:HD23	1:C:68:VAL:HG12	2.00	0.42
1:C:355:ASP:OD1	1:C:355:ASP:N	2.51	0.42
2:D:501:NAD:H2D	2:D:501:NAD:H6N	1.81	0.42
2:A:501:NAD:H2D	2:A:501:NAD:H6N	1.81	0.42
1:B:219:LEU:O	1:B:245:MET:HG2	2.19	0.42
2:C:501:NAD:H2D	2:C:501:NAD:H6N	1.83	0.42
1:A:171:ARG:O	1:A:175:MET:HG3	2.19	0.42
1:C:62:MET:HE2	1:C:95:ALA:HA	2.01	0.42
2:B:501:NAD:H2D	2:B:501:NAD:H6N	1.78	0.41
1:A:130:PRO:HB3	1:A:154:MET:SD	2.60	0.41
1:A:433:LEU:HG	1:A:437:LYS:HE3	2.02	0.41
1:B:126:LYS:HG2	1:B:127:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASN:HA	1:A:158:ILE:HA	2.01	0.41
1:B:175:MET:O	1:B:179:GLY:N	2.54	0.41
1:C:39:MET:HE1	1:C:42:ARG:CZ	2.50	0.41
1:C:463:LYS:NZ	8:C:601:HOH:O	2.49	0.41
1:A:108:TRP:O	1:A:111:GLU:HG3	2.20	0.41
1:A:196:LYS:HE3	1:D:468:ARG:HB2	2.02	0.41
1:B:468:ARG:HB2	1:C:196[A]:LYS:NZ	2.35	0.41
1:D:424:PRO:HD2	1:D:427:LEU:HD12	2.03	0.41
1:B:318:VAL:HG12	1:B:328:ILE:HD13	2.03	0.41
1:A:323:HIS:HA	1:A:373:LEU:HD21	2.02	0.41
1:C:8:ALA:C	1:C:10:PHE:H	2.28	0.41
1:D:55:LYS:HB3	1:D:131:TRP:CH2	2.56	0.41
1:C:28:LEU:O	1:C:32:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/472 (98%)	454 (98%)	8 (2%)	0	100	100
1	B	463/472 (98%)	444 (96%)	17 (4%)	2 (0%)	30	23
1	C	463/472 (98%)	452 (98%)	11 (2%)	0	100	100
1	D	461/472 (98%)	451 (98%)	10 (2%)	0	100	100
All	All	1849/1888 (98%)	1801 (97%)	46 (2%)	2 (0%)	48	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	405	LYS
1	B	422	VAL

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	379/385 (98%)	378 (100%)	1 (0%)	86	89
1	B	381/385 (99%)	379 (100%)	2 (0%)	81	85
1	C	380/385 (99%)	373 (98%)	7 (2%)	51	51
1	D	379/385 (98%)	375 (99%)	4 (1%)	65	68
All	All	1519/1540 (99%)	1505 (99%)	14 (1%)	73	74

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	B	354	LYS
1	B	421	GLU
1	C	76	LEU
1	C	117	GLU
1	C	196[A]	LYS
1	C	196[B]	LYS
1	C	217	HIS
1	C	288	LEU
1	C	355	ASP
1	D	76	LEU
1	D	173	LEU
1	D	174[A]	ASP
1	D	174[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	170	HIS
1	B	400	HIS
1	C	347	HIS
1	C	404	GLN
1	D	48	GLN

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Mol	Chain	Res	Type
1	D	336	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 29 ligands modelled in this entry, 4 are monoatomic - leaving 25 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	SY4	A	508	-	16,16,16	1.57	4 (25%)	21,23,23	3.30	9 (42%)
6	PO4	C	504	-	4,4,4	0.97	0	6,6,6	0.42	0
6	PO4	D	504	-	4,4,4	0.99	0	6,6,6	0.45	0
6	PO4	A	507	-	4,4,4	0.93	0	6,6,6	0.60	0
6	PO4	B	505	-	4,4,4	0.98	0	6,6,6	0.46	0
6	PO4	A	506	-	4,4,4	0.92	0	6,6,6	0.55	0
6	PO4	C	505	-	4,4,4	0.98	0	6,6,6	0.44	0
6	PO4	D	505	-	4,4,4	0.96	0	6,6,6	0.47	0
6	PO4	C	507	-	4,4,4	0.96	0	6,6,6	0.41	0
3	ADE	B	502	-	11,11,11	0.37	0	15,15,15	0.42	0
3	ADE	A	502	-	11,11,11	0.41	0	15,15,15	0.42	0
6	PO4	D	508	-	4,4,4	0.95	0	6,6,6	0.43	0
6	PO4	D	507	-	4,4,4	0.94	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PO4	B	506	-	4,4,4	0.97	0	6,6,6	0.44	0
2	NAD	B	501	-	46,48,48	0.35	0	64,73,73	0.41	0
2	NAD	A	501	-	46,48,48	0.37	0	64,73,73	0.44	0
6	PO4	B	504	-	4,4,4	0.97	0	6,6,6	0.44	0
3	ADE	C	502	-	11,11,11	0.39	0	15,15,15	0.42	0
6	PO4	D	506	-	4,4,4	0.94	0	6,6,6	0.49	0
2	NAD	C	501	-	46,48,48	0.37	0	64,73,73	0.42	0
6	PO4	A	505	-	4,4,4	0.94	0	6,6,6	0.49	0
6	PO4	C	506	-	4,4,4	0.96	0	6,6,6	0.45	0
4	DMS	A	503	-	3,3,3	0.67	0	3,3,3	0.61	0
3	ADE	D	502	-	11,11,11	0.40	0	15,15,15	0.42	0
2	NAD	D	501	-	46,48,48	0.35	0	64,73,73	0.42	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	ADE	C	502	-	-	-	0/2/2/2
3	ADE	B	502	-	-	-	0/2/2/2
7	SY4	A	508	-	-	1/9/9/9	0/1/1/1
2	NAD	C	501	-	-	5/30/62/62	0/5/5/5
3	ADE	A	502	-	-	-	0/2/2/2
2	NAD	B	501	-	-	4/30/62/62	0/5/5/5
2	NAD	A	501	-	-	5/30/62/62	0/5/5/5
3	ADE	D	502	-	-	-	0/2/2/2
2	NAD	D	501	-	-	5/30/62/62	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	508	SY4	S-N	3.98	1.70	1.62
7	A	508	SY4	O-S	2.57	1.47	1.43
7	A	508	SY4	O1-S	2.38	1.46	1.43
7	A	508	SY4	C5-N1	2.28	1.45	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	508	SY4	O1-S-O	-12.63	101.68	119.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	508	SY4	C7-C6-C5	-3.51	120.21	123.35
7	A	508	SY4	C7-C8-C3	-3.37	119.98	123.43
7	A	508	SY4	C4-C3-C8	2.93	120.46	117.65
7	A	508	SY4	O-S-C2	2.73	112.19	107.86
7	A	508	SY4	O1-S-C2	2.62	112.02	107.86
7	A	508	SY4	C3-N-S	-2.16	118.34	123.58
7	A	508	SY4	C2-S-N	2.15	109.78	106.72
7	A	508	SY4	O-S-N	2.12	112.36	107.23

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	O4D-C1D-N1N-C2N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	C	501	NAD	C2D-C1D-N1N-C2N
2	C	501	NAD	C2D-C1D-N1N-C6N
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C2N
2	D	501	NAD	C2D-C1D-N1N-C6N
7	A	508	SY4	C1-C2-S-O1
2	A	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	O4B-C4B-C5B-O5B
2	D	501	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

8 monomers are involved in 10 short contacts:

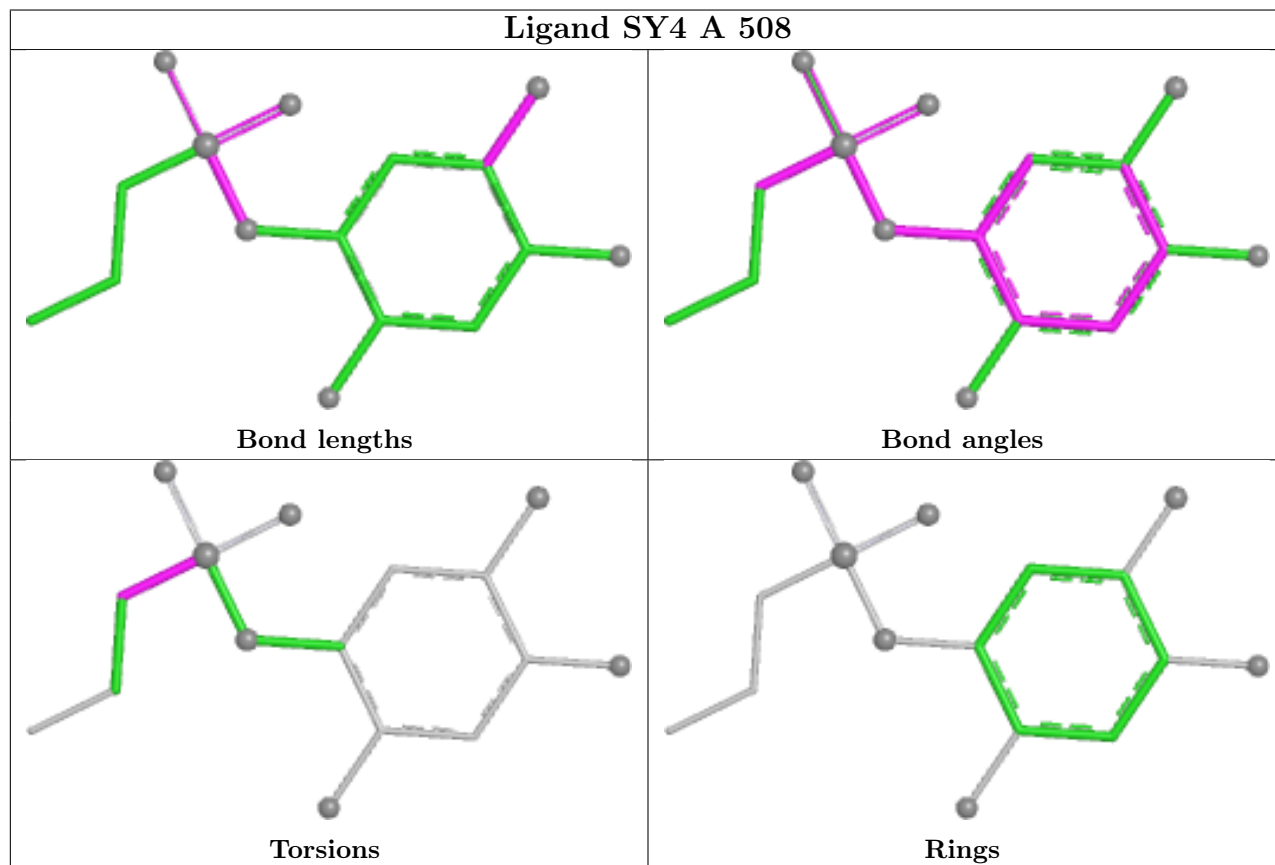
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	508	SY4	2	0
6	C	504	PO4	1	0
6	D	504	PO4	1	0

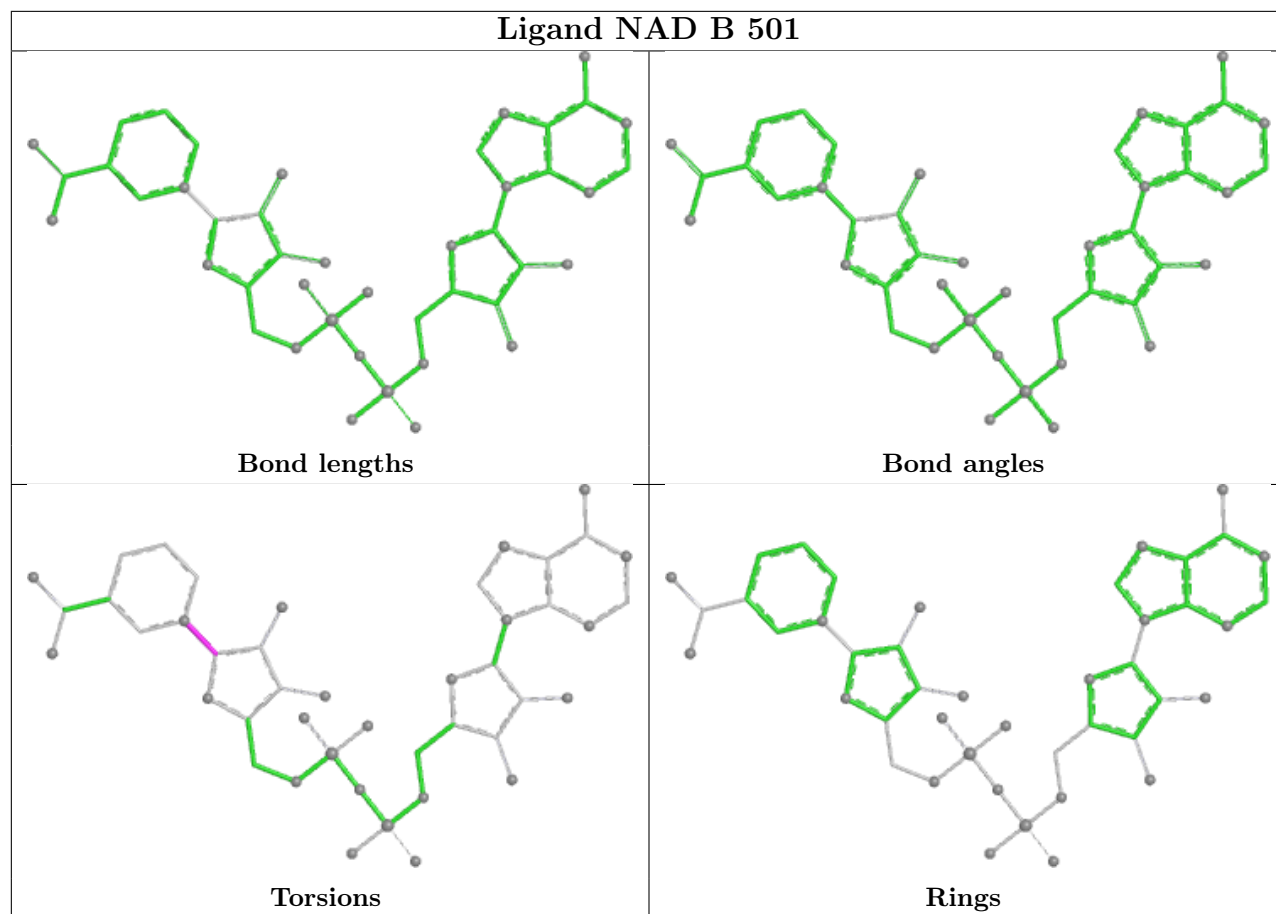
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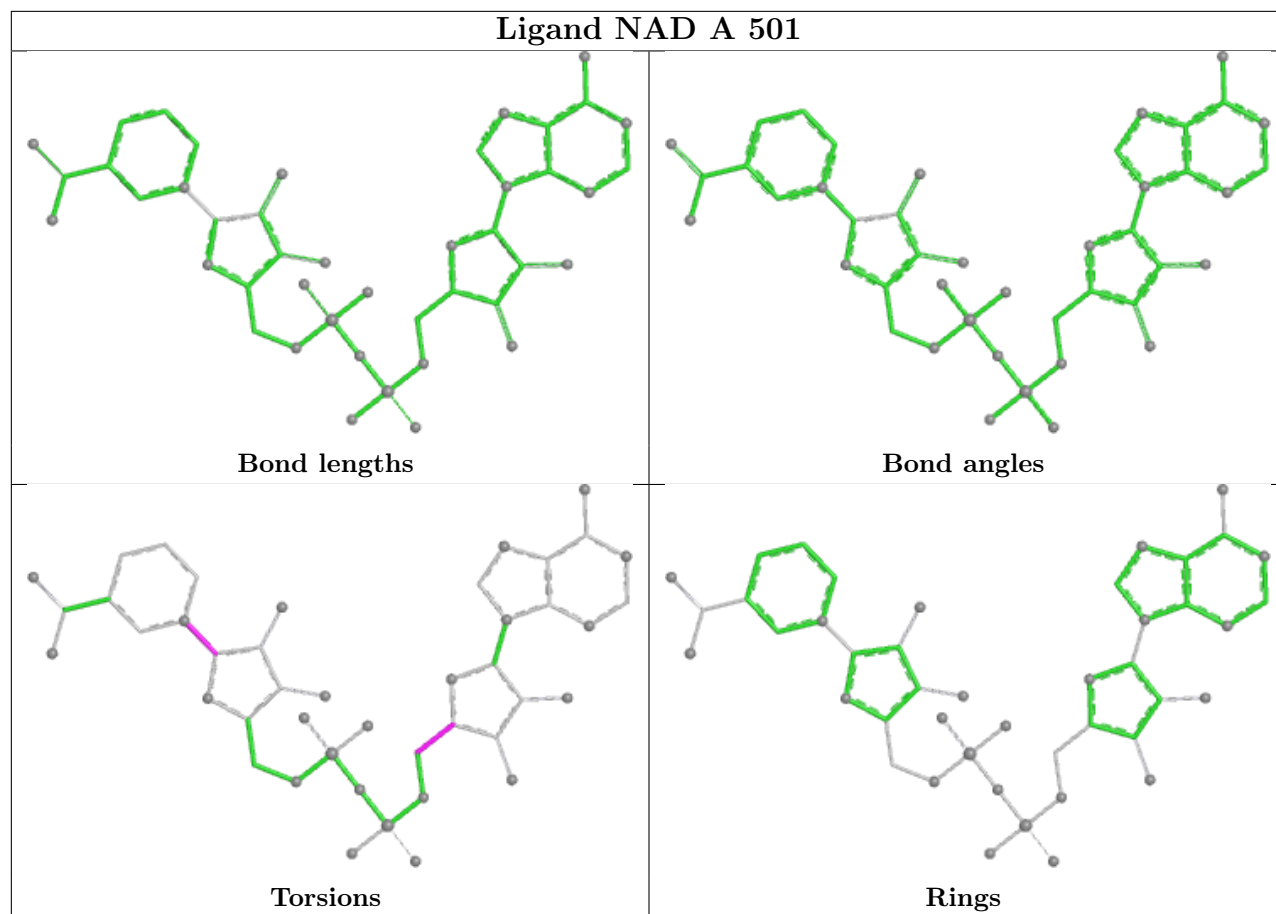
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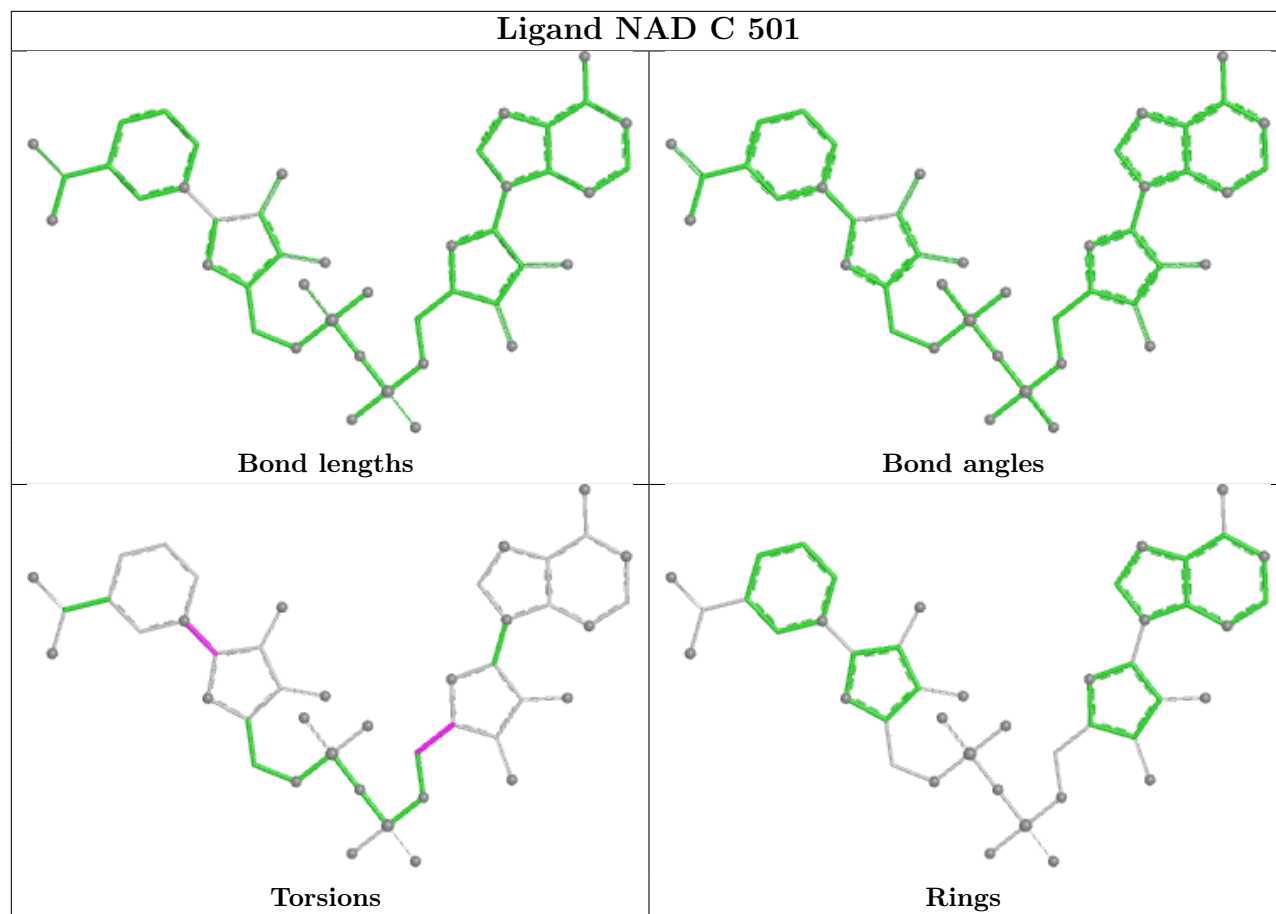
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	505	PO4	1	0
2	B	501	NAD	1	0
2	A	501	NAD	1	0
2	C	501	NAD	2	0
2	D	501	NAD	1	0

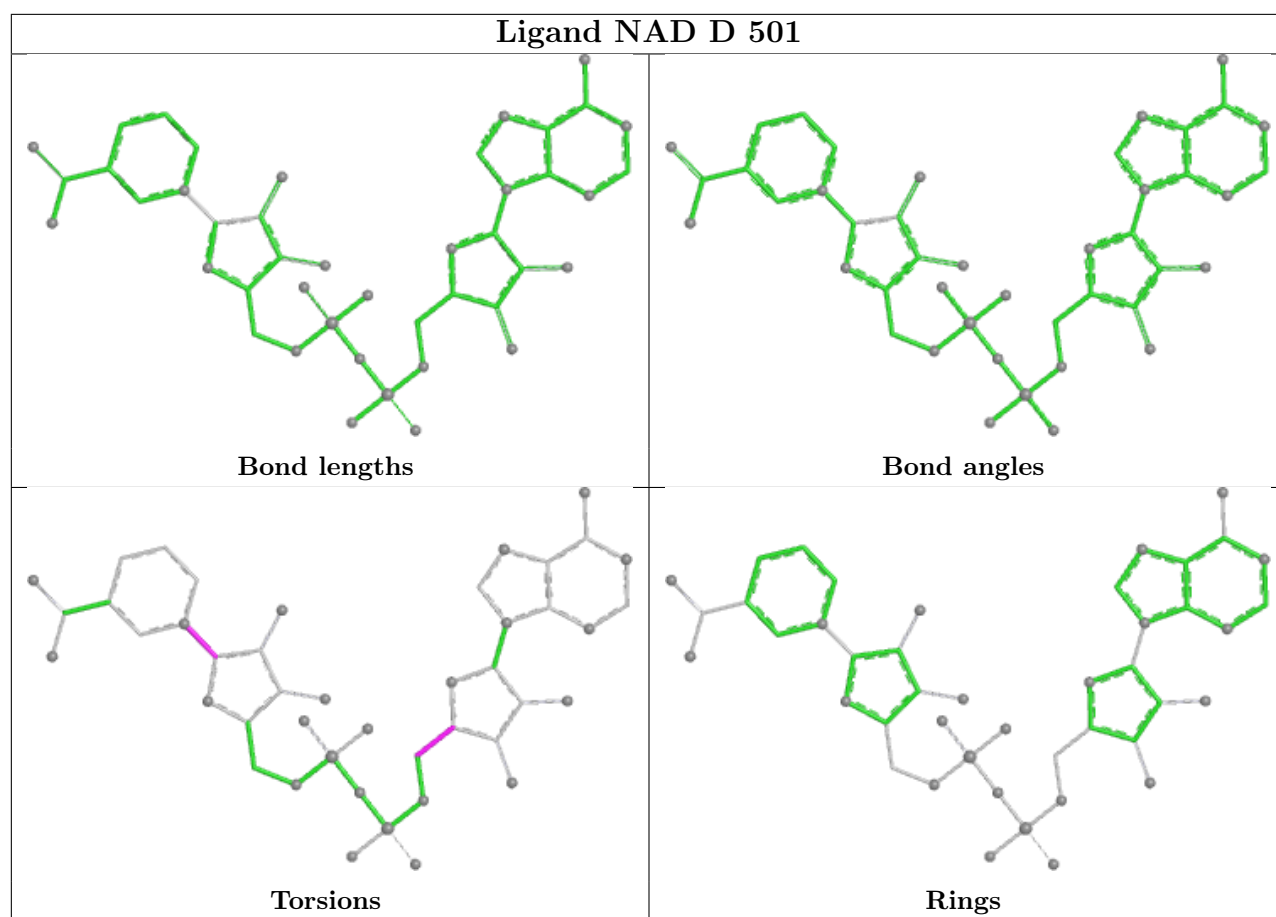
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	462/472 (97%)	-0.05	1 (0%) 91 93	27, 50, 69, 104	2 (0%)
1	B	461/472 (97%)	0.63	29 (6%) 26 25	29, 72, 126, 163	4 (0%)
1	C	462/472 (97%)	1.24	96 (20%) 2 2	33, 94, 126, 166	3 (0%)
1	D	461/472 (97%)	0.80	57 (12%) 8 8	23, 74, 110, 164	2 (0%)
All	All	1846/1888 (97%)	0.66	183 (9%) 13 13	23, 72, 120, 166	11 (0%)

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	PRO	4.3
1	D	409	LEU	4.1
1	B	406	TYR	4.0
1	C	107	ALA	3.9
1	C	90	THR	3.9
1	C	15	VAL	3.8
1	C	105	VAL	3.8
1	C	84	SER	3.7
1	D	10	PHE	3.7
1	D	407	ALA	3.5
1	D	76	LEU	3.4
1	B	418	LEU	3.4
1	B	183	VAL	3.3
1	C	110	GLY	3.3
1	B	176	LEU	3.3
1	C	106	PHE	3.3
1	C	99	ALA	3.3
1	C	96	ALA	3.2
1	C	133	ALA	3.2
1	C	104	PRO	3.2
1	C	88	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	183	VAL	3.1
1	C	125	LEU	3.1
1	C	131	TRP	3.1
1	D	75	ALA	3.1
1	D	384	SER	3.1
1	D	24	GLY	3.0
1	D	95	ALA	3.0
1	C	349	ILE	3.0
1	C	184	PRO	3.0
1	B	412	ALA	2.9
1	C	13	TYR	2.9
1	C	9	GLY	2.9
1	D	415	ALA	2.9
1	D	20	LEU	2.9
1	C	158	ILE	2.9
1	C	356	GLY	2.9
1	D	57	LEU	2.8
1	C	116	TYR	2.8
1	C	143	LEU	2.8
1	D	118	TRP	2.8
1	D	106	PHE	2.8
1	C	407	ALA	2.8
1	D	100	ALA	2.8
1	C	118	TRP	2.8
1	D	80	VAL	2.8
1	B	45	TYR	2.8
1	D	96	ALA	2.8
1	C	155	LEU	2.8
1	D	131	TRP	2.8
1	D	133	ALA	2.7
1	D	13	TYR	2.7
1	C	420	VAL	2.7
1	B	160	GLY	2.7
1	C	67	GLY	2.7
1	C	124	ILE	2.7
1	D	82	TRP	2.7
1	D	410	PRO	2.7
1	D	15	VAL	2.7
1	D	56	ILE	2.7
1	C	412	ALA	2.6
1	D	16	ALA	2.6
1	D	46	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	155	LEU	2.6
1	C	364	TYR	2.6
1	D	59	CYS	2.6
1	C	422	VAL	2.6
1	D	105	VAL	2.6
1	B	401	LEU	2.6
1	C	120	ILE	2.6
1	D	29	ILE	2.6
1	C	304	CYS	2.6
1	D	128	GLY	2.6
1	C	379	ALA	2.6
1	D	412	ALA	2.6
1	D	18	ILE	2.5
1	C	359	ALA	2.5
1	D	94	ALA	2.5
1	C	73	LEU	2.5
1	D	28	LEU	2.5
1	B	179	GLY	2.5
1	B	125	LEU	2.5
1	C	406	TYR	2.5
1	C	147	LEU	2.5
1	C	301	VAL	2.4
1	A	411	ALA	2.4
1	D	137	LEU	2.4
1	C	85	CYS	2.4
1	D	90	THR	2.4
1	B	411	ALA	2.4
1	D	102	GLY	2.4
1	C	132	ASP	2.4
1	C	87	ILE	2.4
1	D	70	ILE	2.4
1	B	11	THR	2.4
1	C	63	THR	2.4
1	C	383	PRO	2.4
1	C	60	ILE	2.4
1	C	68	VAL	2.4
1	C	352	THR	2.4
1	C	410	PRO	2.4
1	D	45	TYR	2.3
1	C	75	ALA	2.3
1	B	181	LEU	2.3
1	C	140	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	154	MET	2.3
1	C	402	PHE	2.3
1	D	103	ILE	2.3
1	C	80	VAL	2.3
1	C	119	CYS	2.3
1	B	407	ALA	2.3
1	D	99	ALA	2.3
1	D	116	TYR	2.3
1	D	406	TYR	2.3
1	C	178	ASN	2.3
1	B	409	LEU	2.3
1	C	373	LEU	2.3
1	C	409	LEU	2.3
1	B	158	ILE	2.3
1	C	103	ILE	2.3
1	C	11	THR	2.3
1	C	16	ALA	2.3
1	C	108	TRP	2.3
1	C	160	GLY	2.3
1	B	146	ILE	2.3
1	C	56	ILE	2.3
1	B	420	VAL	2.3
1	C	123	THR	2.3
1	C	306	ALA	2.3
1	C	102	GLY	2.3
1	C	168	GLY	2.3
1	C	335	LYS	2.3
1	D	127	ASP	2.3
1	C	339	TRP	2.3
1	B	466	THR	2.2
1	C	342	VAL	2.2
1	C	8	ALA	2.2
1	C	100	ALA	2.2
1	C	311	ALA	2.2
1	C	401	LEU	2.2
1	B	151	TYR	2.2
1	B	402	PHE	2.2
1	C	307	ASN	2.2
1	B	141	GLY	2.2
1	C	331	ALA	2.2
1	B	172	LEU	2.2
1	C	367	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	418	LEU	2.2
1	B	422	VAL	2.2
1	C	338	ALA	2.2
1	C	322	GLY	2.1
1	C	69	LEU	2.1
1	C	134	ASN	2.1
1	C	129	GLN	2.1
1	C	94	ALA	2.1
1	C	57	LEU	2.1
1	D	104	PRO	2.1
1	D	146	ILE	2.1
1	C	332	PHE	2.1
1	D	183	VAL	2.1
1	B	143	LEU	2.1
1	C	162	THR	2.1
1	B	188	VAL	2.1
1	D	88	PHE	2.1
1	D	23	TRP	2.1
1	C	185	ALA	2.1
1	D	176	LEU	2.0
1	C	153	GLN	2.0
1	C	350	HIS	2.0
1	D	123	THR	2.0
1	C	353	GLY	2.0
1	B	186	ILE	2.0
1	D	87	ILE	2.0
1	C	10	PHE	2.0
1	D	74	VAL	2.0
1	D	402	PHE	2.0
1	C	62	MET	2.0
1	D	359	ALA	2.0
1	C	368	LEU	2.0
1	D	408	ASP	2.0
1	D	14	LYS	2.0
1	D	50	PRO	2.0
1	C	128	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

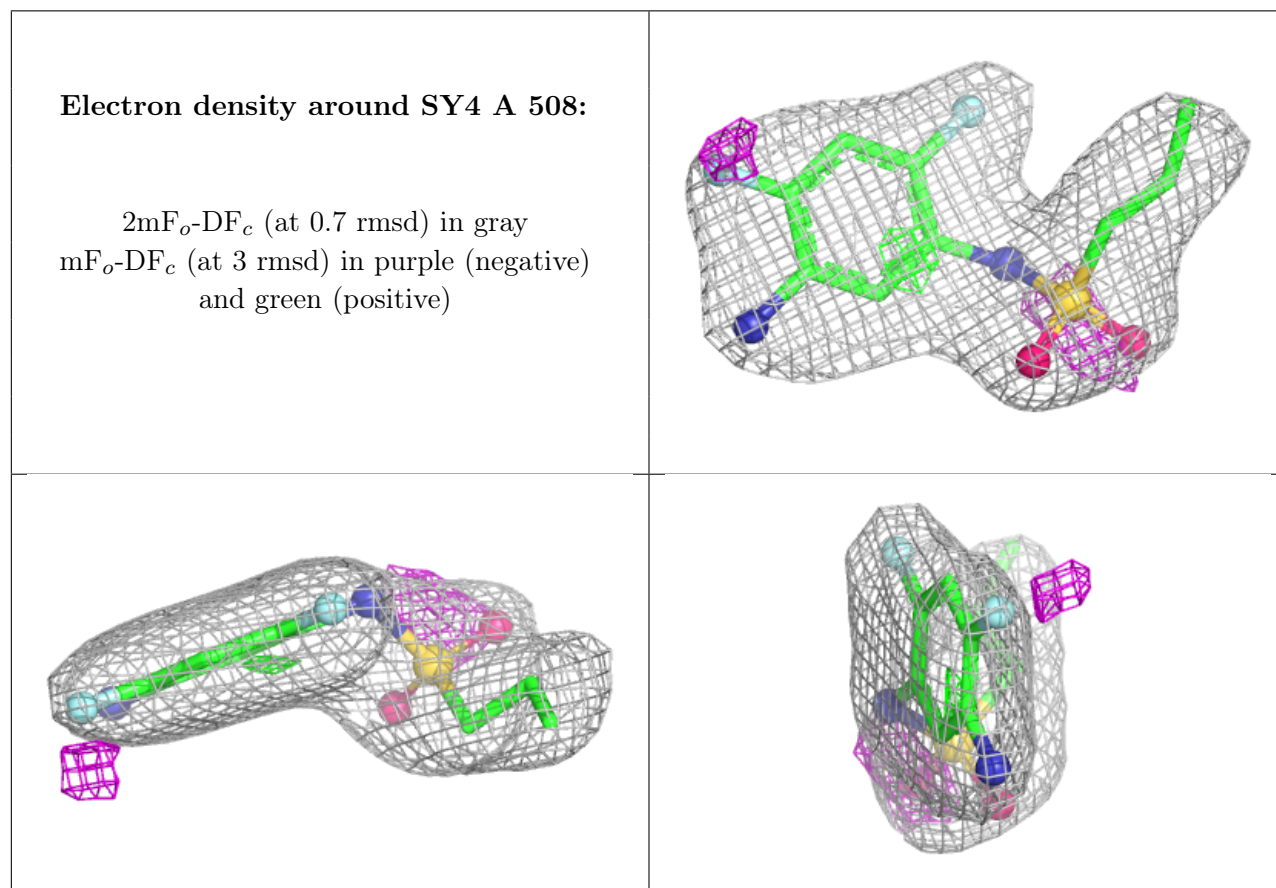
6.4 Ligands [i](#)

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
6	PO4	C	507	5/5	0.56	0.13	76,83,90,93	5
6	PO4	C	504	5/5	0.64	0.12	86,91,99,101	0
6	PO4	D	505	5/5	0.78	0.11	91,94,98,100	0
6	PO4	C	506	5/5	0.80	0.13	75,79,84,87	5
6	PO4	D	504	5/5	0.81	0.11	68,73,77,77	5
6	PO4	C	505	5/5	0.82	0.15	81,81,86,88	0
3	ADE	C	502	10/10	0.83	0.14	78,82,86,87	0
6	PO4	B	506	5/5	0.85	0.16	62,70,72,76	5
7	SY4	A	508	16/16	0.86	0.13	45,51,68,69	0
6	PO4	A	505	5/5	0.87	0.10	56,58,63,66	5
2	NAD	C	501	44/44	0.87	0.14	58,75,80,84	0
2	NAD	B	501	44/44	0.87	0.12	56,64,68,75	0
4	DMS	A	503	4/4	0.88	0.15	59,68,69,72	4
6	PO4	B	505	5/5	0.88	0.11	60,61,63,71	5
6	PO4	D	506	5/5	0.89	0.13	64,66,72,73	5
5	K	D	503	1/1	0.90	0.11	54,54,54,54	0
6	PO4	B	504	5/5	0.90	0.08	71,72,75,79	0
6	PO4	D	508	5/5	0.91	0.11	52,54,60,62	5
5	K	C	503	1/1	0.91	0.10	64,64,64,64	0
6	PO4	D	507	5/5	0.92	0.09	53,57,61,65	5
3	ADE	B	502	10/10	0.93	0.10	56,59,61,62	0
6	PO4	A	506	5/5	0.94	0.13	55,57,58,59	0
6	PO4	A	507	5/5	0.94	0.09	45,45,50,58	0
2	NAD	D	501	44/44	0.94	0.08	44,52,64,65	0
3	ADE	A	502	10/10	0.95	0.06	38,43,45,46	0
3	ADE	D	502	10/10	0.96	0.08	63,66,69,70	0
2	NAD	A	501	44/44	0.96	0.07	37,45,51,52	0
5	K	B	503	1/1	0.96	0.08	48,48,48,48	0
5	K	A	504	1/1	0.99	0.06	40,40,40,40	0

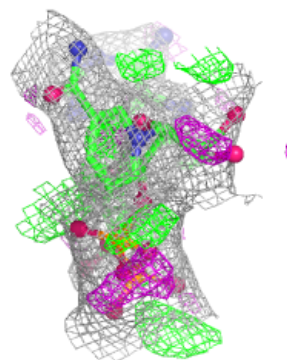
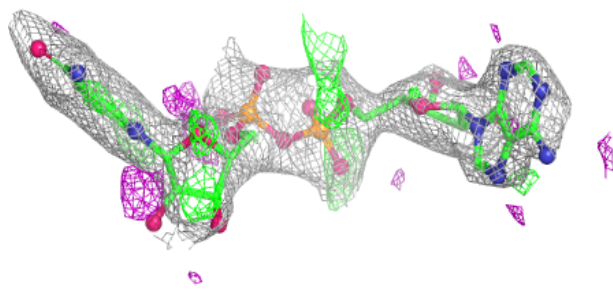
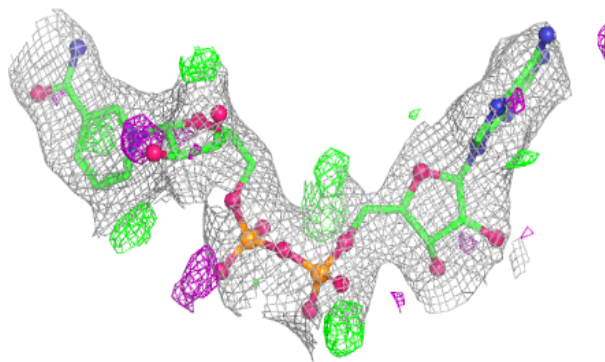
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

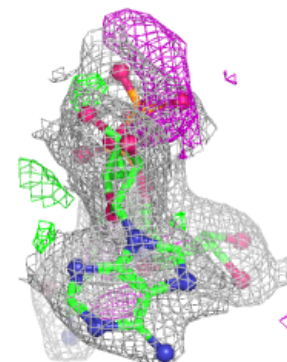
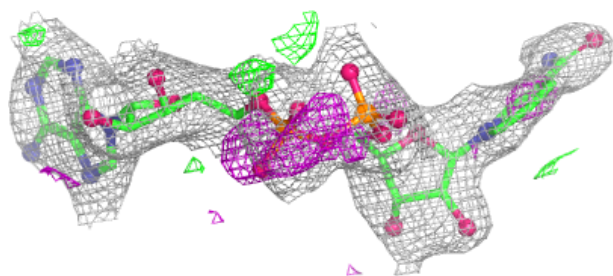
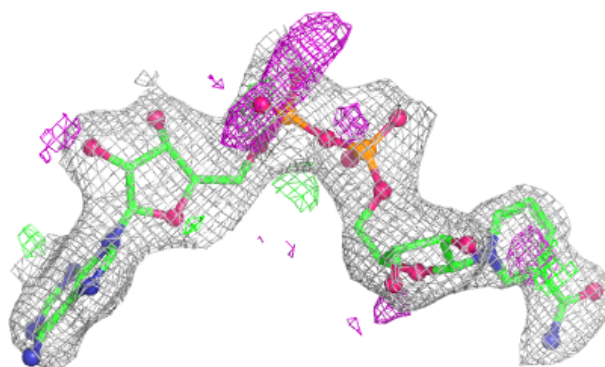


Electron density around NAD C 501:

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

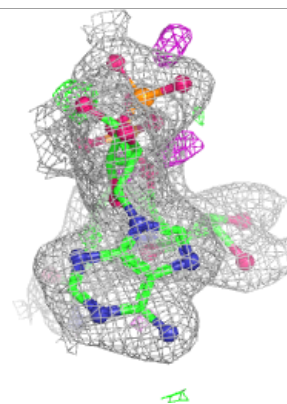
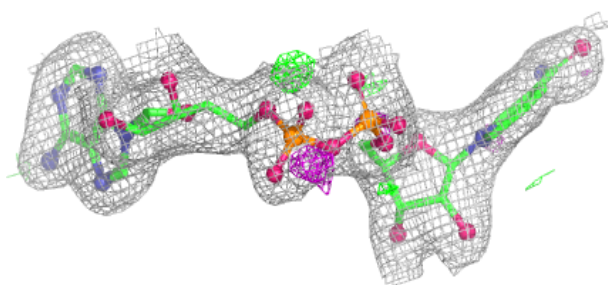
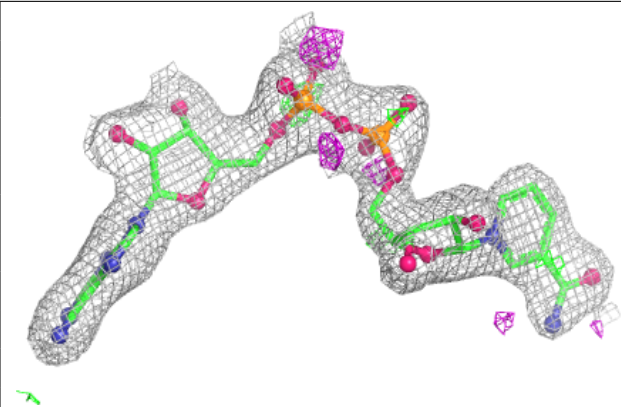
**Electron density around NAD B 501:**

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

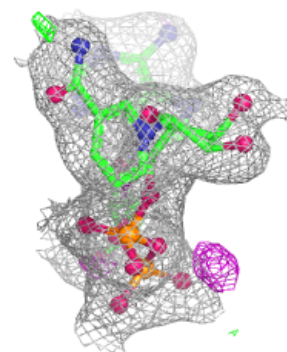
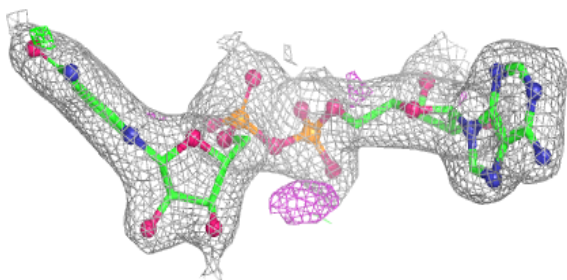
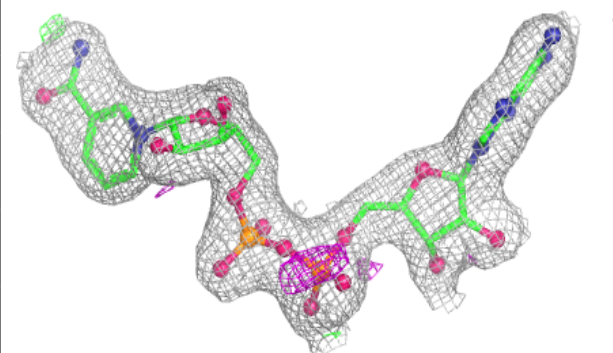


Electron density around NAD D 501:

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

**Electron density around NAD A 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.