



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:01 PM UTC

PDB ID : 5SA0 / pdb_00005sa0
Title : PanDDA analysis group deposition – Crystal Structure of Trypanosoma brucei
Trypanothione reductase in complex with Z1506050651
Authors : Fiorillo, A.; Ilari, A.
Deposited on : 2021-05-18
Resolution : 1.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

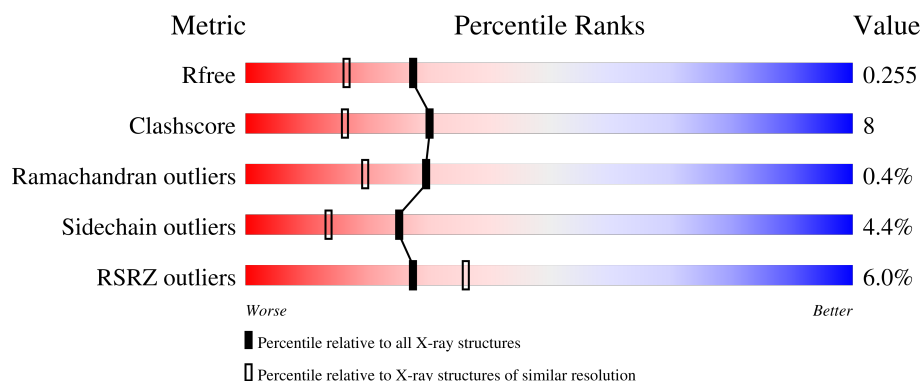
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	495	9% 78% 19% ..
1	B	495	3% 79% 18% ..

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.

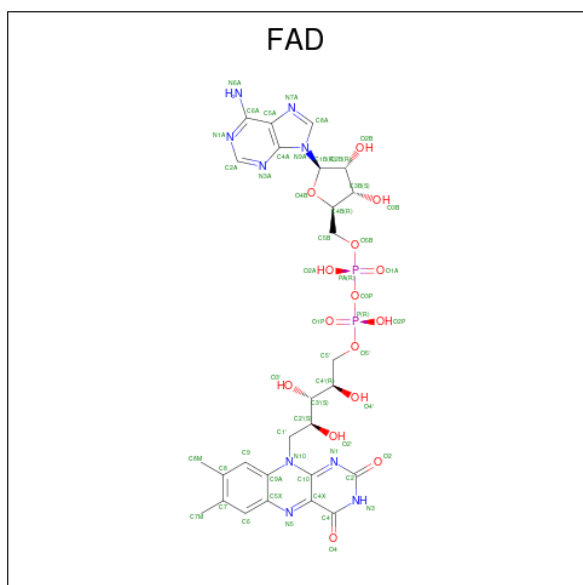
- Molecule 1 is a protein called N(1),N(8)-bis(glutathionyl)spermidine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total 3741	C 2383	N 636	O 703	S 19	0	6	0
1	B	483	Total 3679	C 2339	N 627	O 694	S 19	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A3L6KZJ1
A	-1	SER	-	expression tag	UNP A0A3L6KZJ1
A	0	HIS	-	expression tag	UNP A0A3L6KZJ1
B	-2	GLY	-	expression tag	UNP A0A3L6KZJ1
B	-1	SER	-	expression tag	UNP A0A3L6KZJ1
B	0	HIS	-	expression tag	UNP A0A3L6KZJ1

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



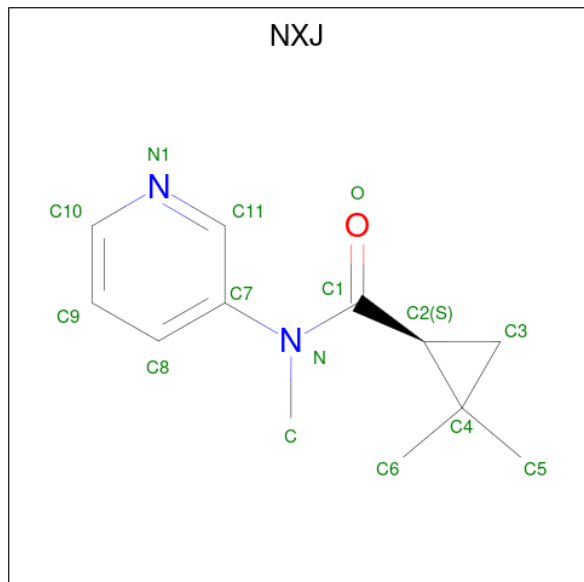
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

- Molecule 4 is (1S)-N,2,2-trimethyl-N-(pyridin-3-yl)cyclopropane-1-carboxamide (CCD ID: NXJ) (formula: C₁₂H₁₆N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	12	2	1		
4	B	1	Total	C	N	O	0	0
			15	12	2	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Br	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	257	Total	O	0	0
			257	257		

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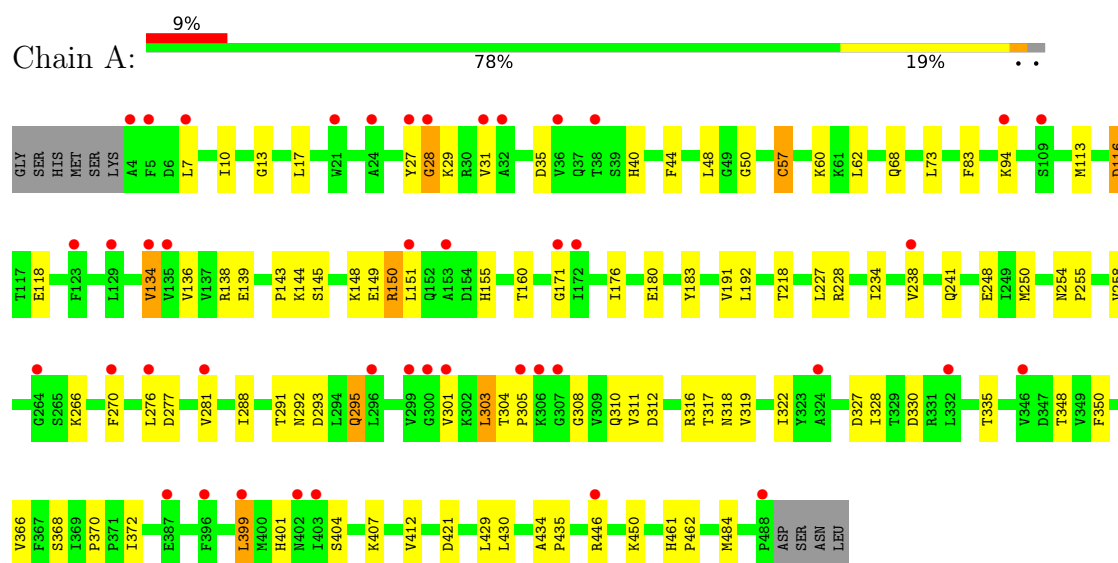
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	263	Total 263	O 263	0	0

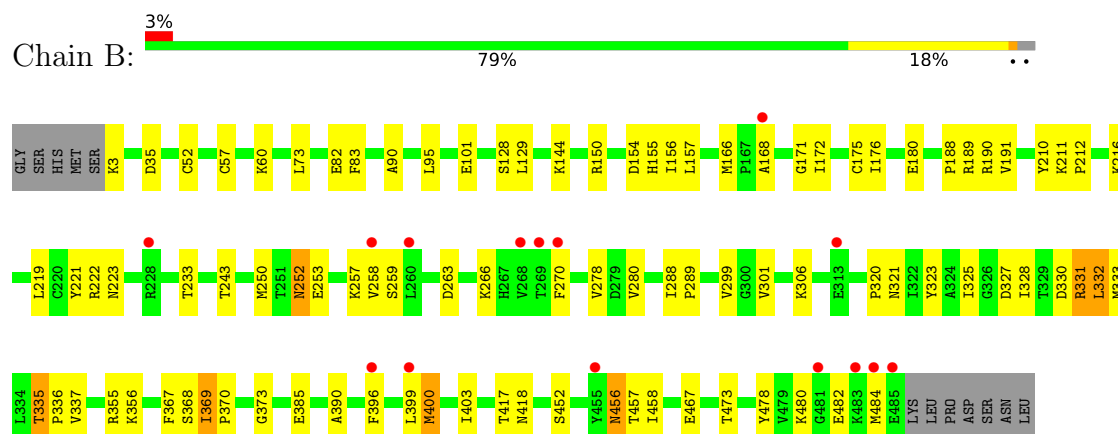
3 Residue-property plots [i](#)

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: N(1),N(8)-bis(glutathionyl)spermidine reductase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.58Å 108.28Å 112.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.97 – 1.97 77.97 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.8 (77.97-1.97) 99.8 (77.97-1.97)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.193 , 0.251 0.206 , 0.255	Depositor DCC
R_{free} test set	3422 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8119	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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: DMS, NXJ, BR, MG, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.12	1/3821 (0.0%)	1.43	4/5185 (0.1%)
1	B	1.10	1/3756 (0.0%)	1.43	11/5095 (0.2%)
All	All	1.11	2/7577 (0.0%)	1.43	15/10280 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	VAL	C-O	5.25	1.29	1.24
1	B	35	ASP	C-O	5.18	1.30	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	458	ILE	CA-C-N	6.96	126.71	120.10
1	B	458	ILE	C-N-CA	6.96	126.71	120.10
1	B	233	THR	CA-CB-OG1	-6.17	100.35	109.60
1	B	327	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	327	ASP	CA-CB-CG	5.77	118.37	112.60
1	B	369	ILE	CB-CA-C	5.69	116.49	111.08
1	B	368	SER	N-CA-C	-5.67	103.44	110.41
1	A	348	THR	CA-C-N	5.61	128.14	120.46
1	A	348	THR	C-N-CA	5.61	128.14	120.46
1	B	456	ASN	CA-CB-CG	-5.43	107.17	112.60
1	B	457	THR	CA-CB-OG1	-5.40	101.50	109.60
1	B	367	PHE	CA-CB-CG	-5.32	108.48	113.80
1	B	473	THR	CA-CB-OG1	-5.16	101.86	109.60
1	B	373	GLY	CA-C-O	-5.01	117.03	120.94
1	A	308	GLY	CA-C-O	-5.00	117.04	121.64

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	3741	0	3746	71	0
1	B	3679	0	3684	59	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
3	A	24	0	36	3	0
3	B	16	0	24	4	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	1	0	0	0	0
7	A	257	0	0	7	1
7	B	263	0	0	15	1
All	All	8119	0	7552	127	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 8.

All (127) 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:446[B]:ARG:HH21	1:A:446[B]:ARG:HB2	1.19	1.03
1:B:250:MET:HE1	1:B:270:PHE:CE1	2.05	0.90
1:A:446[B]:ARG:HB2	1:A:446[B]:ARG:NH2	1.92	0.84
1:B:399:LEU:N	7:B:605:HOH:O	2.23	0.72
1:B:101:GLU:HG3	7:B:857:HOH:O	1.90	0.71
1:A:44:PHE:HD2	7:A:621:HOH:O	1.73	0.71
1:B:83:PHE:CE2	3:B:502:DMS:H13	2.27	0.69
1:A:295:GLN:HE21	1:A:295:GLN:HA	1.58	0.67
1:B:222:ARG:O	1:B:252:ASN:HA	1.94	0.67
1:A:407:LYS:HB2	7:A:622:HOH:O	1.94	0.66
1:A:138:ARG:NH1	1:A:145:SER:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:HA	1:A:248:GLU:OE1	2.00	0.62
1:A:68:GLN:HG2	7:A:839:HOH:O	2.01	0.60
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.35	0.60
1:B:396:PHE:CE1	1:B:467:GLU:HG3	2.37	0.60
1:A:83:PHE:CE2	3:A:502:DMS:H13	2.38	0.59
1:A:150:ARG:CZ	1:A:150:ARG:HB2	2.33	0.59
1:B:176:ILE:HB	1:B:180:GLU:HB2	1.86	0.58
1:B:129:LEU:HD13	1:B:299:VAL:HG21	1.84	0.58
1:B:320:PRO:O	1:B:321:ASN:OD1	2.22	0.58
1:B:355:ARG:NH2	7:B:602:HOH:O	2.18	0.58
3:B:504:DMS:H23	7:B:717:HOH:O	2.02	0.57
1:A:17:LEU:HD22	1:A:113:MET:HE1	1.87	0.57
1:B:250:MET:HE1	1:B:270:PHE:CD1	2.39	0.57
1:A:250:MET:HE1	1:A:270:PHE:CE1	2.39	0.57
3:B:504:DMS:C2	7:B:717:HOH:O	2.52	0.57
1:A:176:ILE:HB	1:A:180:GLU:HB2	1.87	0.56
1:B:171:GLY:HA3	1:B:258:VAL:O	2.05	0.56
1:B:355:ARG:HB3	7:B:694:HOH:O	2.05	0.56
1:B:396:PHE:HE1	1:B:467:GLU:HG3	1.71	0.55
1:B:211:LYS:O	7:B:603:HOH:O	2.18	0.55
1:A:150:ARG:HB2	1:A:150:ARG:NH1	2.22	0.55
1:B:190:ARG:HA	1:B:216:LYS:O	2.06	0.54
1:B:259:SER:HA	7:B:783:HOH:O	2.08	0.54
1:A:318:ASN:OD1	1:A:319:VAL:HG23	2.07	0.54
1:A:155:HIS:ND1	1:A:350:PHE:CE1	2.76	0.54
1:B:129:LEU:CD1	1:B:299:VAL:HG21	2.38	0.54
1:B:219:LEU:C	1:B:219:LEU:HD23	2.32	0.53
1:A:401:HIS:HA	1:A:404:SER:OG	2.09	0.52
1:B:331:ARG:CD	7:B:847:HOH:O	2.56	0.52
1:B:155:HIS:HD2	1:B:323:TYR:OH	1.92	0.52
1:A:171:GLY:HA3	1:A:258:VAL:O	2.09	0.52
1:B:250:MET:HE1	1:B:270:PHE:CZ	2.43	0.52
1:B:166:MET:HB3	1:B:172:ILE:HD11	1.92	0.52
1:A:60:LYS:HG3	7:A:715:HOH:O	2.09	0.51
1:B:243:THR:OG1	7:B:601:HOH:O	2.17	0.51
1:B:330:ASP:OD1	1:B:333:MET:HE3	2.10	0.51
1:B:331:ARG:HD3	7:B:847:HOH:O	2.11	0.51
1:A:228:ARG:NE	3:A:503:DMS:H21	2.24	0.51
1:A:94[A]:LYS:NZ	1:B:82:GLU:OE2	2.39	0.50
1:A:446[B]:ARG:HH21	1:A:446[B]:ARG:CB	2.08	0.50
1:A:40:HIS:ND1	1:A:183:TYR:OH	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLN:NE2	1:A:370:PRO:HG3	2.27	0.50
1:A:73:LEU:HD23	1:B:73:LEU:CD2	2.41	0.50
1:A:27:TYR:O	1:A:29:LYS:HG2	2.12	0.49
1:B:175:CYS:SG	1:B:258:VAL:HG21	2.53	0.49
1:A:303:LEU:N	1:A:303:LEU:HD23	2.27	0.49
1:B:129:LEU:HD21	1:B:156:ILE:HG21	1.94	0.49
1:B:157:LEU:HD11	1:B:325:ILE:HG12	1.94	0.49
1:A:35:ASP:HA	2:A:501:FAD:N3A	2.28	0.48
1:A:317:THR:OG1	1:A:322:ILE:O	2.17	0.48
1:A:238[A]:VAL:HG21	1:A:372:ILE:HD11	1.94	0.48
1:A:304:THR:HB	1:A:305:PRO:CD	2.43	0.48
1:B:83:PHE:CZ	3:B:502:DMS:H13	2.49	0.48
1:A:304:THR:HB	1:A:305:PRO:HD2	1.97	0.47
1:A:234:ILE:O	1:A:238[B]:VAL:HG22	2.14	0.47
1:A:62:LEU:HD13	1:B:403:ILE:CD1	2.44	0.47
1:A:13:GLY:HA2	1:A:50:GLY:HA3	1.97	0.47
1:A:446[B]:ARG:NH2	7:A:617:HOH:O	2.46	0.47
1:B:289:PRO:HB3	1:B:328:ILE:HA	1.97	0.47
1:A:266:LYS:O	1:A:277:ASP:HA	2.15	0.47
1:A:227:LEU:HD12	1:A:238[B]:VAL:HG21	1.96	0.46
1:A:57:CYS:HA	1:A:60:LYS:HE2	1.97	0.46
1:A:311:VAL:HA	1:A:316:ARG:O	2.16	0.46
1:A:73:LEU:HD23	1:B:73:LEU:HD22	1.98	0.46
1:A:134:VAL:HA	1:A:151:LEU:O	2.16	0.46
1:B:252:ASN:C	1:B:253:GLU:HG2	2.41	0.46
1:B:478:TYR:HA	1:B:482:GLU:O	2.16	0.46
1:A:73:LEU:CD2	1:B:73:LEU:HD22	2.46	0.46
1:A:241:GLN:NE2	1:A:370:PRO:CG	2.79	0.46
1:A:330:ASP:O	1:A:330:ASP:CG	2.58	0.46
1:A:155:HIS:HD1	1:A:350:PHE:HE1	1.64	0.45
1:A:148:LYS:C	1:A:149:GLU:HG2	2.42	0.45
1:A:7:LEU:O	1:A:31:VAL:HA	2.17	0.44
1:A:399:LEU:N	7:A:619:HOH:O	2.46	0.44
1:A:27:TYR:O	1:A:28:GLY:C	2.60	0.44
1:B:191:VAL:HA	1:B:280:VAL:O	2.18	0.44
1:B:299:VAL:HG23	1:B:301:VAL:HG23	1.99	0.44
1:A:238[B]:VAL:HG13	1:A:430:LEU:HD13	2.00	0.44
1:A:254:ASN:OD1	1:A:255:PRO:HD2	2.18	0.44
1:B:399:LEU:O	1:B:400:MET:C	2.61	0.43
1:A:434:ALA:HB3	1:A:435:PRO:HD3	1.99	0.43
1:A:304:THR:HG22	1:A:310:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:SER:OG	7:B:604:HOH:O	2.21	0.43
1:B:418:ASN:ND2	7:B:619:HOH:O	2.45	0.43
1:B:52:CYS:HB3	7:B:654:HOH:O	2.18	0.43
1:A:143:PRO:HB3	1:A:295:GLN:OE1	2.19	0.43
1:A:192:LEU:HA	1:A:218:THR:O	2.19	0.43
1:B:452:SER:O	1:B:456:ASN:HB2	2.19	0.43
1:B:332:LEU:HD13	1:B:337:VAL:HG21	2.02	0.42
1:A:228:ARG:HE	3:A:503:DMS:H21	1.84	0.42
1:B:189:ARG:HG3	1:B:212:PRO:HG2	2.00	0.42
1:B:190:ARG:HB2	1:B:278:VAL:HA	2.01	0.42
1:A:136:VAL:O	1:A:136:VAL:HG13	2.20	0.42
1:A:484:MET:HE2	1:A:484:MET:HB3	1.91	0.42
1:B:331:ARG:HB3	7:B:612:HOH:O	2.18	0.42
1:B:369:ILE:HA	1:B:370:PRO:HA	1.88	0.42
1:A:312:ASP:OD1	1:A:312:ASP:C	2.63	0.42
1:A:366:VAL:C	1:A:368:SER:H	2.28	0.42
1:B:188:PRO:HB3	1:B:280:VAL:HG23	2.02	0.41
1:B:263:ASP:OD1	1:B:263:ASP:C	2.63	0.41
1:B:95:LEU:HD22	1:B:210:TYR:CZ	2.55	0.41
1:A:139:GLU:HG3	1:A:148:LYS:HG2	2.03	0.41
1:A:292:ASN:HD22	1:A:292:ASN:N	2.17	0.41
1:A:407:LYS:N	7:A:622:HOH:O	2.49	0.41
1:A:421:ASP:O	1:A:450:LYS:HE3	2.20	0.41
1:B:418:ASN:C	1:B:418:ASN:HD22	2.28	0.41
1:A:116:ASP:N	1:A:116:ASP:OD1	2.53	0.41
1:B:390:ALA:HB3	1:B:417:THR:OG1	2.21	0.41
1:A:10:ILE:HG22	1:A:160:THR:HG22	2.01	0.41
1:A:461:HIS:HA	1:A:462:PRO:HA	1.84	0.41
1:B:90:ALA:HB1	1:B:210:TYR:CD2	2.55	0.41
1:A:412:VAL:O	1:A:429:LEU:HA	2.21	0.40
1:B:335:THR:N	1:B:336:PRO:CD	2.83	0.40
1:A:60:LYS:HD2	1:A:60:LYS:C	2.45	0.40
1:B:52:CYS:HB2	1:B:335:THR:HG1	1.86	0.40
1:A:227:LEU:CD1	1:A:238[B]:VAL:HG21	2.51	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:834:HOH:O	7:B:622:HOH:O[3_544]	2.14	0.06

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	489/495 (99%)	462 (94%)	25 (5%)	2 (0%)	30	20
1	B	482/495 (97%)	464 (96%)	16 (3%)	2 (0%)	30	20
All	All	971/990 (98%)	926 (95%)	41 (4%)	4 (0%)	30	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	GLY
1	B	331	ARG
1	B	168	ALA
1	A	48	LEU

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	404/407 (99%)	387 (96%)	17 (4%)	26	15
1	B	397/407 (98%)	379 (96%)	18 (4%)	24	13
All	All	801/814 (98%)	766 (96%)	35 (4%)	25	14

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	CYS
1	A	116	ASP

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Mol	Chain	Res	Type
1	A	118	GLU
1	A	134	VAL
1	A	144	LYS
1	A	150	ARG
1	A	191	VAL
1	A	276	LEU
1	A	288	ILE
1	A	291	THR
1	A	293	ASP
1	A	295	GLN
1	A	301	VAL
1	A	303	LEU
1	A	328	ILE
1	A	335	THR
1	A	399	LEU
1	B	3	LYS
1	B	57	CYS
1	B	60	LYS
1	B	144	LYS
1	B	150	ARG
1	B	154	ASP
1	B	252	ASN
1	B	257	LYS
1	B	266	LYS
1	B	288	ILE
1	B	306	LYS
1	B	332	LEU
1	B	335	THR
1	B	356	LYS
1	B	385	GLU
1	B	400	MET
1	B	480	LYS
1	B	484	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	152	GLN
1	A	224	ASN
1	A	241	GLN
1	A	252	ASN

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Mol	Chain	Res	Type
1	A	292	ASN
1	A	295	GLN
1	A	340	ASN
1	A	352	ASN
1	A	359	HIS
1	A	419	HIS
1	A	448	ASN
1	B	68	GLN
1	B	155	HIS
1	B	208	ASN
1	B	352	ASN
1	B	418	ASN
1	B	448	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 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	DMS	A	505	-	3,3,3	0.37	0	3,3,3	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DMS	A	503	-	3,3,3	0.31	0	3,3,3	0.12	0
3	DMS	B	502	-	3,3,3	0.29	0	3,3,3	0.12	0
3	DMS	A	504	-	3,3,3	0.24	0	3,3,3	0.11	0
3	DMS	A	506	-	3,3,3	0.34	0	3,3,3	0.05	0
3	DMS	B	503	-	3,3,3	0.46	0	3,3,3	0.35	0
4	NXJ	A	508	-	16,16,16	1.12	2 (12%)	22,24,24	0.77	0
3	DMS	A	507	-	3,3,3	0.31	0	3,3,3	0.15	0
3	DMS	A	502	-	3,3,3	0.26	0	3,3,3	0.36	0
3	DMS	B	505	-	3,3,3	0.33	0	3,3,3	0.11	0
4	NXJ	B	506	-	16,16,16	1.17	2 (12%)	22,24,24	0.76	0
2	FAD	A	501	-	58,58,58	0.73	0	85,89,89	0.89	3 (3%)
2	FAD	B	501	-	58,58,58	0.76	1 (1%)	85,89,89	0.74	2 (2%)
3	DMS	B	504	-	3,3,3	0.26	0	3,3,3	0.07	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
4	NXJ	B	506	-	-	0/12/20/20	0/2/2/2
2	FAD	B	501	-	-	5/34/50/50	0/6/6/6
4	NXJ	A	508	-	-	0/12/20/20	0/2/2/2
2	FAD	A	501	-	-	6/34/50/50	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	P-O3P	3.89	1.63	1.59
4	A	508	NXJ	C2-C1	-3.24	1.47	1.52
4	B	506	NXJ	C2-C1	-3.12	1.48	1.52
4	B	506	NXJ	C1-N	2.74	1.39	1.35
4	A	508	NXJ	C1-N	2.14	1.38	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	O2P-P-O1P	2.94	126.14	112.44
2	B	501	FAD	C4-N3-C2	-2.24	121.67	125.64
2	A	501	FAD	O3P-P-O1P	-2.05	104.55	110.70
2	B	501	FAD	O2P-P-O1P	2.04	121.95	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	O2P-P-O3P	2.02	112.73	107.27

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	C3B-C4B-C5B-O5B
2	A	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	C3B-C4B-C5B-O5B
2	A	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	PA-O3P-P-O5'
2	A	501	FAD	PA-O3P-P-O1P
2	B	501	FAD	P-O3P-PA-O2A
2	A	501	FAD	P-O3P-PA-O1A
2	B	501	FAD	P-O3P-PA-O1A
2	A	501	FAD	P-O3P-PA-O2A

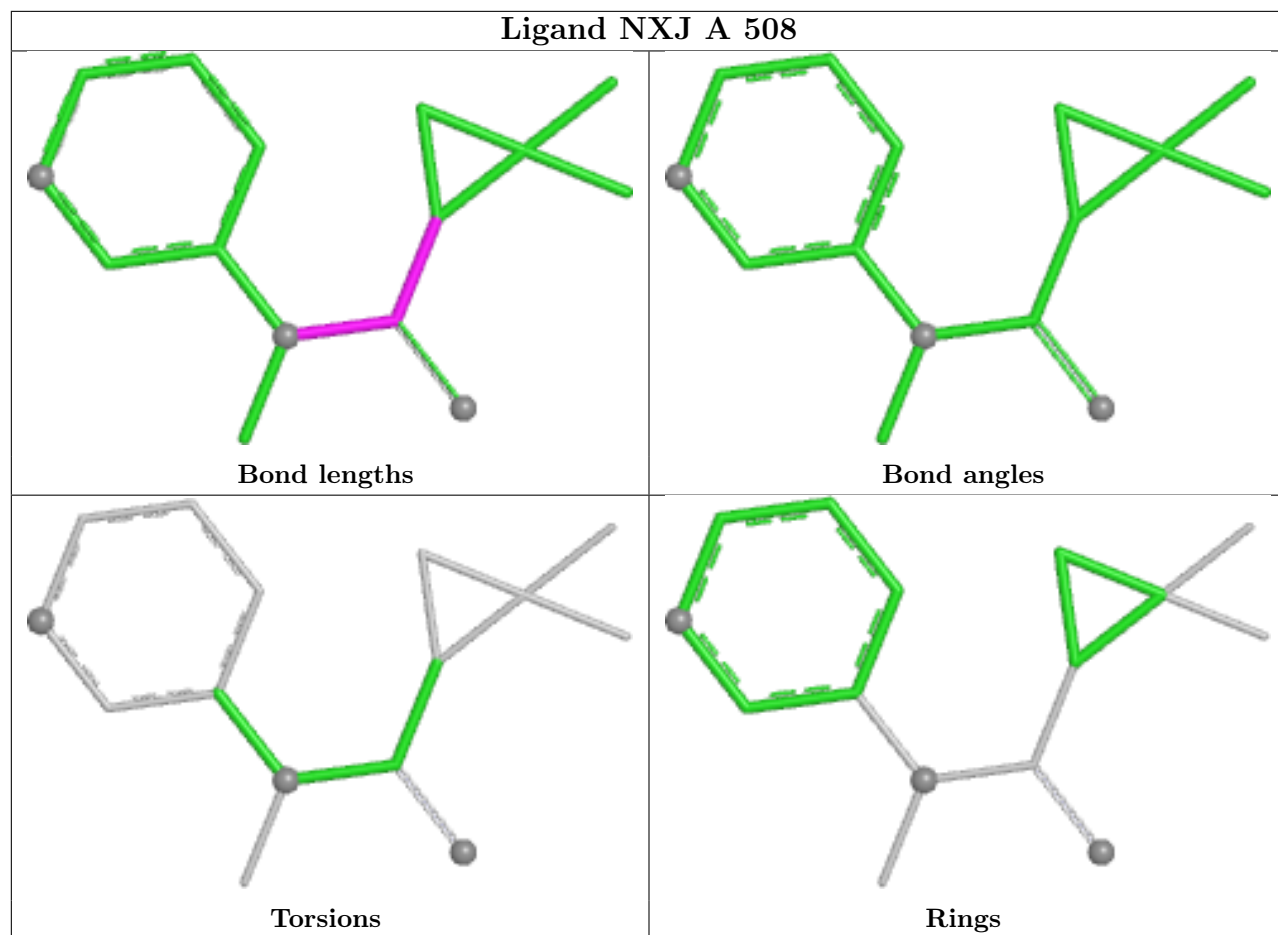
There are no ring outliers.

5 monomers are involved in 8 short contacts:

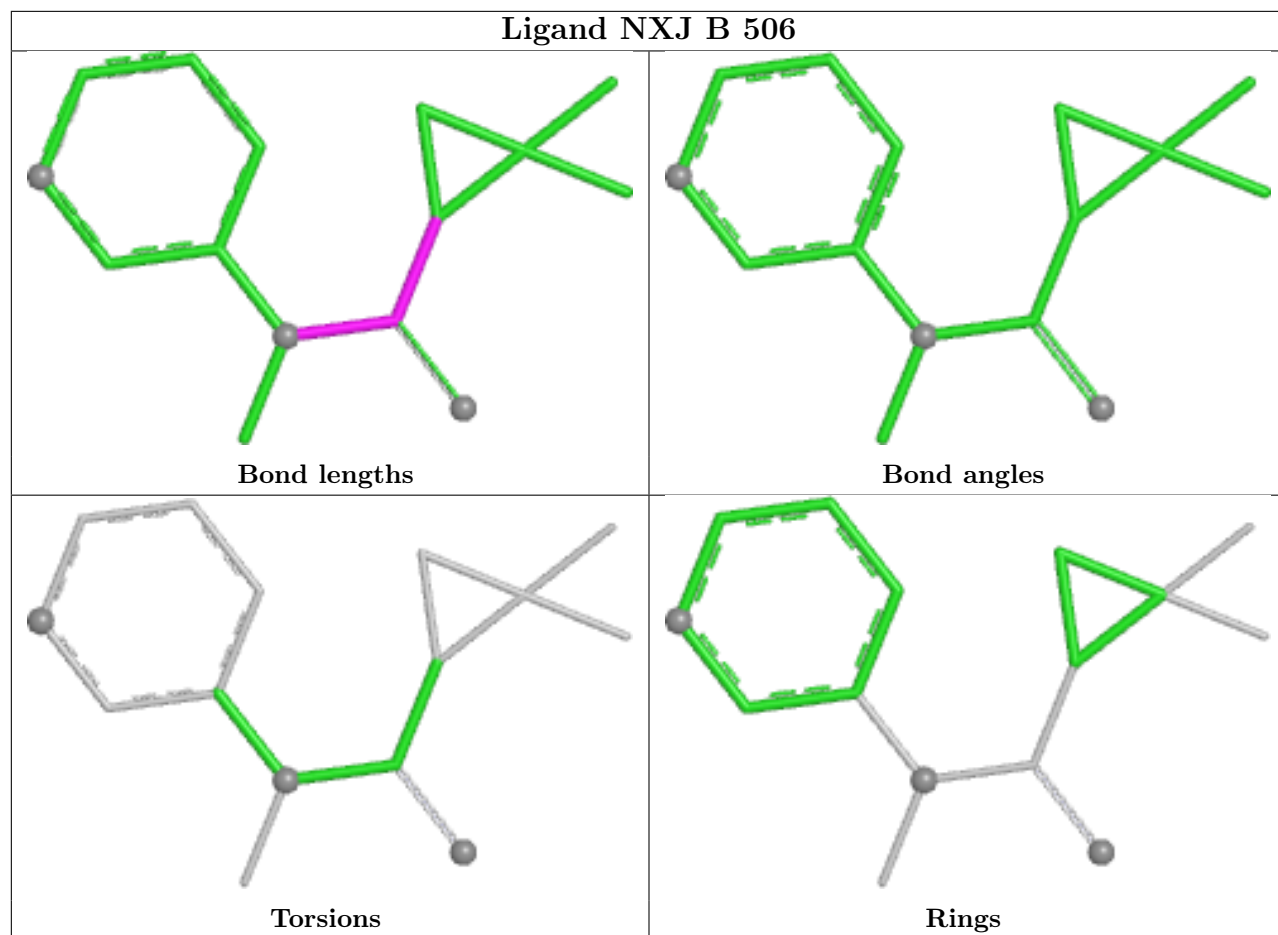
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	DMS	2	0
3	B	502	DMS	2	0
3	A	502	DMS	1	0
2	A	501	FAD	1	0
3	B	504	DMS	2	0

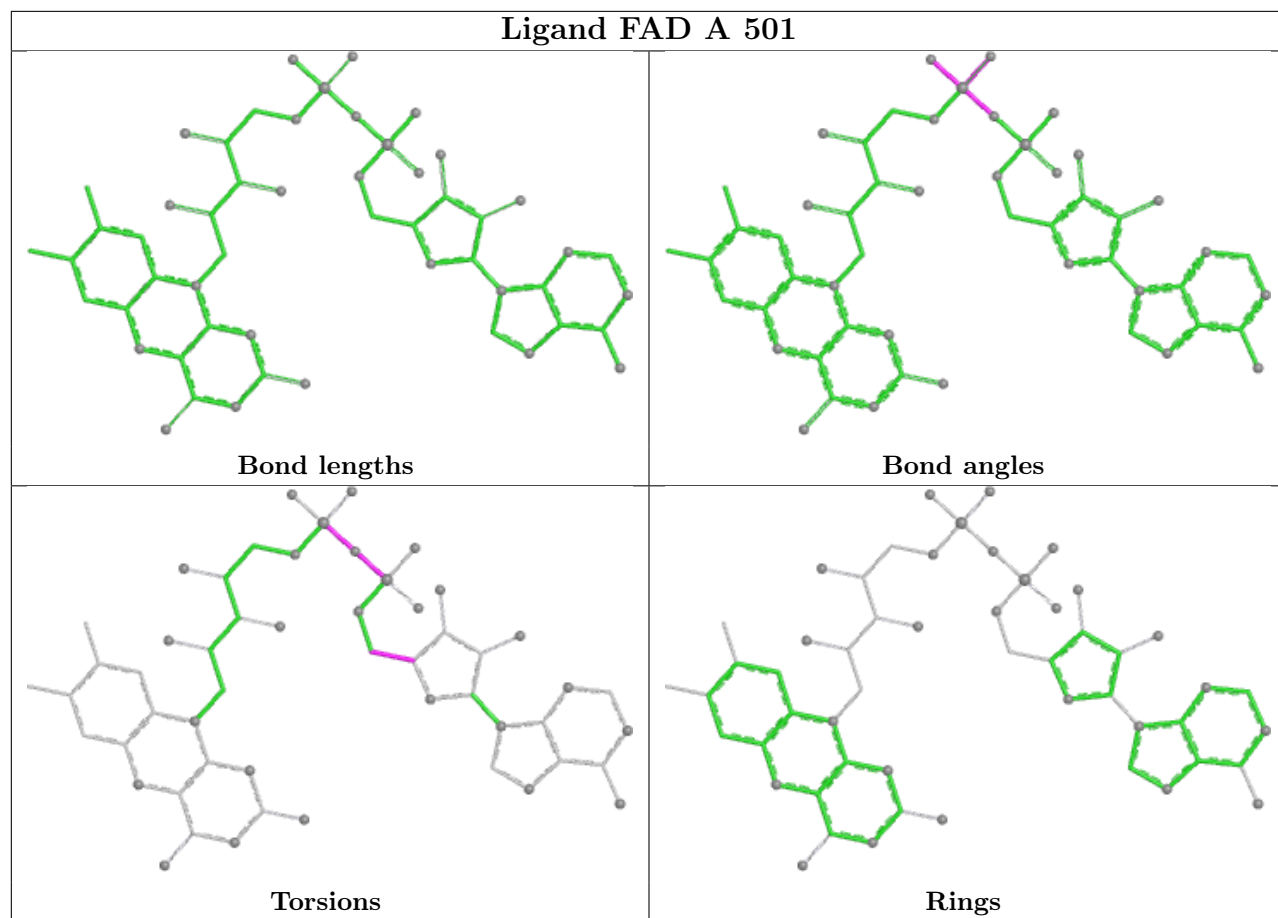
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

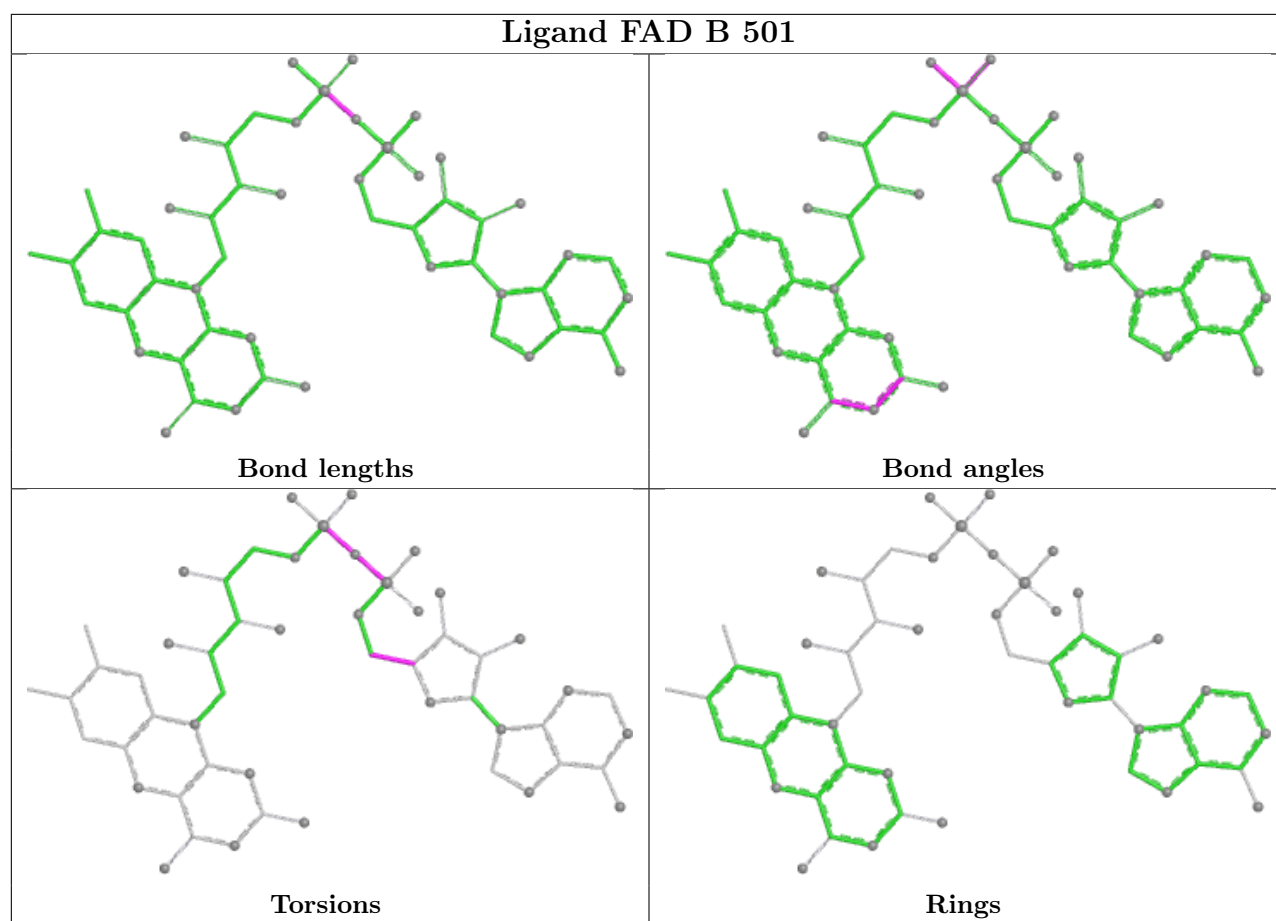
Ligand NXJ A 508



Ligand NXJ B 506







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	485/495 (97%)	0.66	43 (8%) 15 22	10, 48, 81, 114	6 (1%)
1	B	483/495 (97%)	0.37	15 (3%) 51 61	17, 46, 70, 88	6 (1%)
All	All	968/990 (97%)	0.51	58 (5%) 27 36	10, 47, 76, 114	12 (1%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21[A]	TRP	16.4
1	A	94[A]	LYS	11.9
1	A	446[A]	ARG	11.6
1	A	332[A]	LEU	10.7
1	A	387[A]	GLU	10.3
1	B	455	TYR	10.1
1	A	238[A]	VAL	10.0
1	B	484	MET	9.7
1	B	483	LYS	8.6
1	B	485	GLU	8.0
1	B	313	GLU	5.9
1	B	228[A]	ARG	5.3
1	A	296	LEU	4.3
1	A	5	PHE	4.2
1	A	32	ALA	3.9
1	B	399	LEU	3.9
1	A	488	PRO	3.9
1	A	399	LEU	3.8
1	B	396	PHE	3.5
1	A	129	LEU	3.5
1	A	4	ALA	3.4
1	A	300	GLY	3.3
1	A	151	LEU	3.2
1	A	299	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	260	LEU	3.0
1	A	123	PHE	2.9
1	A	346	VAL	2.8
1	B	269	THR	2.8
1	A	109	SER	2.7
1	A	38	THR	2.6
1	B	268	VAL	2.6
1	A	172	ILE	2.6
1	A	306	LYS	2.5
1	B	168	ALA	2.3
1	A	28	GLY	2.3
1	A	134	VAL	2.3
1	A	301	VAL	2.3
1	A	276	LEU	2.3
1	A	305	PRO	2.2
1	A	270	PHE	2.2
1	A	402	ASN	2.2
1	B	258	VAL	2.2
1	A	7	LEU	2.2
1	A	307	GLY	2.2
1	A	264	GLY	2.1
1	A	153	ALA	2.1
1	A	403	ILE	2.1
1	A	135	VAL	2.1
1	A	324	ALA	2.1
1	B	481	GLY	2.1
1	A	31	VAL	2.1
1	A	36	VAL	2.1
1	A	24	ALA	2.1
1	A	396	PHE	2.0
1	B	270	PHE	2.0
1	A	171	GLY	2.0
1	A	27	TYR	2.0
1	A	281	VAL	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

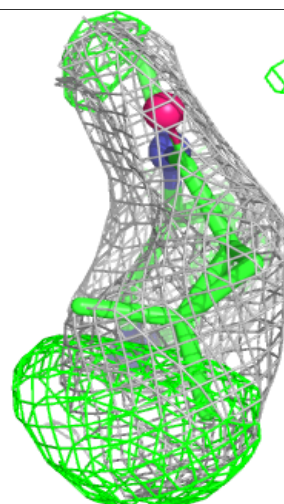
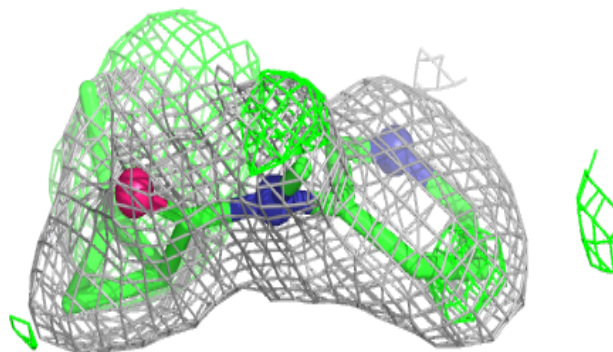
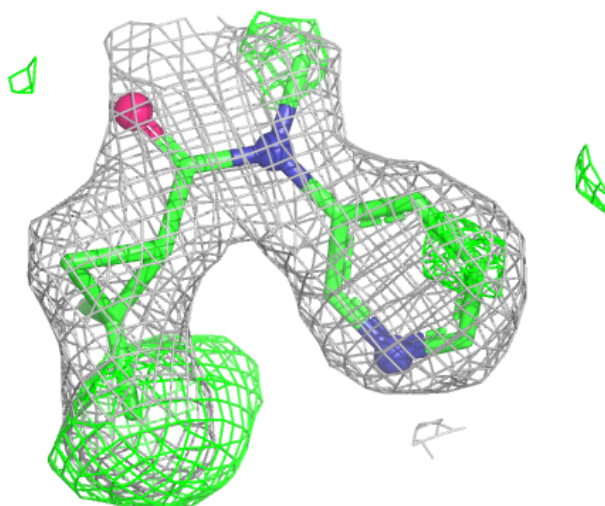
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	A	509	1/1	0.61	0.12	90,90,90,90	0
3	DMS	A	505	4/4	0.70	0.18	83,90,94,104	0
3	DMS	B	503	4/4	0.78	0.18	70,74,75,79	0
3	DMS	B	505	4/4	0.79	0.22	74,87,95,97	0
3	DMS	A	507	4/4	0.83	0.20	71,92,102,110	0
4	NXJ	A	508	15/15	0.86	0.20	43,46,51,51	15
4	NXJ	B	506	15/15	0.86	0.21	45,56,63,63	15
3	DMS	A	504	4/4	0.86	0.14	84,98,100,101	0
3	DMS	A	506	4/4	0.87	0.15	77,83,84,91	0
3	DMS	B	502	4/4	0.88	0.14	71,74,82,87	0
3	DMS	A	503	4/4	0.88	0.14	66,73,74,78	0
3	DMS	B	504	4/4	0.90	0.12	67,71,74,77	0
3	DMS	A	502	4/4	0.91	0.13	63,69,77,78	0
5	MG	B	508	1/1	0.92	0.06	63,63,63,63	0
6	BR	B	507	1/1	0.95	0.12	88,88,88,88	0
2	FAD	A	501	53/53	0.96	0.07	29,38,53,57	0
2	FAD	B	501	53/53	0.97	0.05	30,35,49,52	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.

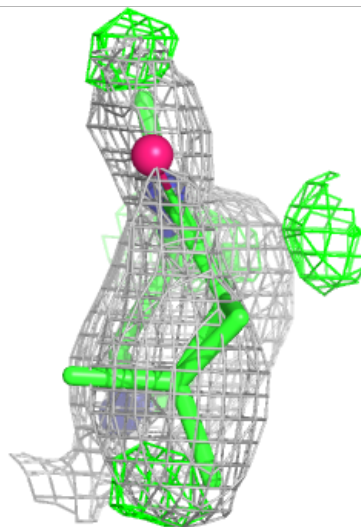
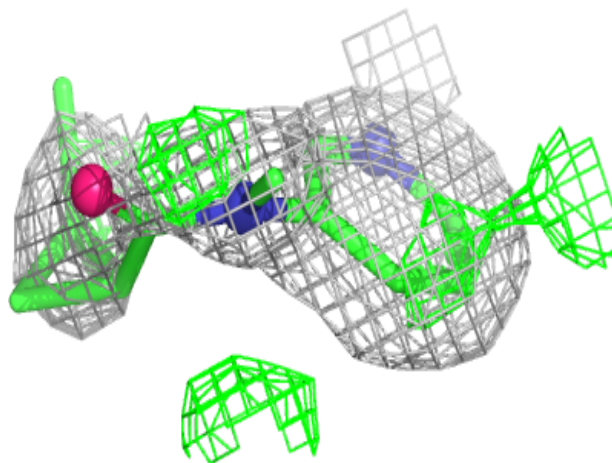
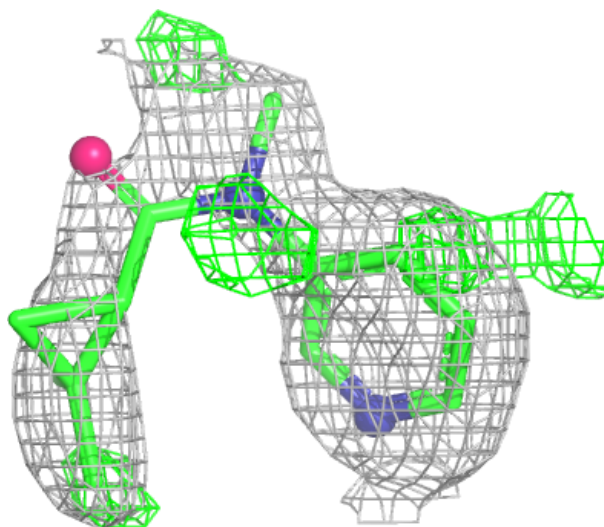
Electron density around NXJ A 508:

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



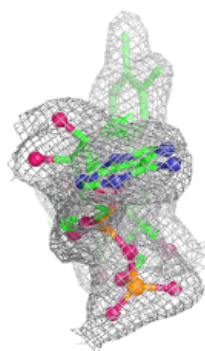
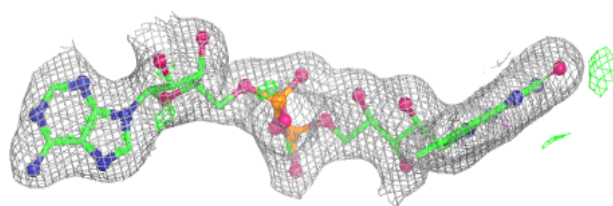
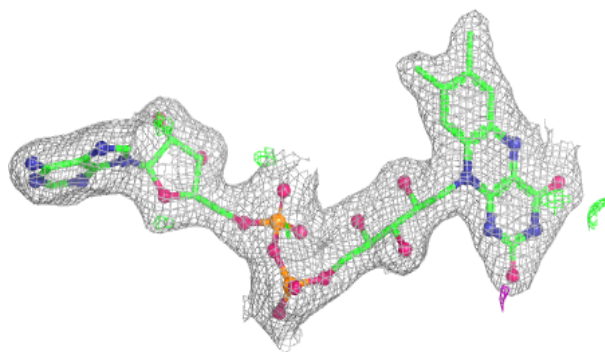
Electron density around NXJ B 506:

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

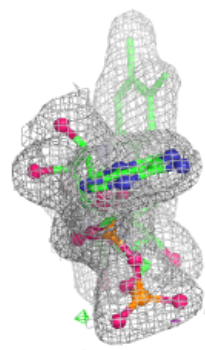
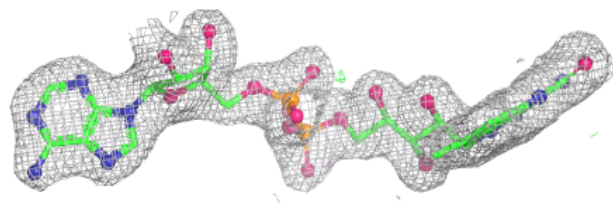
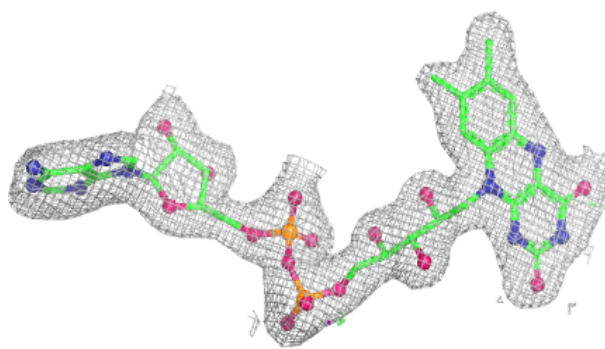


Electron density around FAD A 501:

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

**Electron density around FAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.