



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 03:43 pm GMT

PDB ID : 8CFR
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *P. aeruginosa* in complex with F2X-Entry library fragment G03
Authors : Malecki, P.H.; Gawel, M.; Stepniewska, M.; Brzezinski, K.
Deposited on : 2023-02-03
Resolution : 1.89 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

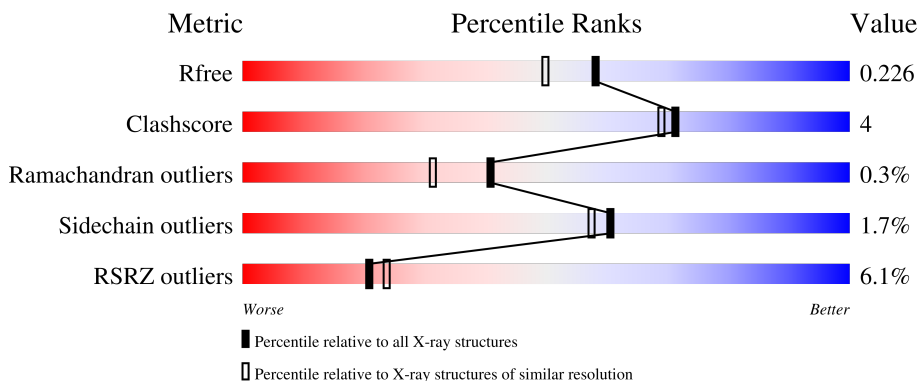
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	 2% 91% 7% .
1	B	472	 11% 85% 12% .
1	C	472	 5% 88% 9% .
1	D	472	 5% 88% 10% .

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15819 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	3578	2255	619	681	23	0	3	0
1	B	461	3571	2251	618	680	22	0	3	0
1	C	462	3590	2263	620	684	23	0	5	0
1	D	464	3610	2277	624	686	23	0	6	0

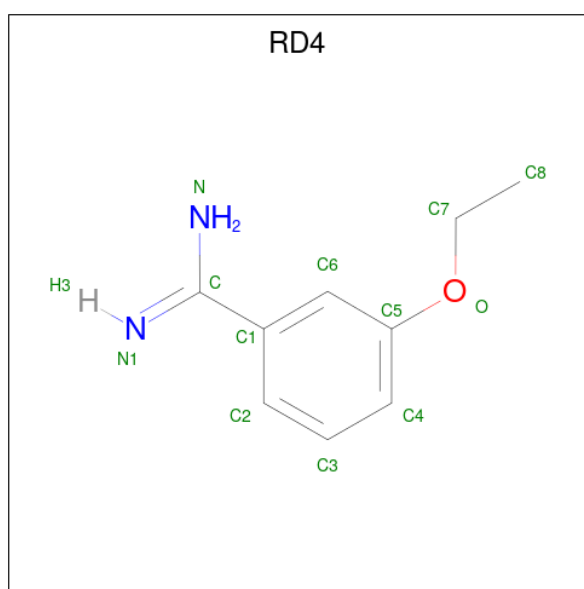
There are 12 discrepancies between the modelled and reference sequences:

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 (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).

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

- Molecule 4 is 3-ethoxybenzene-1-carboximidamide (three-letter code: RD4) (formula: $C_9H_{12}N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	9	2	1		
4	B	1	Total	C	N	O	0	0
			12	9	2	1		
4	C	1	Total	C	N	O	0	0
			12	9	2	1		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

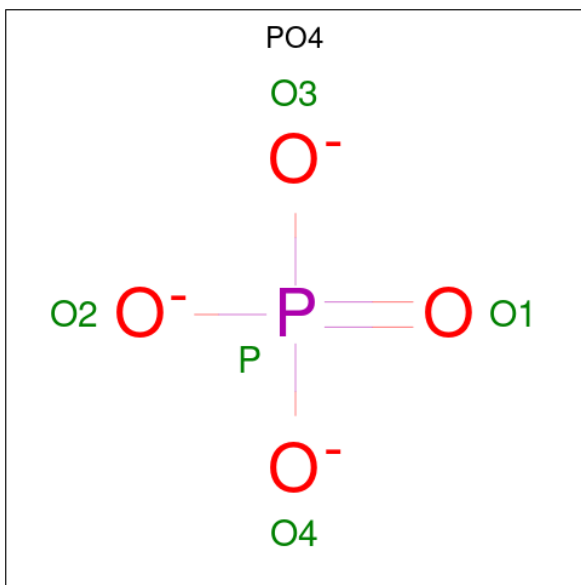
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		

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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



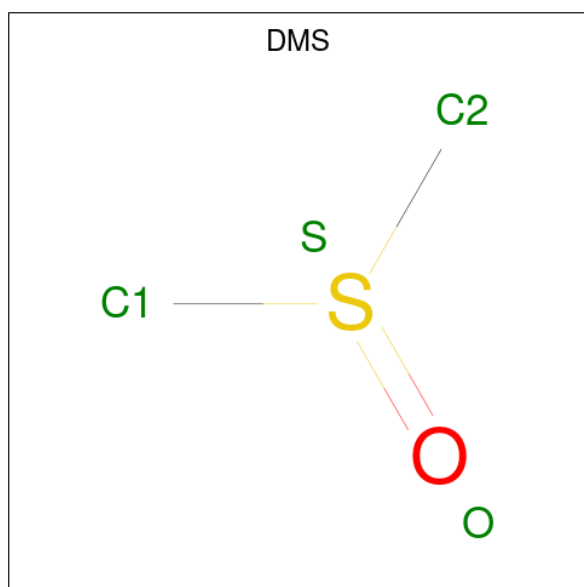
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			5	4	1		
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 DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

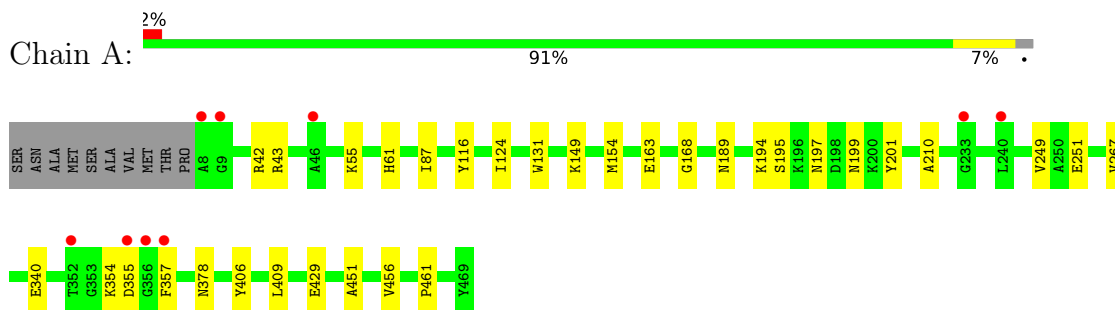
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	341	Total	O	0	9
			350	350		
8	B	216	Total	O	0	1
			217	217		
8	C	284	Total	O	0	3
			287	287		
8	D	292	Total	O	0	4
			296	296		

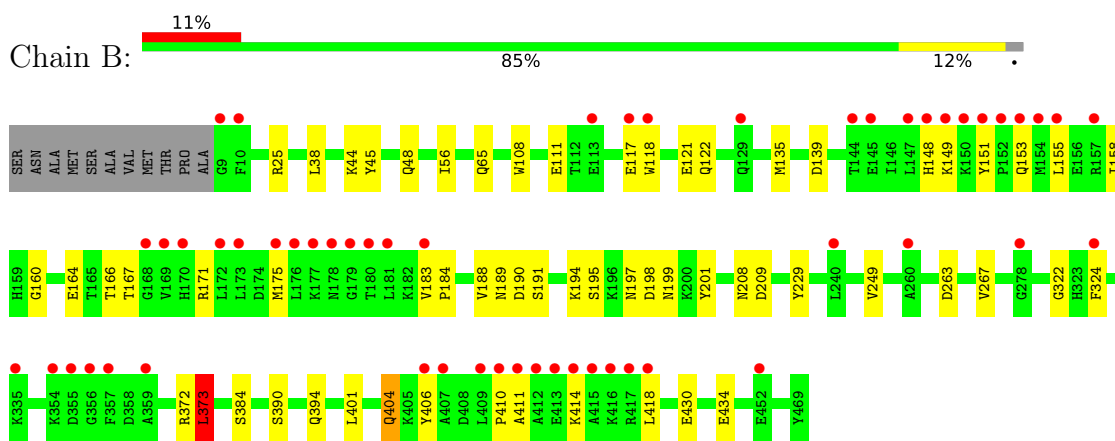
3 Residue-property plots [i](#)

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.

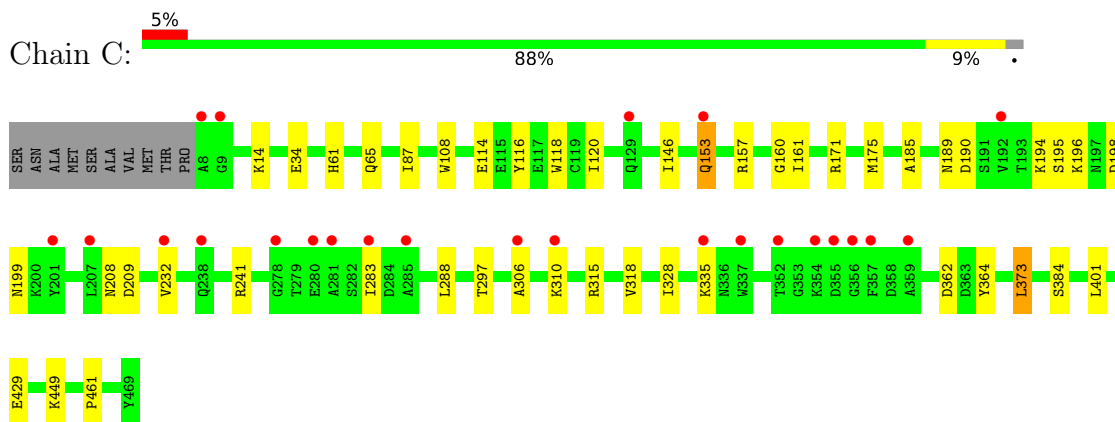
- Molecule 1: Adenosylhomocysteinase



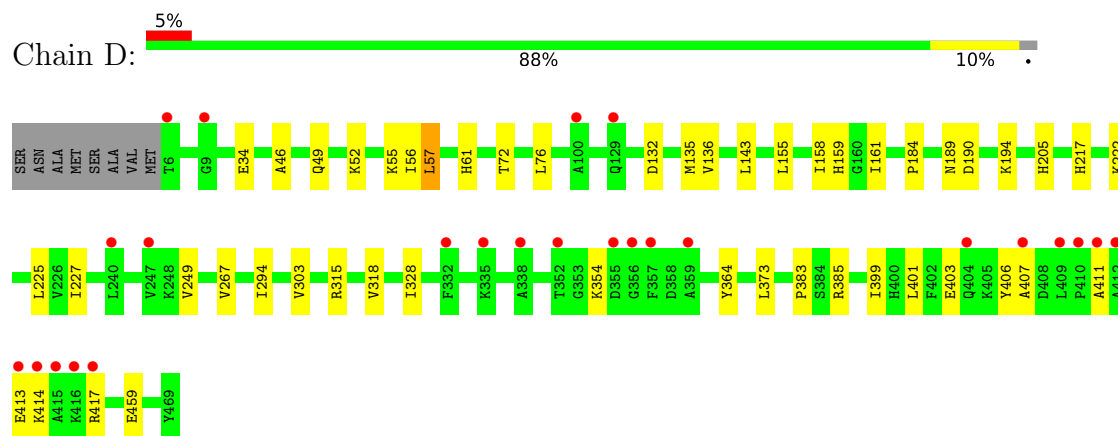
- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.21Å 101.49Å 110.70Å 90.00° 114.42° 90.00°	Depositor
Resolution (Å)	37.03 – 1.89 47.77 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.03-1.89) 99.2 (47.77-1.89)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, R_{free}	0.186 , 0.225 0.187 , 0.226	Depositor DCC
R_{free} test set	1042 reflections (0.72%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtrriage
Anisotropy	0.739	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15819	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0748e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAD, ADE, K, DMS, PO4, RD4

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	0.45	0/3644	0.64	0/4926
1	B	0.42	0/3640	0.61	1/4921 (0.0%)
1	C	0.44	0/3662	0.63	2/4950 (0.0%)
1	D	0.43	0/3680	0.61	0/4975
All	All	0.43	0/14626	0.62	3/19772 (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	C	198	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	373	LEU	CA-CB-CG	5.44	127.82	115.30
1	C	373	LEU	CA-CB-CG	5.37	127.65	115.30

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	3578	0	3584	14	0
1	B	3571	0	3579	37	0
1	C	3590	0	3598	27	0
1	D	3610	0	3624	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
4	C	12	0	0	1	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	1	0
6	C	20	0	0	0	0
6	D	10	0	0	0	0
7	C	4	0	6	1	0
8	A	350	0	0	1	0
8	B	217	0	0	2	0
8	C	287	0	0	6	0
8	D	296	0	0	0	0
All	All	15819	0	14511	103	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 (103) 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:155:LEU:HA	1:B:158:ILE:HD12	1.63	0.79
1:C:189:ASN:HA	1:C:194:LYS:HD2	1.74	0.69
1:B:189:ASN:HA	1:B:194:LYS:HD2	1.73	0.69
1:D:189:ASN:HA	1:D:194:LYS:HD2	1.75	0.68
1:C:196:LYS:HE2	8:C:613:HOH:O	1.95	0.67
1:D:46:ALA:O	1:D:49:GLN:NE2	2.28	0.66
1:D:373:LEU:HD12	1:D:373:LEU:H	1.60	0.65
1:A:189:ASN:HA	1:A:194:LYS:HD2	1.81	0.62
1:B:197:ASN:HA	1:B:201:TYR:HD2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:TYR:CE1	1:B:414:LYS:HB3	2.37	0.59
1:B:118:TRP:O	1:B:122:GLN:HG2	2.04	0.58
1:A:43:ARG:NH2	8:A:603:HOH:O	2.36	0.57
1:B:322:GLY:O	1:B:373:LEU:HD13	2.05	0.57
1:C:196:LYS:HE3	8:C:675:HOH:O	2.04	0.57
1:B:404:GLN:NE2	8:B:602:HOH:O	2.39	0.56
1:D:155:LEU:HD23	1:D:158:ILE:HD12	1.87	0.56
1:A:451:ALA:HB1	1:A:456:VAL:O	2.07	0.54
1:D:413:GLU:OE1	1:D:417:ARG:NH1	2.40	0.54
1:D:399:ILE:O	1:D:403:GLU:HG3	2.08	0.54
1:D:57[A]:LEU:HB3	1:D:143:LEU:HD21	1.89	0.53
1:B:56:ILE:HG12	1:B:135:MET:HB2	1.91	0.51
1:B:171:ARG:O	1:B:175:MET:HG3	2.10	0.51
1:C:157:ARG:NH1	8:C:607:HOH:O	2.44	0.51
1:A:340:GLU:HB2	1:A:357:PHE:CZ	2.47	0.50
1:C:283:ILE:HG23	1:C:288:LEU:HD12	1.93	0.50
1:D:56:ILE:HG12	1:D:135:MET:HB2	1.93	0.50
1:B:410:PRO:O	1:B:414:LYS:HG3	2.12	0.50
1:B:194:LYS:HG2	1:B:390:SER:HB3	1.94	0.50
1:D:136:VAL:HB	1:D:161:ILE:HG12	1.94	0.49
1:D:184:PRO:HD3	1:D:406:TYR:CG	2.48	0.49
1:A:87:ILE:HG22	1:A:116:TYR:HB2	1.94	0.48
1:B:167:THR:HG21	1:B:324:PHE:HE2	1.78	0.48
1:C:195:SER:O	1:C:199:ASN:HB2	2.14	0.48
1:A:197:ASN:HA	1:A:201:TYR:HD2	1.78	0.48
1:B:434:GLU:HG3	8:B:738:HOH:O	2.14	0.48
1:C:190:ASP:OD2	4:C:501:RD4:N1	2.46	0.48
1:D:249:VAL:O	1:D:267:VAL:HA	2.14	0.48
1:C:318:VAL:HG12	1:C:328:ILE:HD13	1.95	0.48
1:D:205:HIS:CD2	1:D:383:PRO:HD3	2.49	0.47
1:B:194:LYS:O	1:B:198:ASP:HB3	2.14	0.47
1:B:188:VAL:HG11	1:B:394:GLN:HG2	1.96	0.47
1:B:229:TYR:OH	1:B:263:ASP:OD2	2.26	0.47
1:C:171:ARG:O	1:C:175:MET:HG3	2.15	0.47
1:A:406:TYR:HA	1:A:409:LEU:HD12	1.97	0.47
1:C:161:ILE:O	1:C:185:ALA:HA	2.15	0.46
1:B:44:LYS:NZ	1:B:430:GLU:OE2	2.47	0.46
1:B:197:ASN:O	1:B:201:TYR:HB2	2.16	0.46
1:A:249:VAL:O	1:A:267:VAL:HA	2.16	0.46
1:D:194:LYS:HD3	1:D:194:LYS:C	2.36	0.46
1:A:429:GLU:OE1	1:A:461:PRO:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:VAL:HG12	1:B:194:LYS:HG3	1.97	0.46
1:A:195:SER:O	1:A:199:ASN:HB2	2.16	0.45
1:C:315:ARG:NH1	1:C:362:ASP:HB2	2.30	0.45
1:C:153:GLN:HB2	8:C:793:HOH:O	2.15	0.45
1:D:159:HIS:CE1	1:D:407:ALA:HB3	2.52	0.45
1:B:167:THR:HG21	1:B:324:PHE:CE2	2.51	0.45
1:B:167:THR:O	1:B:171:ARG:HG3	2.16	0.45
1:B:406:TYR:CZ	1:B:414:LYS:HB3	2.52	0.45
1:C:232:VAL:HG12	1:C:297:THR:HB	1.98	0.45
1:D:318:VAL:HG12	1:D:328:ILE:HD13	1.97	0.45
1:C:14:LYS:HD3	1:C:108:TRP:CZ3	2.52	0.45
1:B:249:VAL:O	1:B:267:VAL:HA	2.17	0.45
1:C:208[B]:ASN:OD1	1:C:209:ASP:N	2.50	0.44
1:D:55:LYS:HE2	1:D:132:ASP:OD2	2.18	0.44
1:A:124:ILE:HG23	1:A:154:MET:SD	2.57	0.44
1:D:315:ARG:HG2	1:D:364:TYR:CZ	2.52	0.44
1:D:227:ILE:HG21	1:D:303:VAL:HB	1.99	0.44
1:B:208[A]:ASN:OD1	1:B:209:ASP:N	2.51	0.43
1:D:401:LEU:HD23	1:D:401:LEU:HA	1.87	0.43
1:A:210:ALA:HB1	1:A:378:ASN:HB2	2.00	0.43
1:B:139:ASP:HA	1:B:164:GLU:HB3	1.99	0.43
1:B:195:SER:O	1:B:199:ASN:HB2	2.18	0.43
1:C:14:LYS:HD2	1:C:118:TRP:CH2	2.54	0.43
7:C:504:DMS:H23	8:C:845:HOH:O	2.18	0.43
1:B:160:GLY:HA3	1:B:401:LEU:HD13	2.02	0.42
1:D:225:LEU:O	1:D:294:ILE:HA	2.20	0.42
1:B:148:HIS:HA	1:B:155:LEU:HD11	2.02	0.42
1:C:429:GLU:OE1	1:C:461:PRO:HA	2.20	0.42
1:C:87:ILE:HG22	1:C:116:TYR:HB2	2.00	0.42
1:C:315:ARG:HG2	1:C:364:TYR:CZ	2.54	0.42
1:D:411:ALA:O	1:D:414:LYS:HB2	2.20	0.42
1:B:25:ARG:NH1	6:B:505:PO4:O3	2.53	0.41
1:C:160:GLY:HA3	1:C:401:LEU:HD13	2.02	0.41
1:D:72:THR:O	1:D:76:LEU:HG	2.20	0.41
1:B:194:LYS:HG2	1:B:390:SER:CB	2.50	0.41
1:C:306:ALA:O	1:C:310:LYS:HG3	2.21	0.41
1:A:55:LYS:HB3	1:A:131:TRP:CH2	2.55	0.41
1:C:241:ARG:HD2	8:C:834:HOH:O	2.20	0.41
1:C:288:LEU:HD23	1:C:288:LEU:HA	1.92	0.41
1:B:108:TRP:O	1:B:111:GLU:HG3	2.21	0.41
1:D:184:PRO:HD3	1:D:406:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ARG:O	1:B:373:LEU:C	2.59	0.41
1:C:120:ILE:HG21	1:C:146:ILE:HD12	2.03	0.41
1:B:44:LYS:HE2	1:B:45:TYR:CE1	2.56	0.41
1:B:65:GLN:HG3	1:B:384:SER:HA	2.03	0.41
1:C:34:GLU:OE1	1:D:222:LYS:NZ	2.48	0.40
1:C:114:GLU:H	1:C:114:GLU:CD	2.24	0.40
1:D:34:GLU:O	1:D:385:ARG:HA	2.21	0.40
1:A:163:GLU:CD	1:A:168:GLY:HA3	2.40	0.40
1:B:183:VAL:HB	1:B:184:PRO:HD2	2.04	0.40
1:C:65:GLN:HG3	1:C:384:SER:HA	2.02	0.40
1:B:151:TYR:C	1:B:153:GLN:H	2.25	0.40
1:B:197:ASN:HA	1:B:201:TYR:CD2	2.50	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	463/472 (98%)	449 (97%)	12 (3%)	2 (0%)	34	24
1	B	462/472 (98%)	445 (96%)	15 (3%)	2 (0%)	34	24
1	C	465/472 (98%)	454 (98%)	10 (2%)	1 (0%)	47	38
1	D	468/472 (99%)	451 (96%)	16 (3%)	1 (0%)	47	38
All	All	1858/1888 (98%)	1799 (97%)	53 (3%)	6 (0%)	41	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	373	LEU
1	C	61	HIS
1	D	61	HIS

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Mol	Chain	Res	Type
1	A	61	HIS
1	A	355	ASP
1	B	411	ALA

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	380/385 (99%)	376 (99%)	4 (1%)	73	73
1	B	380/385 (99%)	369 (97%)	11 (3%)	42	35
1	C	382/385 (99%)	378 (99%)	4 (1%)	76	76
1	D	384/385 (100%)	377 (98%)	7 (2%)	59	55
All	All	1526/1540 (99%)	1500 (98%)	26 (2%)	60	57

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	149	LYS
1	A	251	GLU
1	A	354	LYS
1	B	38	LEU
1	B	48	GLN
1	B	117	GLU
1	B	121	GLU
1	B	149	LYS
1	B	166	THR
1	B	190	ASP
1	B	191	SER
1	B	373	LEU
1	B	404	GLN
1	B	418	LEU
1	C	153	GLN
1	C	335	LYS
1	C	373	LEU

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Mol	Chain	Res	Type
1	C	449	LYS
1	D	52	LYS
1	D	57[A]	LEU
1	D	57[B]	LEU
1	D	190	ASP
1	D	217	HIS
1	D	354	LYS
1	D	459	GLU

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PO4	D	505	-	4,4,4	0.93	0	6,6,6	0.50	0
3	ADE	B	503	-	9,11,11	0.96	0	7,15,15	1.12	0
6	PO4	B	507	-	4,4,4	0.69	0	6,6,6	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PO4	A	507	-	4,4,4	1.01	0	6,6,6	0.98	0
3	ADE	D	502	-	9,11,11	0.79	0	7,15,15	1.16	1 (14%)
6	PO4	C	507	-	4,4,4	0.93	0	6,6,6	0.88	0
3	ADE	C	503	-	9,11,11	1.16	2 (22%)	7,15,15	1.14	1 (14%)
3	ADE	A	502	-	9,11,11	0.97	0	7,15,15	1.03	0
6	PO4	B	505	-	4,4,4	0.85	0	6,6,6	0.81	0
2	NAD	C	502	-	42,48,48	0.54	0	50,73,73	0.80	2 (4%)
4	RD4	B	501	-	12,12,12	1.83	3 (25%)	12,15,15	0.97	0
4	RD4	C	501	-	12,12,12	1.97	3 (25%)	12,15,15	0.97	1 (8%)
4	RD4	A	503	-	12,12,12	1.98	3 (25%)	12,15,15	1.31	1 (8%)
6	PO4	C	506	-	4,4,4	0.91	0	6,6,6	0.28	0
7	DMS	C	504	-	3,3,3	0.70	0	3,3,3	0.59	0
6	PO4	C	508	-	4,4,4	0.71	0	6,6,6	0.80	0
2	NAD	D	501	-	42,48,48	0.59	0	50,73,73	0.76	1 (2%)
6	PO4	C	509	-	4,4,4	0.81	0	6,6,6	0.74	0
2	NAD	B	502	-	42,48,48	0.59	0	50,73,73	0.75	2 (4%)
6	PO4	A	506	-	4,4,4	1.06	0	6,6,6	0.37	0
6	PO4	B	506	-	4,4,4	0.94	0	6,6,6	0.51	0
2	NAD	A	501	-	42,48,48	0.58	0	50,73,73	0.81	1 (2%)
6	PO4	A	505	-	4,4,4	0.84	0	6,6,6	0.47	0
6	PO4	D	504	-	4,4,4	0.76	0	6,6,6	0.63	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	503	-	-	-	0/2/2/2
2	NAD	D	501	-	-	5/26/62/62	0/5/5/5
2	NAD	B	502	-	-	5/26/62/62	0/5/5/5
3	ADE	A	502	-	-	-	0/2/2/2
3	ADE	B	503	-	-	-	0/2/2/2
2	NAD	C	502	-	-	5/26/62/62	0/5/5/5
4	RD4	B	501	-	-	4/7/7/7	0/1/1/1
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5
3	ADE	D	502	-	-	-	0/2/2/2
4	RD4	C	501	-	-	2/7/7/7	0/1/1/1
4	RD4	A	503	-	-	0/7/7/7	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	RD4	C-N1	4.33	1.46	1.28
4	C	501	RD4	C-N1	4.29	1.46	1.28
4	B	501	RD4	C-N1	4.16	1.45	1.28
4	C	501	RD4	C1-C	3.98	1.54	1.47
4	A	503	RD4	C1-C	3.65	1.54	1.47
4	A	503	RD4	C-N	-3.05	1.26	1.33
4	B	501	RD4	C-N	-3.03	1.26	1.33
4	C	501	RD4	C-N	-2.81	1.26	1.33
4	B	501	RD4	C1-C	2.81	1.52	1.47
3	C	503	ADE	C4-N9	2.39	1.39	1.34
3	C	503	ADE	C4-N3	-2.23	1.34	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAD	C5A-C6A-N6A	2.41	124.01	120.35
2	C	502	NAD	C5A-C6A-N6A	2.38	123.97	120.35
2	A	501	NAD	C5A-C6A-N6A	2.36	123.94	120.35
3	C	503	ADE	C5-C6-N6	2.33	123.89	120.35
2	B	502	NAD	C5A-C6A-N6A	2.29	123.83	120.35
2	C	502	NAD	PN-O3-PA	-2.21	125.24	132.83
3	D	502	ADE	C5-C6-N6	2.16	123.63	120.35
4	A	503	RD4	O-C7-C8	2.13	115.50	108.21
4	C	501	RD4	C1-C-N	2.06	121.16	118.05
2	B	502	NAD	PN-O3-PA	-2.06	125.76	132.83

There are no chirality outliers.

All (26) 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	502	NAD	O4D-C1D-N1N-C2N
2	B	502	NAD	O4D-C1D-N1N-C6N
2	B	502	NAD	C2D-C1D-N1N-C2N
2	B	502	NAD	C2D-C1D-N1N-C6N
2	C	502	NAD	O4D-C1D-N1N-C2N
2	C	502	NAD	O4D-C1D-N1N-C6N
2	C	502	NAD	C2D-C1D-N1N-C2N

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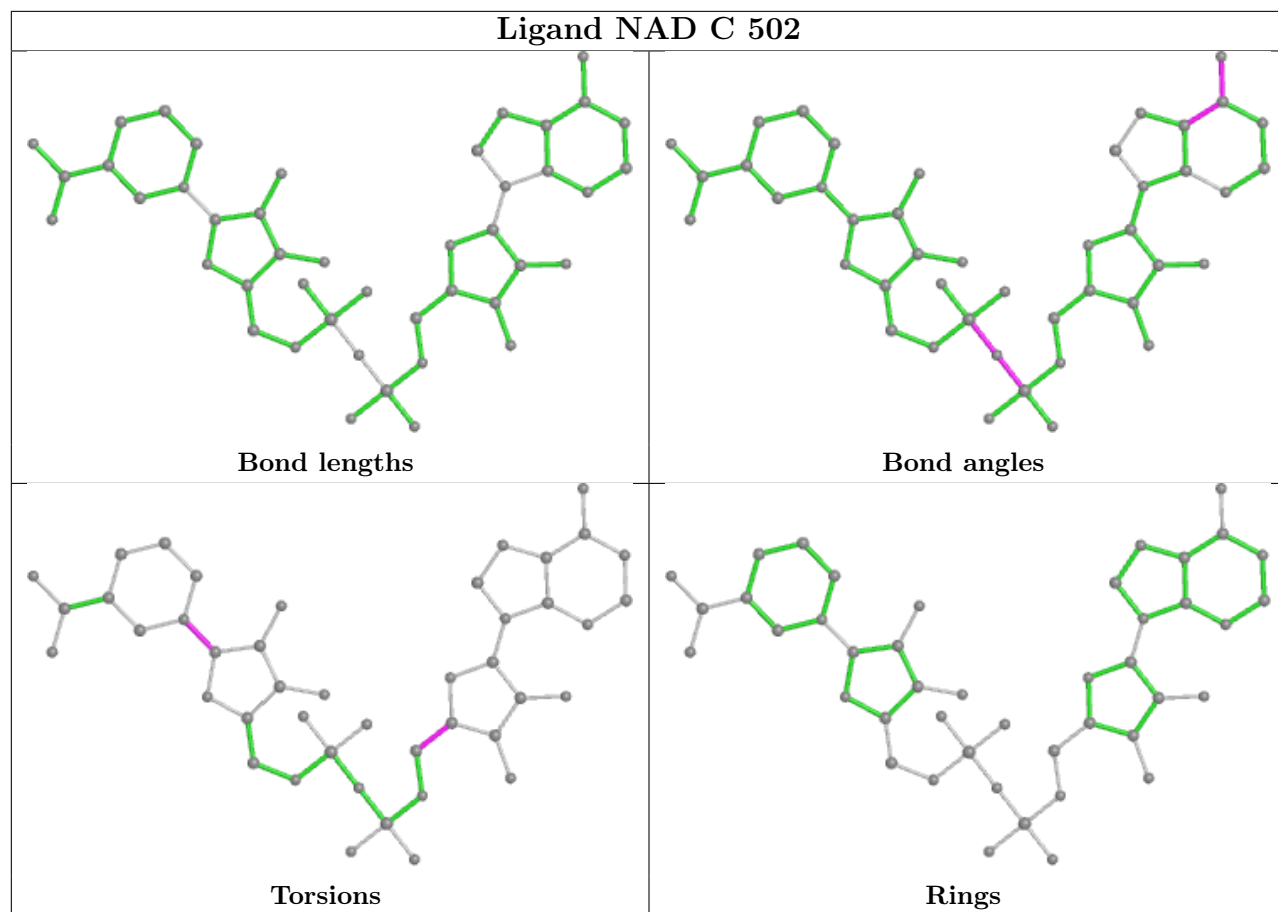
Mol	Chain	Res	Type	Atoms
2	C	502	NAD	C2D-C1D-N1N-C6N
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C2N
2	D	501	NAD	C2D-C1D-N1N-C6N
2	D	501	NAD	O4B-C4B-C5B-O5B
4	B	501	RD4	N-C-C1-C6
4	B	501	RD4	N-C-C1-C2
2	A	501	NAD	O4B-C4B-C5B-O5B
4	C	501	RD4	C4-C5-O-C7
2	B	502	NAD	O4B-C4B-C5B-O5B
2	C	502	NAD	O4B-C4B-C5B-O5B
4	B	501	RD4	N1-C-C1-C6
4	B	501	RD4	N1-C-C1-C2
4	C	501	RD4	C6-C5-O-C7

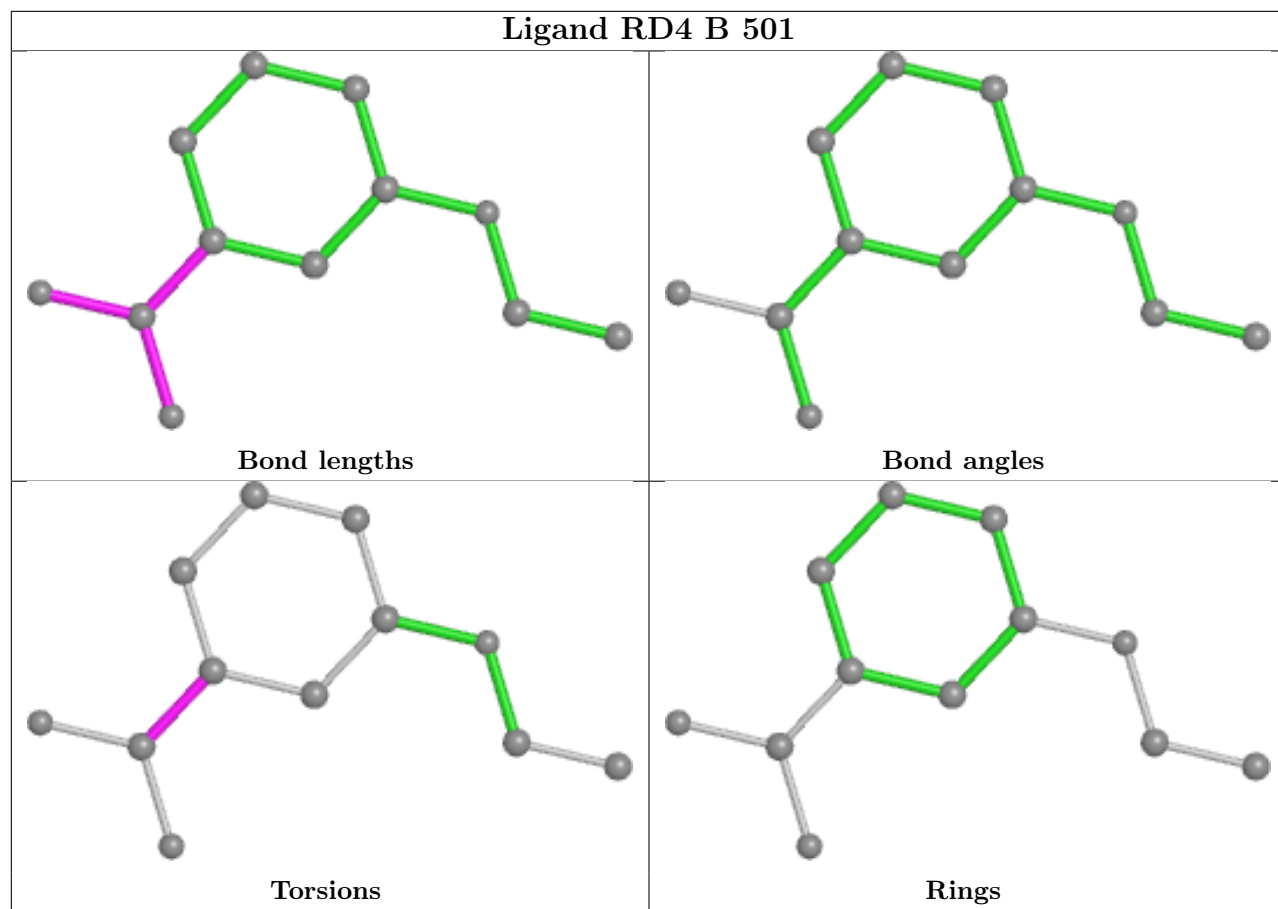
There are no ring outliers.

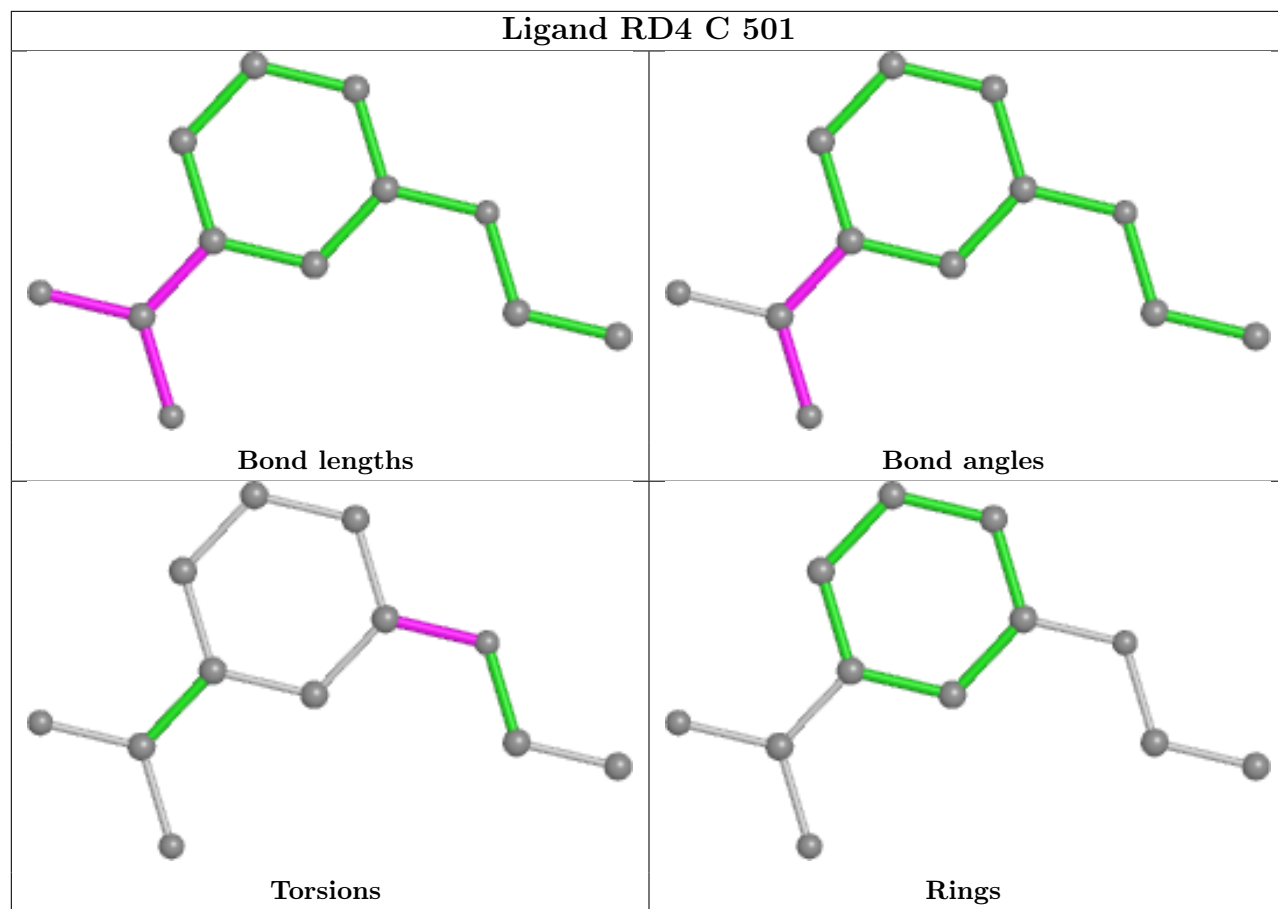
3 monomers are involved in 3 short contacts:

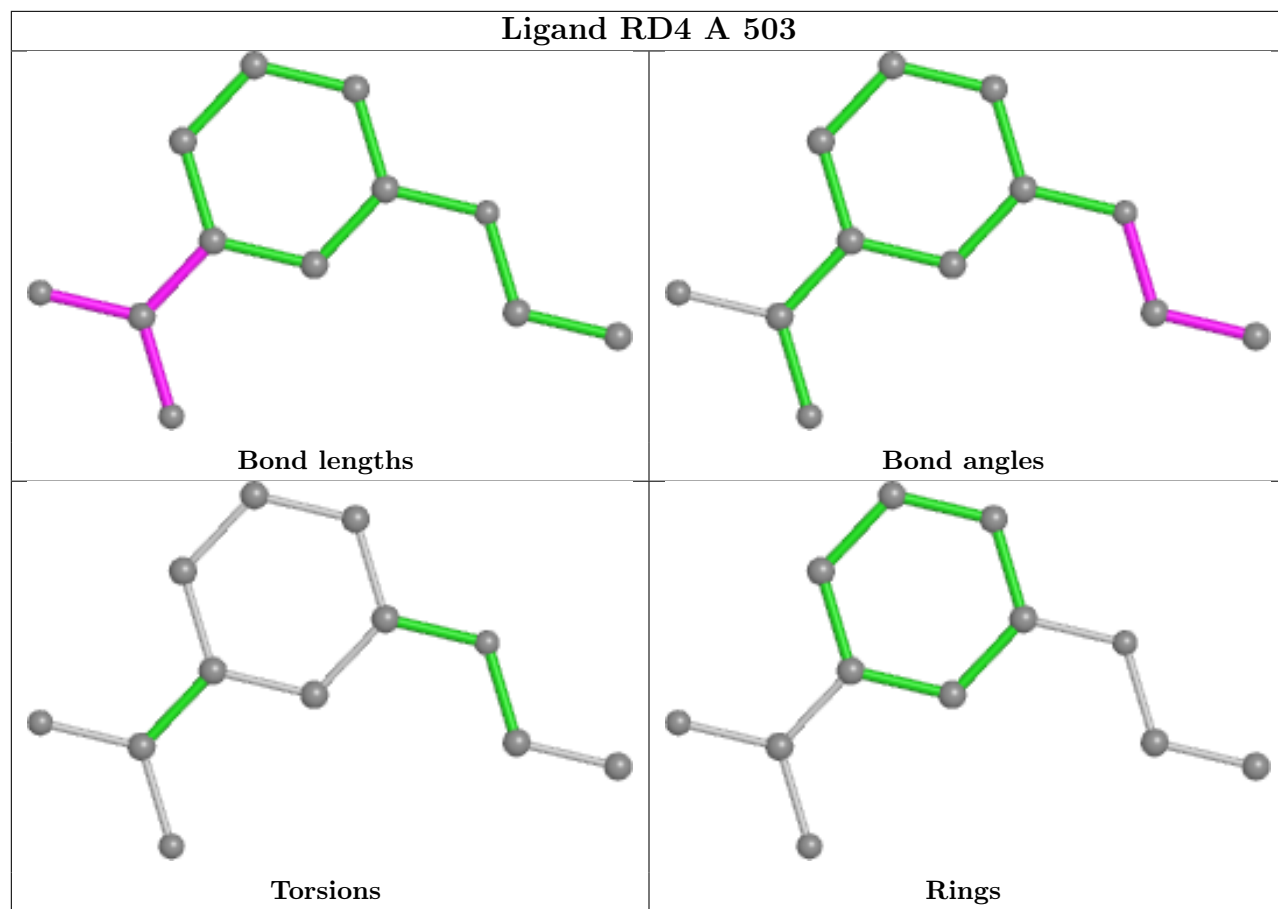
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	505	PO4	1	0
4	C	501	RD4	1	0
7	C	504	DMS	1	0

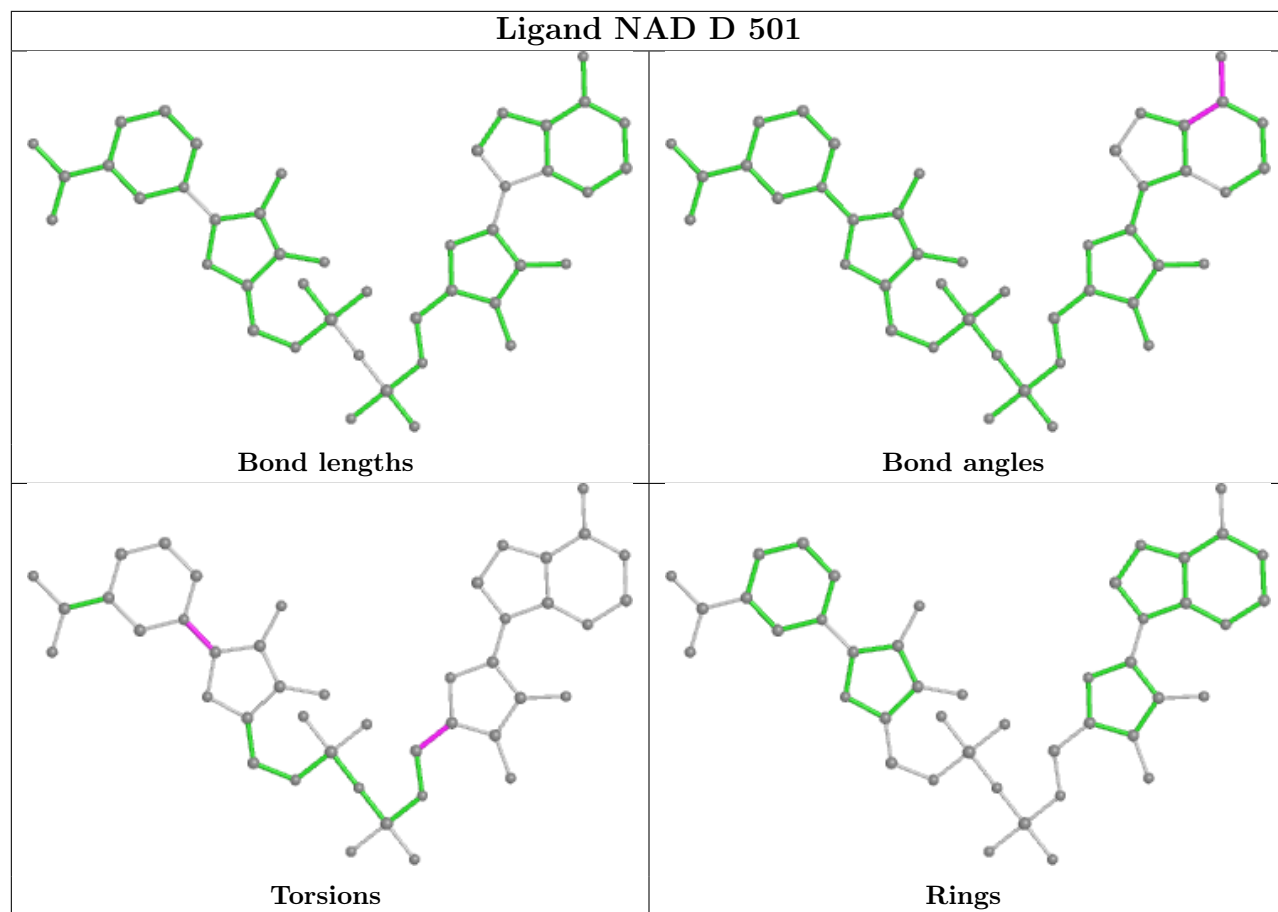
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

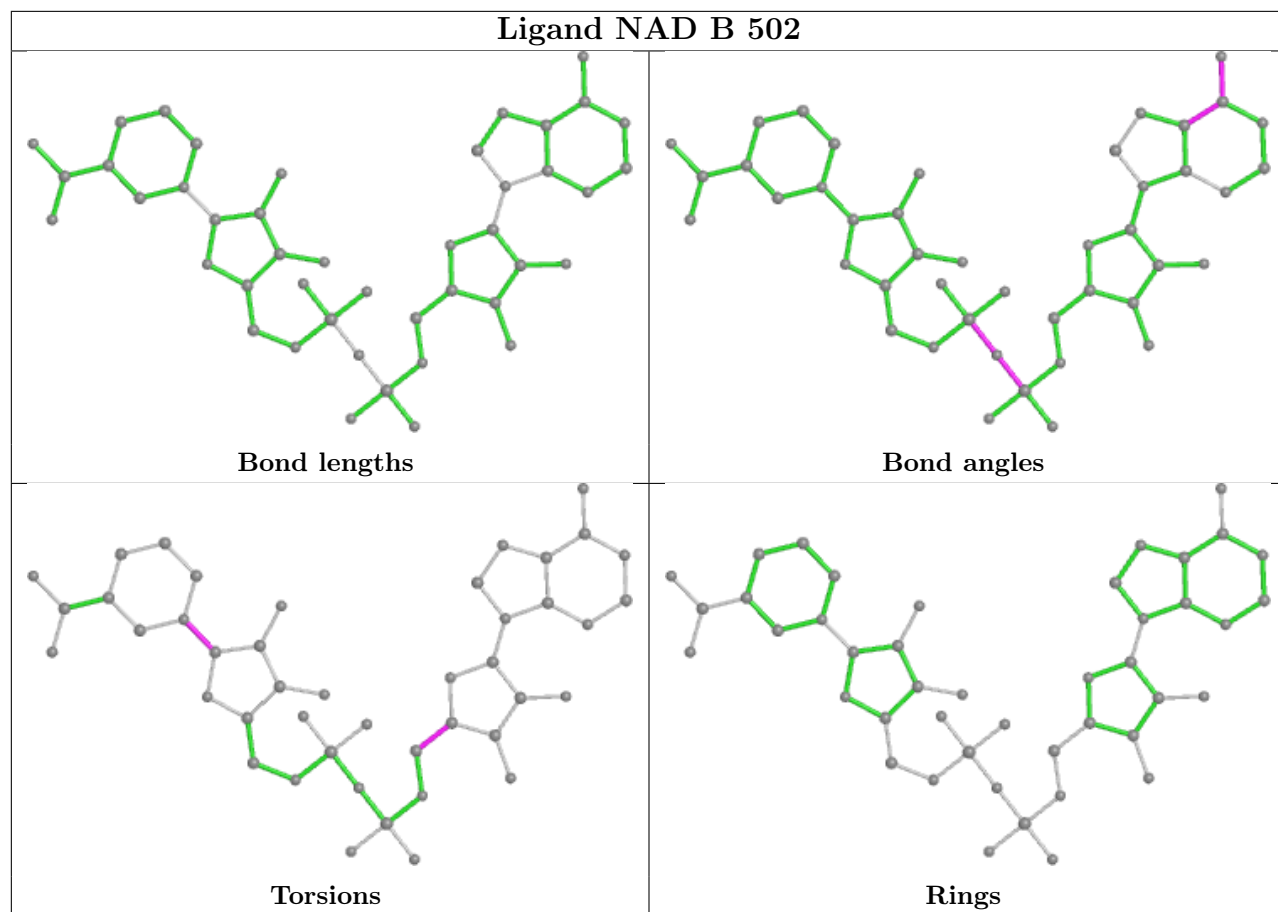


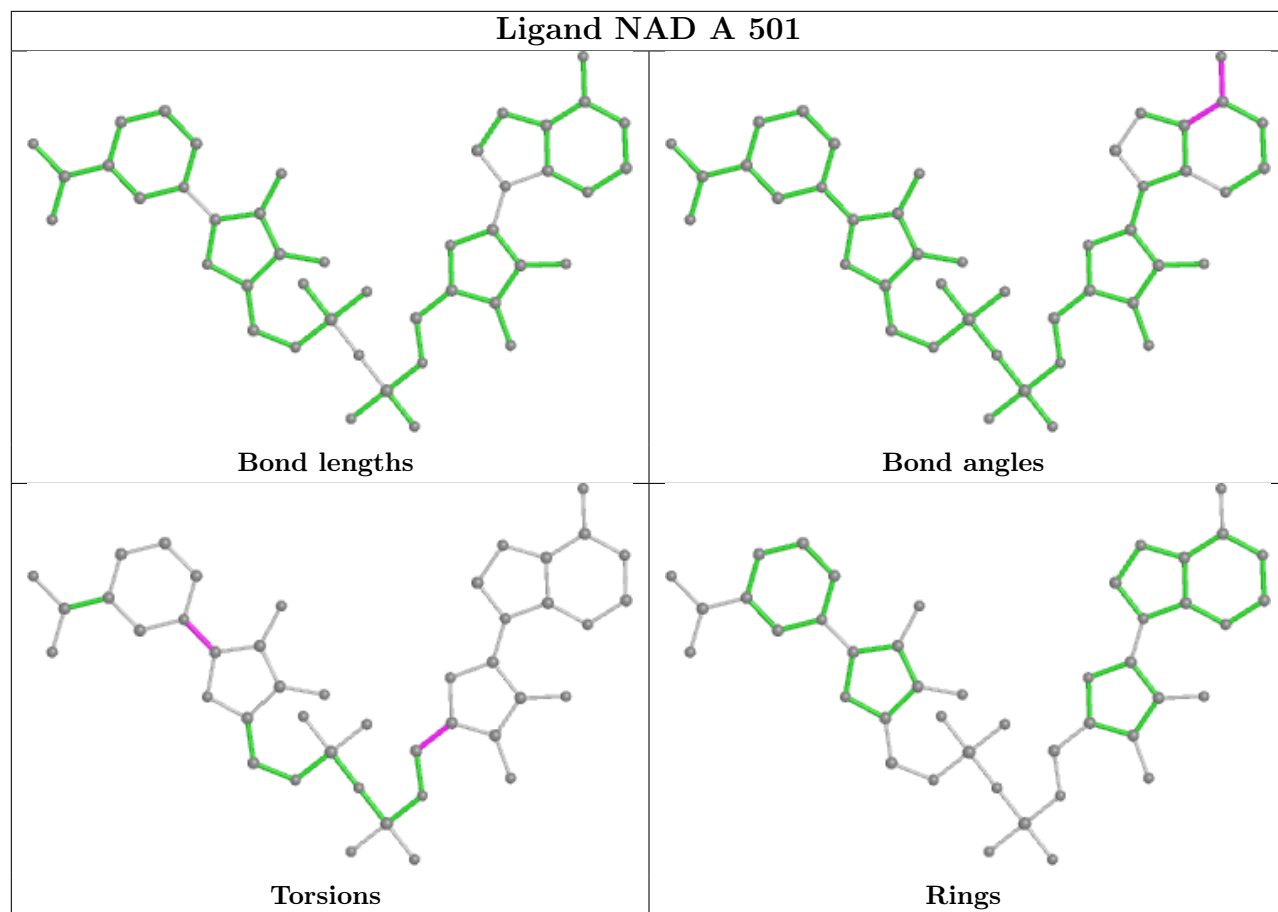












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	462/472 (97%)	-0.02	9 (1%) 66 69	20, 31, 52, 92	0
1	B	461/472 (97%)	0.64	54 (11%) 4 5	21, 41, 88, 145	0
1	C	462/472 (97%)	0.26	24 (5%) 27 30	25, 40, 62, 124	0
1	D	464/472 (98%)	0.22	25 (5%) 25 29	21, 38, 67, 135	0
All	All	1849/1888 (97%)	0.28	112 (6%) 21 24	20, 37, 68, 145	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	412	ALA	17.9
1	C	8	ALA	13.3
1	B	411	ALA	11.4
1	B	181	LEU	9.6
1	B	152	PRO	8.9
1	B	176	LEU	8.4
1	D	412	ALA	8.4
1	D	413	GLU	7.7
1	D	416	LYS	7.5
1	D	409	LEU	7.4
1	B	415	ALA	7.4
1	B	410	PRO	7.0
1	B	355	ASP	6.4
1	B	413	GLU	6.4
1	B	409	LEU	6.3
1	B	179	GLY	6.2
1	D	415	ALA	6.1
1	B	147	LEU	5.7
1	B	180	THR	5.7
1	B	416	LYS	5.7
1	B	177	LYS	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	410	PRO	5.3
1	B	129	GLN	5.2
1	C	359	ALA	5.2
1	B	414	LYS	5.2
1	B	406	TYR	5.1
1	D	417	ARG	4.5
1	C	355	ASP	4.5
1	B	169	VAL	4.3
1	B	417	ARG	4.2
1	B	407	ALA	4.1
1	A	352	THR	4.1
1	B	173	LEU	4.0
1	D	9	GLY	3.9
1	C	285	ALA	3.9
1	C	280	GLU	3.8
1	D	355	ASP	3.8
1	B	359	ALA	3.7
1	B	148	HIS	3.7
1	B	418	LEU	3.7
1	A	46	ALA	3.6
1	B	149	LYS	3.6
1	C	9	GLY	3.4
1	B	183	VAL	3.4
1	D	411	ALA	3.3
1	B	168	GLY	3.2
1	A	8	ALA	3.2
1	B	178	ASN	3.2
1	A	357	PHE	3.1
1	C	281	ALA	3.0
1	D	359	ALA	3.0
1	A	9	GLY	3.0
1	C	283	ILE	2.9
1	B	9	GLY	2.9
1	C	357	PHE	2.9
1	C	306	ALA	2.8
1	B	335	LYS	2.8
1	B	452	GLU	2.8
1	D	414	LYS	2.8
1	B	175	MET	2.8
1	D	357	PHE	2.8
1	B	144	THR	2.7
1	D	407	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	354	LYS	2.6
1	B	157	ARG	2.6
1	C	335	LYS	2.6
1	C	129	GLN	2.6
1	D	356	GLY	2.6
1	C	238[A]	GLN	2.6
1	B	357	PHE	2.5
1	B	354	LYS	2.5
1	C	278	GLY	2.5
1	C	232	VAL	2.5
1	B	153	GLN	2.4
1	A	356	GLY	2.4
1	B	356	GLY	2.4
1	C	207	LEU	2.4
1	B	10	PHE	2.4
1	D	404	GLN	2.4
1	B	240	LEU	2.3
1	D	352	THR	2.3
1	D	332	PHE	2.3
1	C	337	TRP	2.3
1	A	355	ASP	2.3
1	C	352	THR	2.3
1	B	150	LYS	2.2
1	C	356	GLY	2.2
1	D	335	LYS	2.2
1	D	6	THR	2.2
1	B	145	GLU	2.2
1	B	260	ALA	2.2
1	D	100	ALA	2.2
1	D	247	VAL	2.2
1	B	172	LEU	2.2
1	D	240	LEU	2.1
1	D	338	ALA	2.1
1	C	201	TYR	2.1
1	C	192	VAL	2.1
1	B	118	TRP	2.1
1	B	324	PHE	2.1
1	C	310	LYS	2.1
1	B	151	TYR	2.1
1	B	170	HIS	2.1
1	D	129	GLN	2.1
1	B	155	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	113	GLU	2.0
1	A	233	GLY	2.0
1	B	154	MET	2.0
1	B	278	GLY	2.0
1	C	153	GLN	2.0
1	A	240	LEU	2.0
1	B	117	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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.

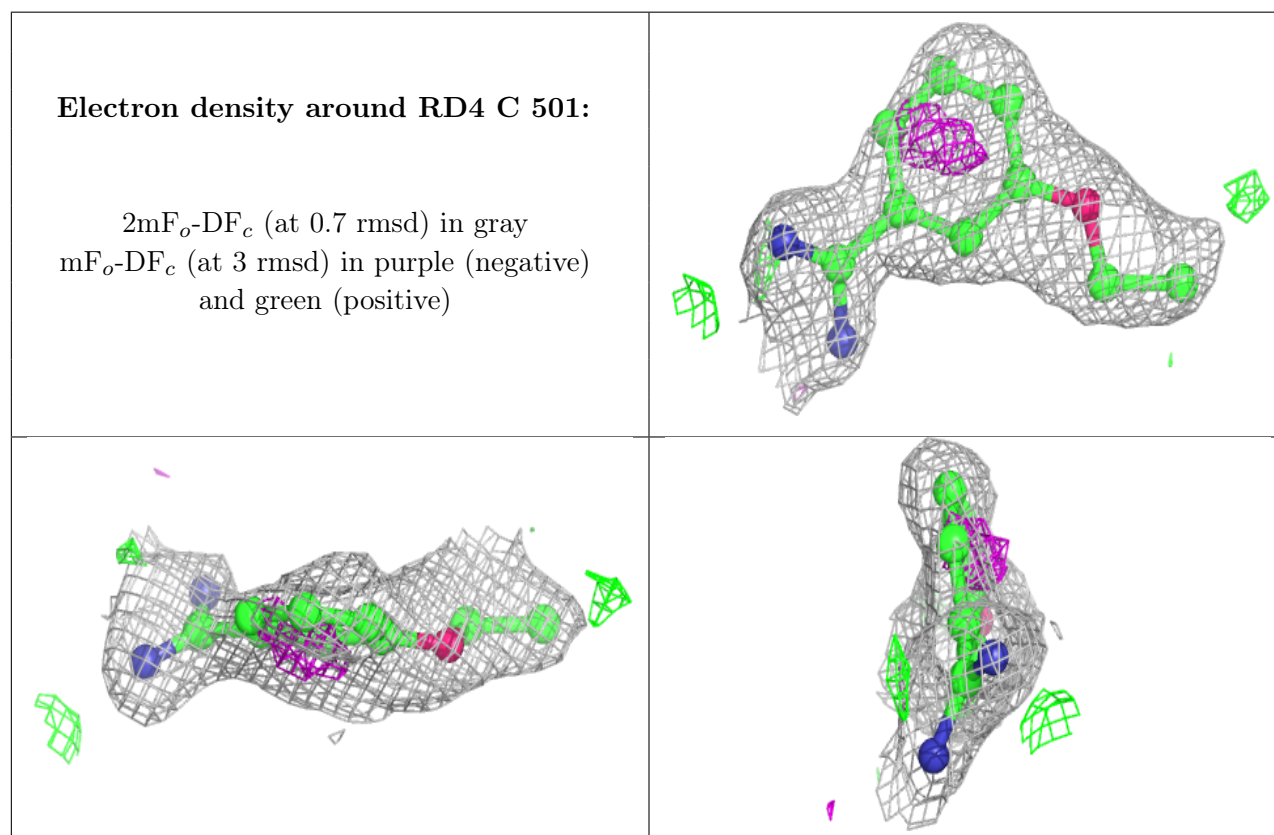
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	RD4	C	501	12/12	0.81	0.17	42,45,48,52	0
4	RD4	A	503	12/12	0.83	0.14	37,43,51,51	0
4	RD4	B	501	12/12	0.86	0.24	39,47,60,64	0
6	PO4	B	507	5/5	0.90	0.11	47,53,57,62	0
6	PO4	A	505	5/5	0.91	0.33	57,63,68,77	0
6	PO4	B	506	5/5	0.95	0.24	52,56,59,67	0
6	PO4	C	508	5/5	0.95	0.10	34,38,41,44	0
6	PO4	D	505	5/5	0.95	0.11	37,38,39,45	0
2	NAD	B	502	44/44	0.96	0.09	23,28,33,37	0
6	PO4	C	509	5/5	0.96	0.22	57,58,68,71	0
6	PO4	D	504	5/5	0.96	0.32	59,62,67,71	0
3	ADE	C	503	10/10	0.96	0.12	28,31,36,36	0
7	DMS	C	504	4/4	0.96	0.27	53,61,64,64	0
6	PO4	C	506	5/5	0.97	0.11	39,44,48,51	0
6	PO4	C	507	5/5	0.97	0.15	43,52,56,57	0
2	NAD	C	502	44/44	0.97	0.09	22,31,36,47	0

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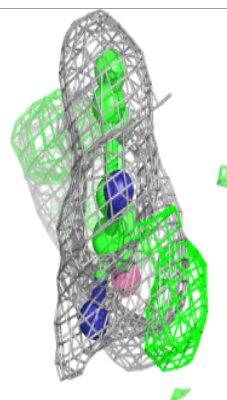
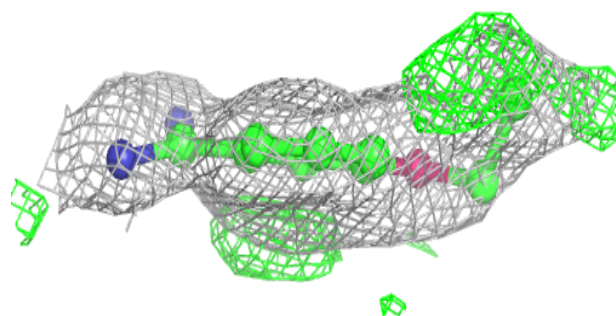
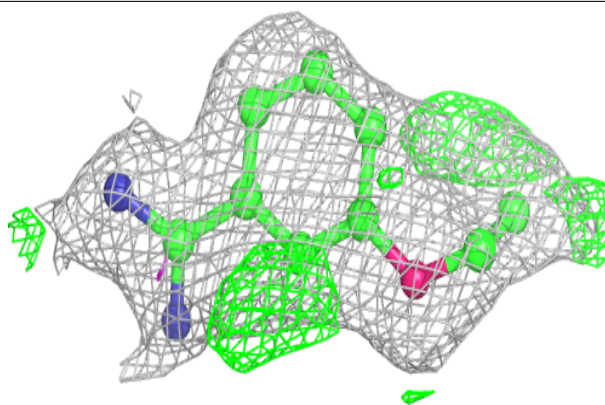
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADE	D	502	10/10	0.97	0.08	32,35,40,41	0
6	PO4	A	507	5/5	0.97	0.10	30,30,37,39	0
3	ADE	A	502	10/10	0.97	0.11	21,22,23,24	0
3	ADE	B	503	10/10	0.97	0.09	32,35,39,42	0
2	NAD	D	501	44/44	0.98	0.08	20,26,31,33	0
2	NAD	A	501	44/44	0.98	0.10	21,26,31,34	0
6	PO4	B	505	5/5	0.98	0.10	40,43,52,52	0
5	K	C	505	1/1	0.99	0.05	29,29,29,29	0
5	K	D	503	1/1	0.99	0.03	24,24,24,24	0
5	K	A	504	1/1	0.99	0.10	26,26,26,26	0
6	PO4	A	506	5/5	0.99	0.08	32,35,40,41	0
5	K	B	504	1/1	0.99	0.03	32,32,32,32	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.

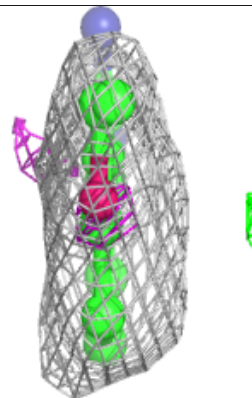
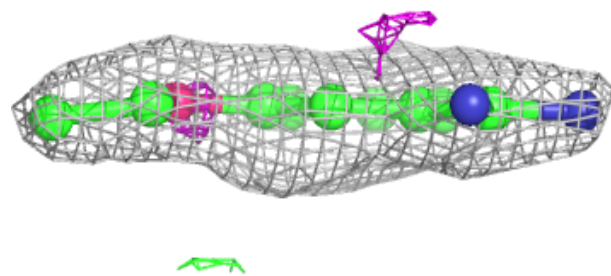
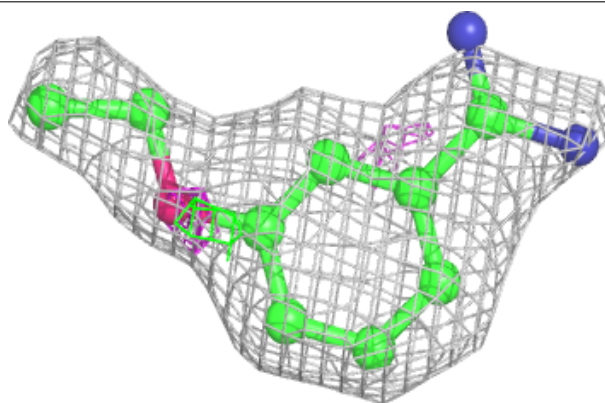


Electron density around RD4 A 503:

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

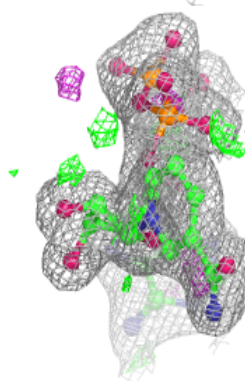
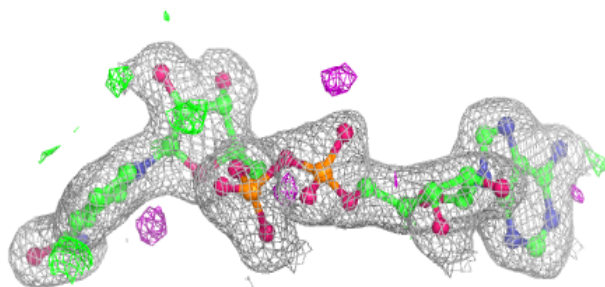
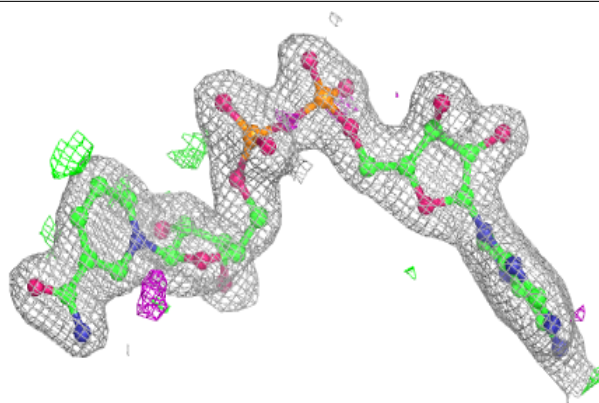
**Electron density around RD4 B 501:**

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

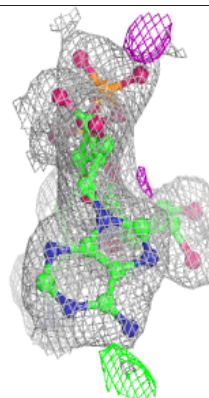
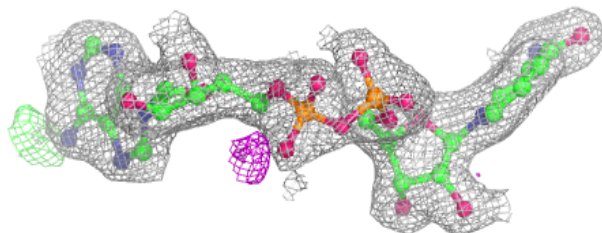
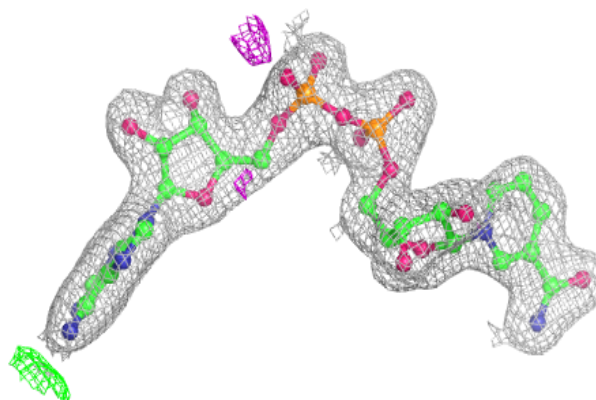


Electron density around NAD B 502:

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

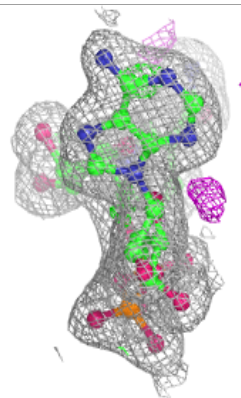
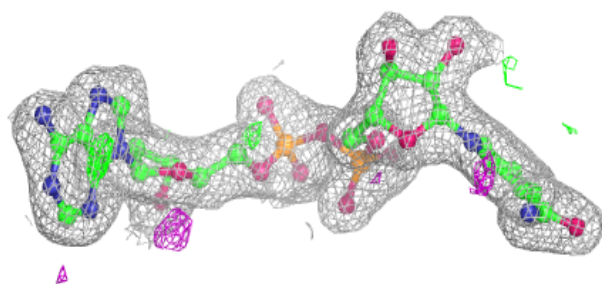
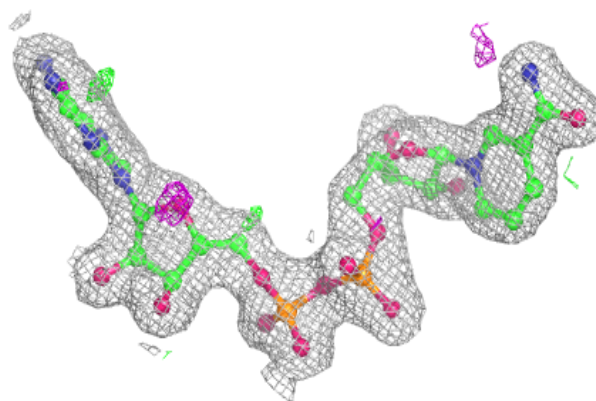
**Electron density around NAD C 502:**

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

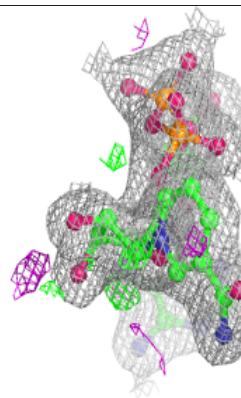
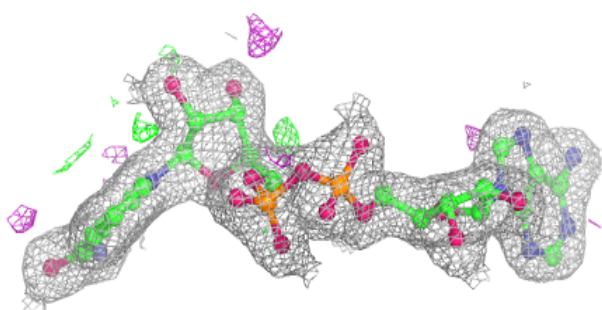
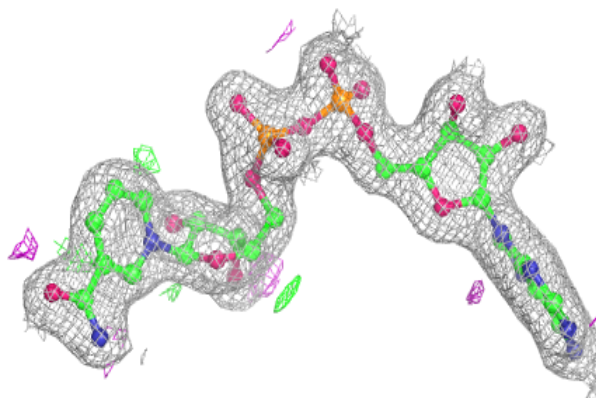


Electron density around NAD D 501:

$2mF_o-DF_c$ (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.