



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:10 PM UTC

PDB ID : 9IFL / pdb\_00009ifl  
Title : PANDDA analysis - Crystal structure of Trypanosoma brucei trypanothione reductase in complex with Z319545618  
Authors : Exertier, C.; Antonelli, L.; Ilari, A.; Fiorillo, A.  
Deposited on : 2025-02-18  
Resolution : 1.71 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](mailto: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>.

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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

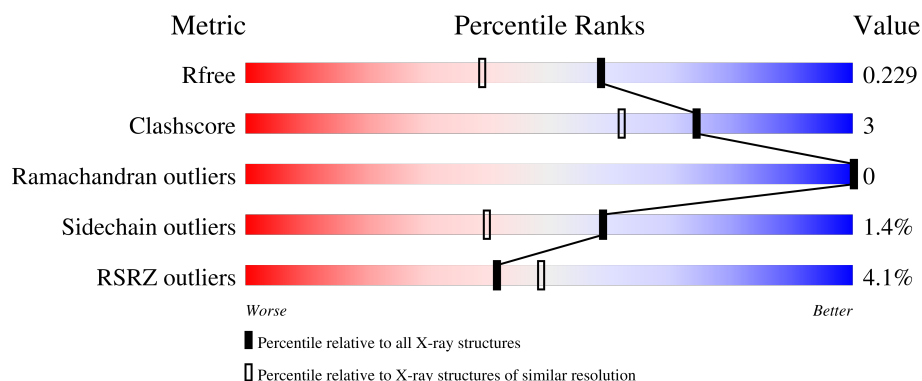
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

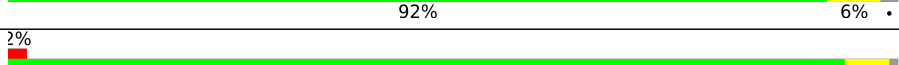
The reported resolution of this entry is 1.71 Å.

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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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  $\geq 3$ , 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	
1	B	495	
1	C	495	
1	D	495	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	A	507	-	-	X	-
4	PEG	B	504	-	-	X	-
6	BR	B	505	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16570 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.

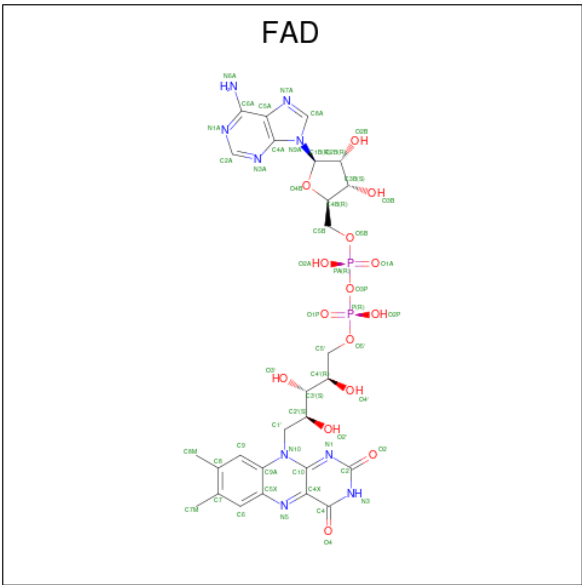
- Molecule 1 is a protein called Trypanothione reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	6	0
			3789	2410	651	706	22			
1	B	488	Total	C	N	O	S	0	6	0
			3793	2413	651	709	20			
1	C	486	Total	C	N	O	S	0	7	0
			3770	2396	643	711	20			
1	D	491	Total	C	N	O	S	0	5	0
			3824	2426	655	722	21			

There are 12 discrepancies between the modelled and reference sequences:

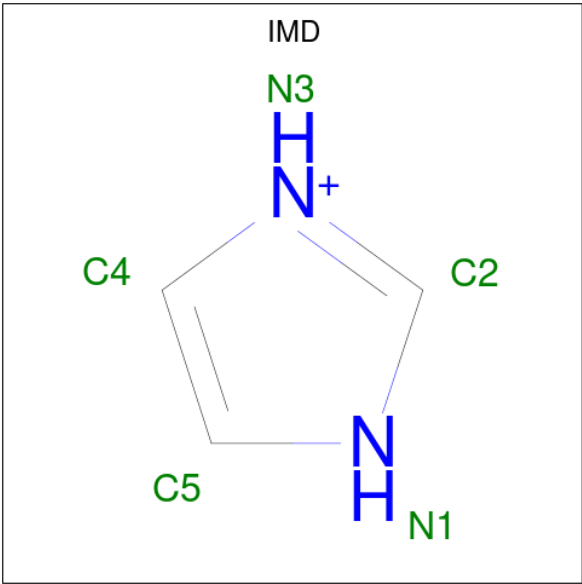
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q389T8
A	-1	SER	-	expression tag	UNP Q389T8
A	0	HIS	-	expression tag	UNP Q389T8
B	-2	GLY	-	expression tag	UNP Q389T8
B	-1	SER	-	expression tag	UNP Q389T8
B	0	HIS	-	expression tag	UNP Q389T8
C	-2	GLY	-	expression tag	UNP Q389T8
C	-1	SER	-	expression tag	UNP Q389T8
C	0	HIS	-	expression tag	UNP Q389T8
D	-2	GLY	-	expression tag	UNP Q389T8
D	-1	SER	-	expression tag	UNP Q389T8
D	0	HIS	-	expression tag	UNP Q389T8

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



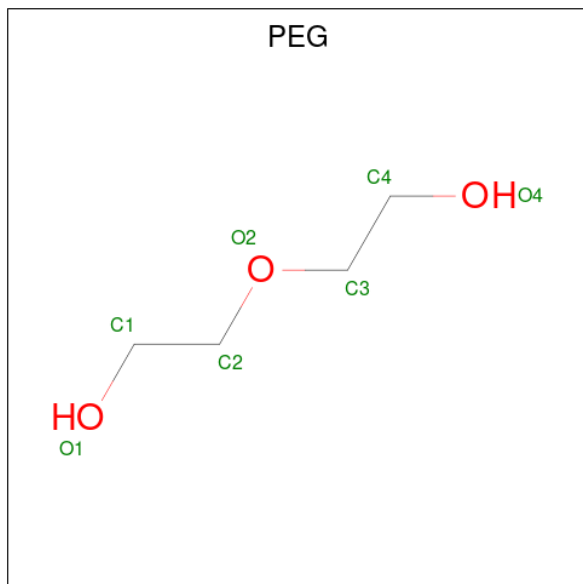
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 5 3 2	0	0
3	A	1	Total C N 5 3 2	0	0
3	B	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0
3	D	1	Total C N 5 3 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



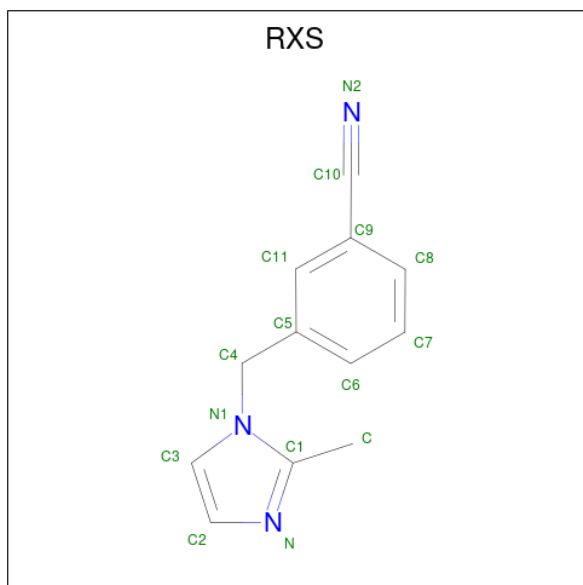
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 3-[(2-methyl-1H-imidazol-1-yl)methyl]benzonitrile (CCD ID: RXS) (formula: C<sub>12</sub>H<sub>11</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			15	12	3		
5	B	1	Total	C	N	0	0
			15	12	3		
5	C	1	Total	C	N	0	0
			15	12	3		
5	D	1	Total	C	N	0	0
			15	12	3		

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

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

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total 1	Na 1	0	0

- Molecule 8 is water.

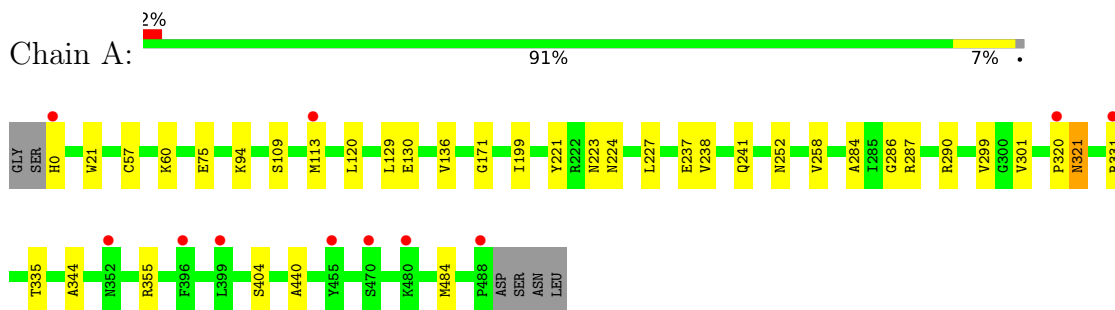
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	305	Total 305	O 305	0	0
8	B	216	Total 216	O 216	0	0
8	C	240	Total 240	O 240	0	0
8	D	279	Total 279	O 279	0	0



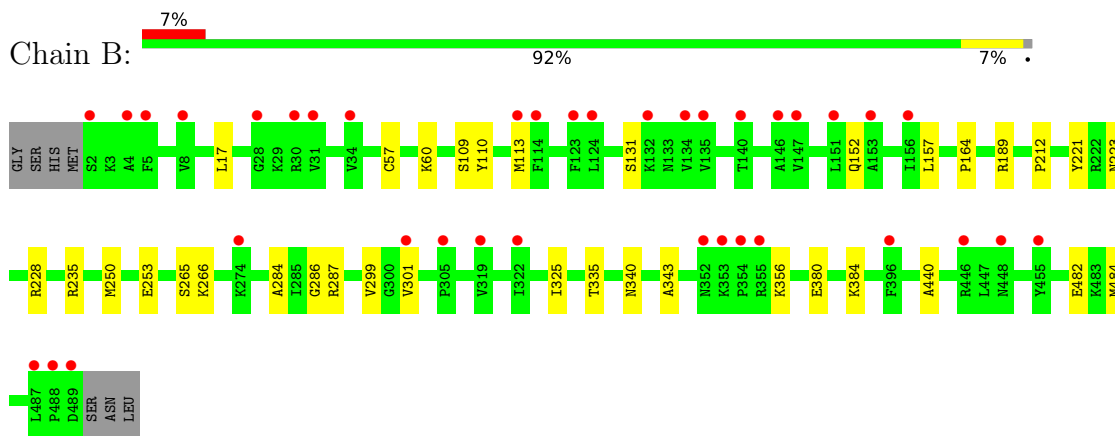
### 3 Residue-property plots

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.

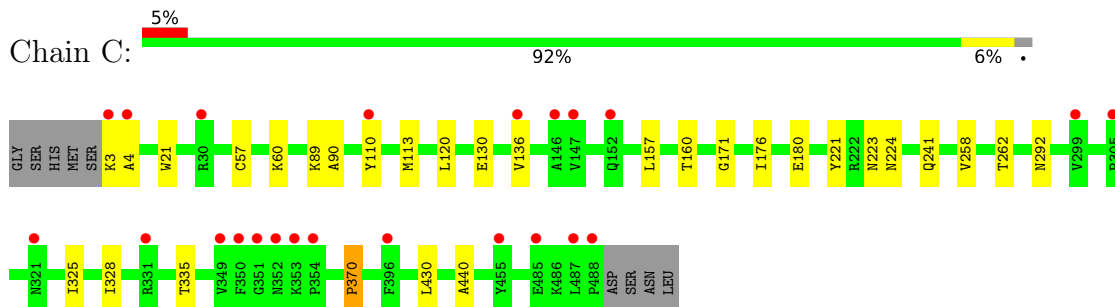
- Molecule 1: Trypanothione reductase



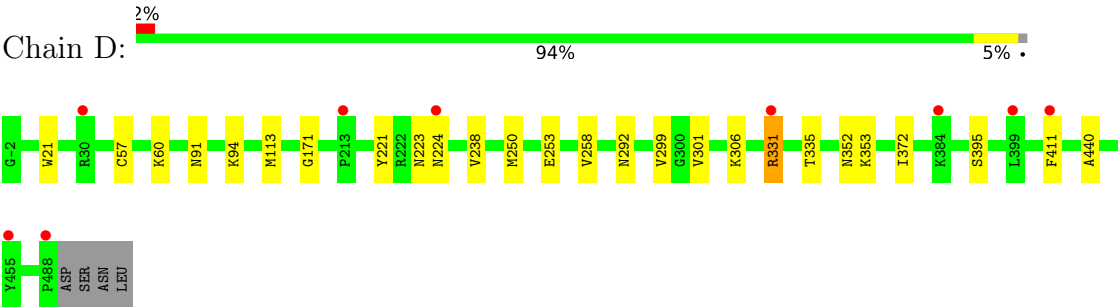
- Molecule 1: Trypanothione reductase



- Molecule 1: Trypanothione reductase



- Molecule 1: Trypanothione reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.00Å 63.83Å 170.25Å 90.00° 97.78° 90.00°	Depositor
Resolution (Å)	84.34 – 1.71 84.34 – 1.71	Depositor EDS
% Data completeness (in resolution range)	97.3 (84.34-1.71) 97.5 (84.34-1.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 1.71Å)	Xtriage
Refinement program	PHENIX 1.21.2	Depositor
R, $R_{free}$	0.194 , 0.229 0.193 , 0.229	Depositor DCC
$R_{free}$ test set	11490 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 31.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16570	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: IMD, NA, PEG, BR, RXS, 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	0.32	0/3879	0.49	0/5257
1	B	0.29	0/3884	0.46	0/5262
1	C	0.31	0/3864	0.49	0/5242
1	D	0.32	0/3910	0.49	0/5300
All	All	0.31	0/15537	0.48	0/21061

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	3789	0	3813	30	0
1	B	3793	0	3825	30	0
1	C	3770	0	3779	20	0
1	D	3824	0	3825	15	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	10	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	5	0	0
3	C	10	0	10	2	0
3	D	5	0	5	0	0
4	A	21	0	30	10	0
4	B	7	0	9	8	0
4	C	14	0	20	0	0
4	D	7	0	10	0	0
5	A	15	0	0	2	0
5	B	15	0	0	4	0
5	C	15	0	0	2	0
5	D	15	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	3	0
7	D	1	0	0	0	0
8	A	305	0	0	4	0
8	B	216	0	0	3	0
8	C	240	0	0	2	0
8	D	279	0	0	1	0
All	All	16570	0	15465	95	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 3.

All (95) 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)
4:B:504:PEG:H22	8:B:626:HOH:O	1.70	0.91
1:A:287:ARG:HG3	4:A:507:PEG:H11	1.64	0.77
1:A:224:ASN:HD22	1:A:252:ASN:HD21	1.35	0.73
1:B:228[B]:ARG:HD3	6:B:505:BR:BR	2.47	0.69
1:B:286:GLY:C	4:B:504:PEG:H42	2.24	0.63
1:D:221:TYR:CE2	1:D:223:ASN:HB2	2.34	0.62
1:A:129:LEU:HD23	1:A:299:VAL:HG21	1.83	0.61
1:B:110:TYR:HD1	5:B:503:RXS:C6	2.13	0.61
1:C:130:GLU:HB2	1:C:136:VAL:CG2	2.32	0.60
1:D:250:MET:HE2	1:D:253:GLU:HG3	1.85	0.59
1:B:340:ASN:HA	8:B:604:HOH:O	2.03	0.59
1:C:370:PRO:HG2	1:C:430:LEU:HD11	1.86	0.58
1:B:284:ALA:C	4:B:504:PEG:H31	2.30	0.56
1:A:94:LYS:HD3	8:A:773:HOH:O	2.06	0.56
1:A:286:GLY:C	4:A:507:PEG:H12	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:ASN:HD22	3:C:506:IMD:H4	1.71	0.55
1:B:343:ALA:HB3	8:B:604:HOH:O	2.06	0.55
1:D:238:VAL:HG21	1:D:372:ILE:HD11	1.89	0.54
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.89	0.54
1:A:221:TYR:CE2	1:A:223:ASN:HB2	2.44	0.53
1:C:440:ALA:HB3	1:D:440:ALA:HB3	1.90	0.53
1:A:355:ARG:NH2	8:A:602:HOH:O	2.41	0.53
1:B:228[B]:ARG:NE	6:B:505:BR:BR	2.97	0.53
1:A:221:TYR:CZ	3:A:506:IMD:H5	2.45	0.52
1:A:320:PRO:O	1:A:321:ASN:OD1	2.27	0.52
1:B:157:LEU:HD11	1:B:325:ILE:HG12	1.90	0.52
1:B:228[B]:ARG:HD3	1:B:235:ARG:HH22	1.76	0.51
1:B:299:VAL:HG23	1:B:301:VAL:HG23	1.93	0.50
1:D:292:ASN:ND2	8:D:602:HOH:O	2.45	0.49
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.95	0.49
1:B:250:MET:HE2	1:B:253:GLU:HG3	1.95	0.49
1:B:228[B]:ARG:CD	6:B:505:BR:BR	3.14	0.48
8:C:601:HOH:O	1:D:91:ASN:ND2	2.47	0.48
1:C:241:GLN:OE1	1:C:370:PRO:HG3	2.14	0.48
1:B:109:SER:O	1:B:113[A]:MET:HE3	2.14	0.47
1:C:120:LEU:HD11	5:C:505:RXS:N2	2.29	0.47
1:A:21:TRP:HB2	5:A:505:RXS:C11	2.44	0.47
1:A:286:GLY:O	4:A:507:PEG:H12	2.13	0.47
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.49	0.47
1:C:110:TYR:CD1	5:C:505:RXS:C6	2.97	0.47
1:A:120:LEU:HD11	5:A:505:RXS:N2	2.30	0.47
1:C:157:LEU:HD11	1:C:325:ILE:HG12	1.96	0.47
1:B:380:GLU:O	1:B:384:LYS:HD2	2.15	0.47
1:B:266:LYS:HD2	1:B:266:LYS:N	2.30	0.47
1:C:292:ASN:H	3:C:506:IMD:H4	1.79	0.47
1:A:344:ALA:HB2	8:A:602:HOH:O	2.14	0.46
1:C:171:GLY:HA3	1:C:258:VAL:O	2.14	0.46
1:D:21:TRP:CE3	1:D:113[B]:MET:SD	3.08	0.46
8:C:601:HOH:O	1:D:94:LYS:HE2	2.16	0.46
1:D:306:LYS:HB3	1:D:306:LYS:HE2	1.68	0.46
1:B:265:SER:C	1:B:266:LYS:HD2	2.41	0.46
1:B:110:TYR:CD1	5:B:503:RXS:C6	2.98	0.46
1:D:395:SER:HA	1:D:411:PHE:O	2.16	0.46
1:B:482:GLU:HG3	1:B:484:MET:HE3	1.97	0.46
1:A:287:ARG:HG3	4:A:507:PEG:C1	2.39	0.45
1:A:290:ARG:HA	8:A:623:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ARG:HG3	4:A:507:PEG:H32	1.98	0.45
1:C:21:TRP:CE3	1:C:113[B]:MET:SD	3.10	0.45
1:D:299:VAL:HG23	1:D:301:VAL:HG23	1.99	0.44
1:C:130:GLU:HB2	1:C:136:VAL:HG23	2.00	0.44
1:A:109:SER:O	1:A:113[A]:MET:HG3	2.18	0.44
1:A:171:GLY:HA3	1:A:258:VAL:O	2.17	0.44
1:A:287:ARG:CG	4:A:507:PEG:H11	2.44	0.43
1:B:110:TYR:HE1	5:B:503:RXS:C4	2.30	0.43
1:B:17:LEU:HD22	5:B:503:RXS:C9	2.48	0.43
1:A:130:GLU:HB2	1:A:136:VAL:HG23	2.00	0.43
1:C:89:LYS:HG3	1:C:90:ALA:N	2.33	0.43
4:A:507:PEG:H11	4:A:507:PEG:H32	1.80	0.43
1:B:286:GLY:CA	4:B:504:PEG:H42	2.49	0.43
1:C:221:TYR:CE2	1:C:223:ASN:HB2	2.54	0.43
1:A:284:ALA:C	4:A:507:PEG:H21	2.44	0.42
1:A:299:VAL:HG23	1:A:301:VAL:HG23	2.01	0.42
1:A:199:ILE:HD12	4:A:507:PEG:H31	2.02	0.42
1:B:228[B]:ARG:HD3	1:B:235:ARG:NH2	2.33	0.42
1:C:176:ILE:HB	1:C:180:GLU:HB2	2.01	0.42
1:B:287:ARG:HG3	4:B:504:PEG:H41	2.01	0.42
1:D:171:GLY:HA3	1:D:258:VAL:O	2.20	0.42
1:C:3:LYS:HG3	1:C:4:ALA:H	1.84	0.41
1:A:199:ILE:HD12	4:A:507:PEG:C3	2.51	0.41
1:B:287:ARG:HG3	4:B:504:PEG:C4	2.50	0.41
1:C:160:THR:OG1	1:C:328:ILE:HD12	2.20	0.41
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.94	0.41
1:B:152:GLN:H	1:B:152:GLN:HG2	1.76	0.41
1:A:237:GLU:O	1:A:241:GLN:HG3	2.21	0.41
1:D:352:ASN:H	1:D:353:LYS:HE2	1.86	0.40
1:C:3:LYS:HE2	1:C:3:LYS:HB2	1.91	0.40
1:A:75:GLU:HB3	1:A:404:SER:HB2	2.02	0.40
1:B:164:PRO:HB3	4:B:504:PEG:C1	2.52	0.40
1:B:164:PRO:HB3	4:B:504:PEG:H11	2.03	0.40
1:C:3:LYS:CG	1:C:4:ALA:H	2.35	0.40
1:A:221:TYR:CZ	3:A:506:IMD:C5	3.05	0.40
1:A:484:MET:HE2	1:A:484:MET:HB3	1.98	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/495 (100%)	481 (97%)	13 (3%)	0	100	100
1	B	496/495 (100%)	483 (97%)	13 (3%)	0	100	100
1	C	495/495 (100%)	483 (98%)	12 (2%)	0	100	100
1	D	500/495 (101%)	485 (97%)	15 (3%)	0	100	100
All	All	1985/1980 (100%)	1932 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/407 (101%)	399 (97%)	11 (3%)	39	17
1	B	411/407 (101%)	406 (99%)	5 (1%)	63	46
1	C	410/407 (101%)	401 (98%)	9 (2%)	45	23
1	D	414/407 (102%)	403 (97%)	11 (3%)	39	17
All	All	1645/1628 (101%)	1609 (98%)	36 (2%)	59	23

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0[A]	HIS
1	A	0[B]	HIS

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Mol	Chain	Res	Type
1	A	57	CYS
1	A	60	LYS
1	A	238	VAL
1	A	321	ASN
1	A	331[A]	ARG
1	A	331[B]	ARG
1	A	331[C]	ARG
1	A	331[D]	ARG
1	A	335	THR
1	B	57	CYS
1	B	60	LYS
1	B	131	SER
1	B	335	THR
1	B	356	LYS
1	C	57	CYS
1	C	60	LYS
1	C	224[A]	ASN
1	C	224[B]	ASN
1	C	224[C]	ASN
1	C	224[D]	ASN
1	C	262	THR
1	C	335	THR
1	C	370	PRO
1	D	57	CYS
1	D	60	LYS
1	D	224[A]	ASN
1	D	224[B]	ASN
1	D	224[C]	ASN
1	D	224[D]	ASN
1	D	331[A]	ARG
1	D	331[B]	ARG
1	D	331[C]	ARG
1	D	331[D]	ARG
1	D	335	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	152	GLN
1	A	223	ASN
1	A	252	ASN

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Mol	Chain	Res	Type
1	A	448	ASN
1	B	107	ASN
1	B	223	ASN
1	B	224	ASN
1	B	252	ASN
1	B	298	ASN
1	C	133	ASN
1	C	223	ASN
1	C	292	ASN
1	C	340	ASN
1	D	22	ASN
1	D	152	GLN
1	D	223	ASN
1	D	252	ASN
1	D	321	ASN
1	D	340	ASN
1	D	352	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 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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	IMD	B	502	-	5,5,5	0.31	0	5,5,5	0.81	0
3	IMD	D	502	-	5,5,5	0.32	0	5,5,5	0.79	0
5	RXS	D	504	-	16,16,16	0.18	0	19,21,21	0.56	0
3	IMD	C	502	-	5,5,5	0.26	0	5,5,5	0.84	0
4	PEG	C	503	-	6,6,6	0.24	0	5,5,5	0.32	0
2	FAD	C	501	-	58,58,58	0.93	2 (3%)	85,89,89	0.94	5 (5%)
4	PEG	A	504	-	6,6,6	0.25	0	5,5,5	0.21	0
5	RXS	A	505	-	16,16,16	0.18	0	19,21,21	0.52	0
3	IMD	C	506	-	5,5,5	0.32	0	5,5,5	0.79	0
3	IMD	A	506	-	5,5,5	0.37	0	5,5,5	0.88	0
4	PEG	B	504	-	6,6,6	0.59	0	5,5,5	1.70	1 (20%)
4	PEG	A	503	-	6,6,6	0.26	0	5,5,5	0.21	0
4	PEG	D	503	-	6,6,6	0.26	0	5,5,5	0.31	0
3	IMD	A	502	-	5,5,5	0.27	0	5,5,5	0.84	0
5	RXS	C	505	-	16,16,16	0.21	0	19,21,21	0.52	0
4	PEG	C	504	-	6,6,6	0.24	0	5,5,5	0.23	0
4	PEG	A	507	-	6,6,6	0.56	0	5,5,5	1.01	0
2	FAD	A	501	-	58,58,58	0.93	2 (3%)	85,89,89	0.98	5 (5%)
2	FAD	D	501	-	58,58,58	0.96	2 (3%)	85,89,89	0.95	5 (5%)
5	RXS	B	503	-	16,16,16	0.16	0	19,21,21	0.46	0
2	FAD	B	501	-	58,58,58	0.98	2 (3%)	85,89,89	0.83	2 (2%)

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	IMD	B	502	-	-	-	0/1/1/1
3	IMD	D	502	-	-	-	0/1/1/1
5	RXS	D	504	-	-	0/6/6/6	0/2/2/2
3	IMD	C	502	-	-	-	0/1/1/1
4	PEG	C	503	-	-	1/4/4/4	-
2	FAD	C	501	-	-	5/34/50/50	0/6/6/6
4	PEG	A	504	-	-	4/4/4/4	-
5	RXS	A	505	-	-	0/6/6/6	0/2/2/2
3	IMD	C	506	-	-	-	0/1/1/1
3	IMD	A	506	-	-	-	0/1/1/1
4	PEG	B	504	-	-	3/4/4/4	-
4	PEG	A	503	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	D	503	-	-	3/4/4/4	-
3	IMD	A	502	-	-	-	0/1/1/1
5	RXS	C	505	-	-	0/6/6/6	0/2/2/2
4	PEG	C	504	-	-	2/4/4/4	-
4	PEG	A	507	-	-	0/4/4/4	-
2	FAD	A	501	-	-	3/34/50/50	0/6/6/6
2	FAD	D	501	-	-	5/34/50/50	0/6/6/6
5	RXS	B	503	-	-	0/6/6/6	0/2/2/2
2	FAD	B	501	-	-	5/34/50/50	0/6/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FAD	P-O3P	4.22	1.64	1.59
2	B	501	FAD	P-O3P	4.20	1.64	1.59
2	D	501	FAD	P-O3P	4.05	1.63	1.59
2	A	501	FAD	P-O3P	3.68	1.63	1.59
2	D	501	FAD	PA-O3P	2.69	1.62	1.59
2	A	501	FAD	PA-O3P	2.56	1.62	1.59
2	B	501	FAD	PA-O3P	2.53	1.62	1.59
2	C	501	FAD	PA-O3P	2.43	1.62	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	FAD	O2P-P-O1P	3.04	126.57	112.44
2	A	501	FAD	C2B-C1B-N9A	2.96	120.66	113.30
2	D	501	FAD	O2P-P-O1P	2.86	125.73	112.44
2	A	501	FAD	O2P-P-O1P	2.75	125.23	112.44
4	B	504	PEG	C3-O2-C2	-2.72	101.34	113.26
2	D	501	FAD	O2P-P-O3P	-2.69	99.99	107.27
2	D	501	FAD	O3P-PA-O1A	-2.50	103.20	110.70
2	D	501	FAD	O2A-PA-O1A	2.44	123.78	112.44
2	C	501	FAD	C10-N1-C2	2.40	122.05	116.85
2	C	501	FAD	O3P-PA-O1A	-2.40	103.48	110.70
2	A	501	FAD	O2'-C2'-C3'	2.34	114.73	109.25
2	B	501	FAD	O2P-P-O1P	2.29	123.10	112.44
2	C	501	FAD	O2A-PA-O1A	2.27	123.02	112.44
2	A	501	FAD	O2A-PA-O1A	2.19	122.62	112.44
2	B	501	FAD	O2A-PA-O1A	2.15	122.43	112.44
2	D	501	FAD	O4B-C1B-N9A	-2.14	103.98	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	O3P-PA-O1A	-2.12	104.34	110.70
2	C	501	FAD	C2B-C1B-N9A	2.07	118.44	113.30

There are no chirality outliers.

All (33) torsion outliers are listed below:

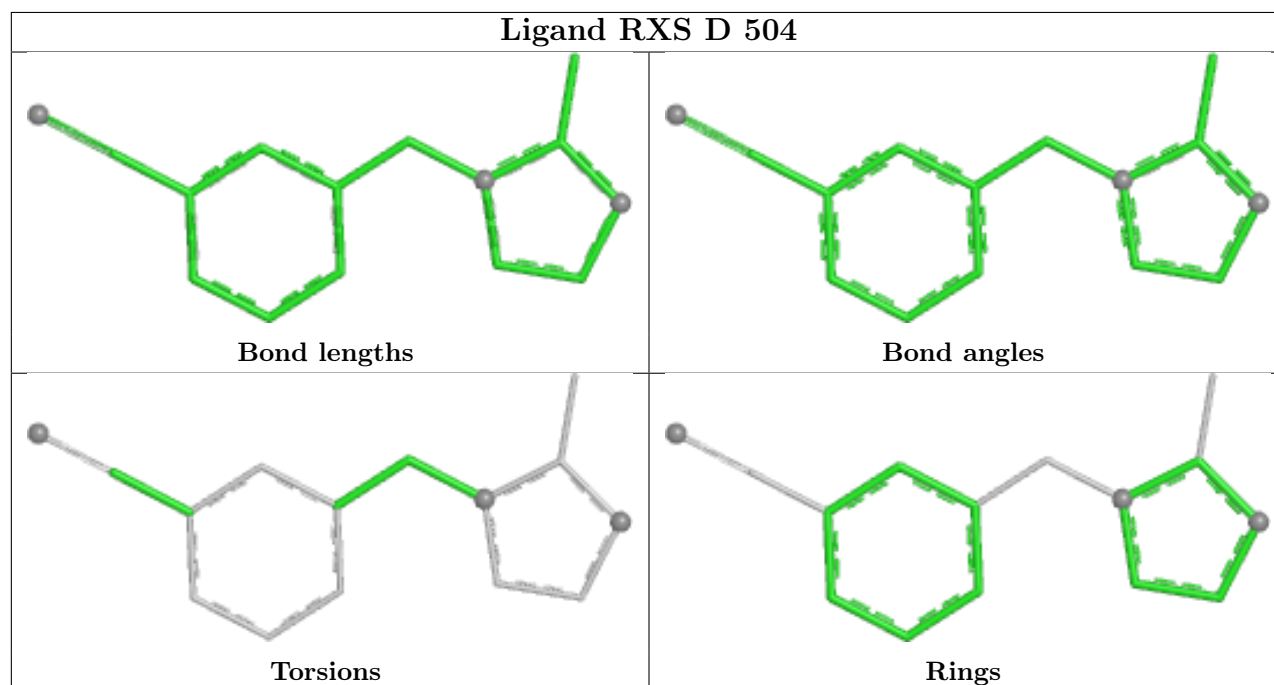
Mol	Chain	Res	Type	Atoms
4	C	504	PEG	O2-C3-C4-O4
4	A	504	PEG	O1-C1-C2-O2
4	A	504	PEG	O2-C3-C4-O4
4	B	504	PEG	O1-C1-C2-O2
4	C	504	PEG	O1-C1-C2-O2
2	C	501	FAD	O4B-C4B-C5B-O5B
4	D	503	PEG	C4-C3-O2-C2
2	B	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	PA-O3P-P-O5'
2	D	501	FAD	PA-O3P-P-O5'
4	D	503	PEG	C1-C2-O2-C3
4	A	504	PEG	C4-C3-O2-C2
2	A	501	FAD	P-O3P-PA-O2A
2	C	501	FAD	P-O3P-PA-O2A
2	D	501	FAD	P-O3P-PA-O2A
4	B	504	PEG	C4-C3-O2-C2
2	C	501	FAD	C3B-C4B-C5B-O5B
4	A	503	PEG	C1-C2-O2-C3
4	A	503	PEG	O2-C3-C4-O4
4	D	503	PEG	O2-C3-C4-O4
2	D	501	FAD	O4B-C4B-C5B-O5B
4	B	504	PEG	C1-C2-O2-C3
2	B	501	FAD	C3B-C4B-C5B-O5B
4	A	504	PEG	C1-C2-O2-C3
4	C	503	PEG	C4-C3-O2-C2
2	A	501	FAD	P-O3P-PA-O1A
2	B	501	FAD	P-O3P-PA-O2A
2	C	501	FAD	P-O3P-PA-O1A
2	D	501	FAD	P-O3P-PA-O1A
2	D	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	PA-O3P-P-O2P

There are no ring outliers.

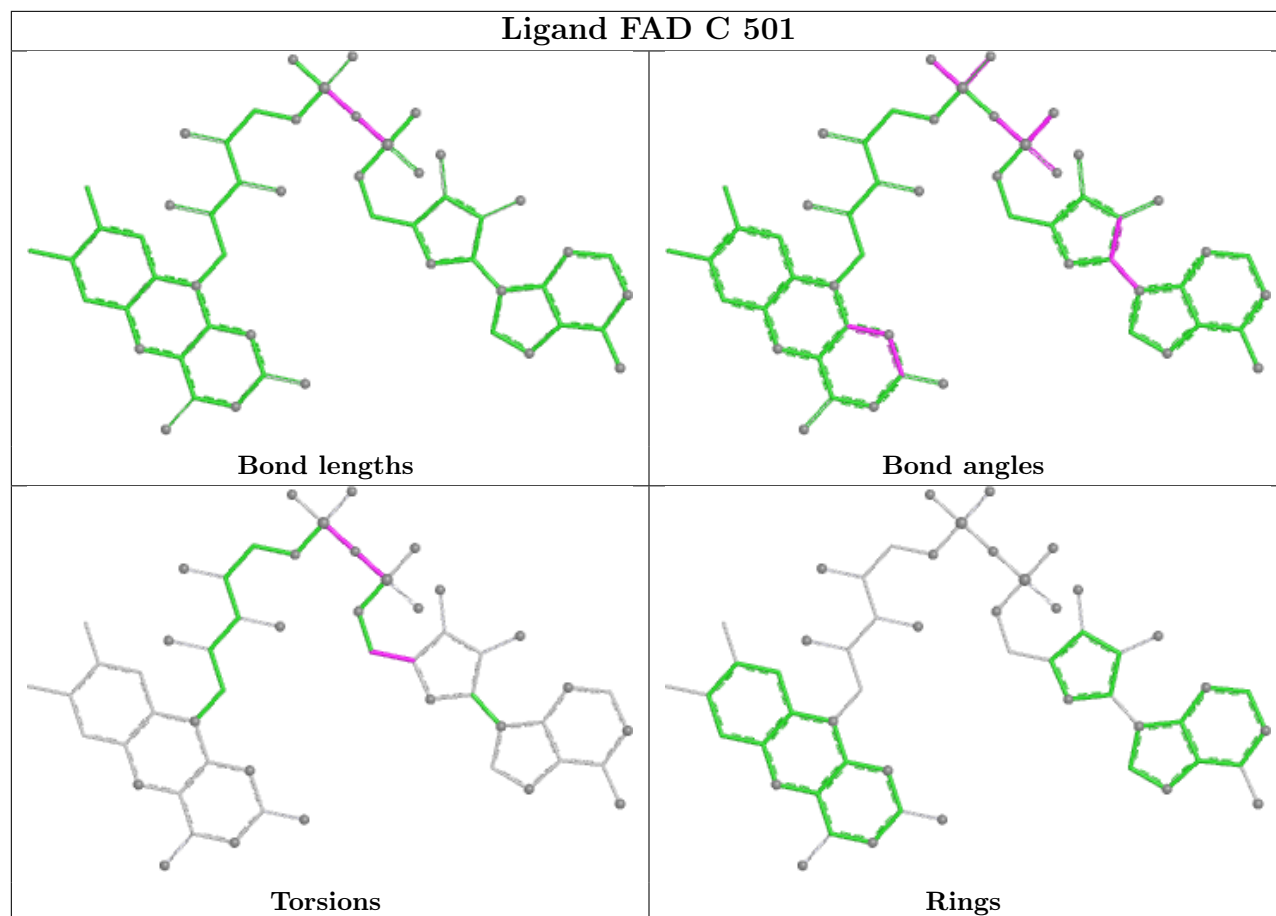
7 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	RXS	2	0
3	C	506	IMD	2	0
3	A	506	IMD	2	0
4	B	504	PEG	8	0
5	C	505	RXS	2	0
4	A	507	PEG	10	0
5	B	503	RXS	4	0

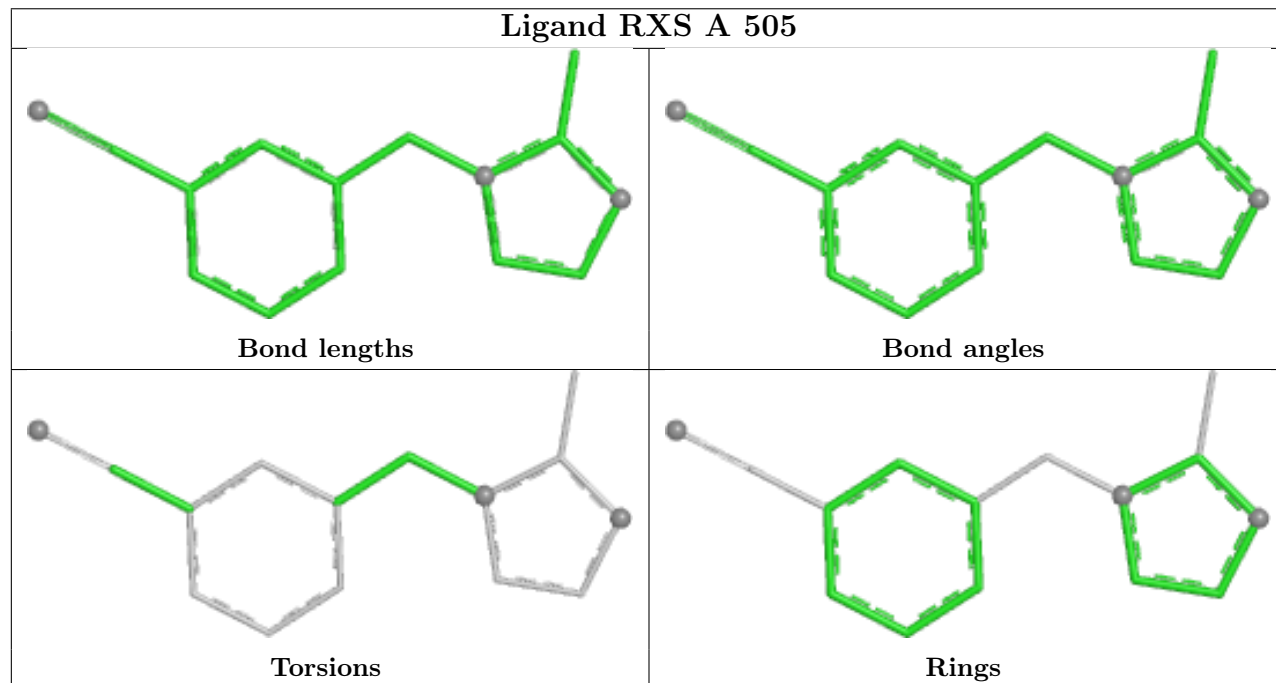
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

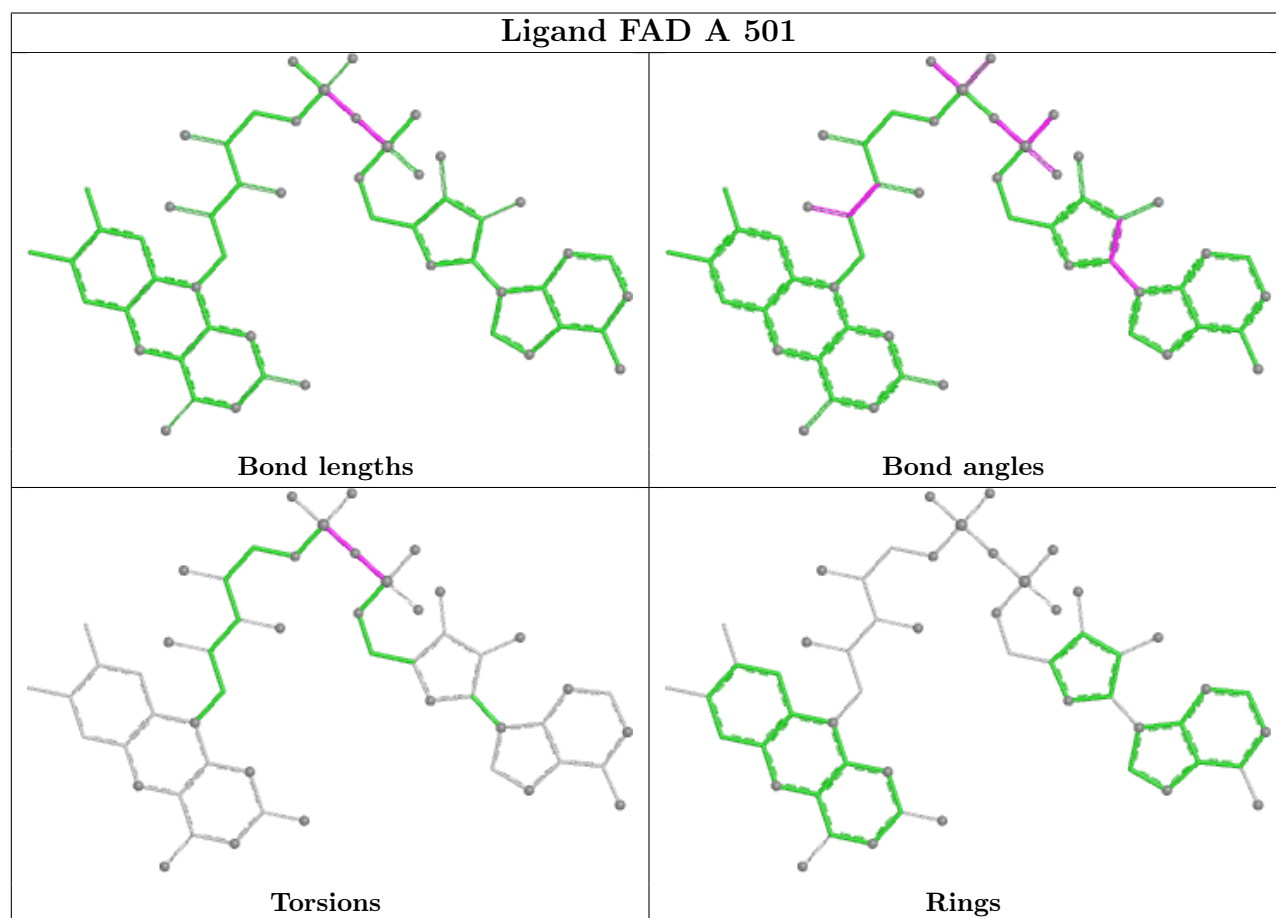
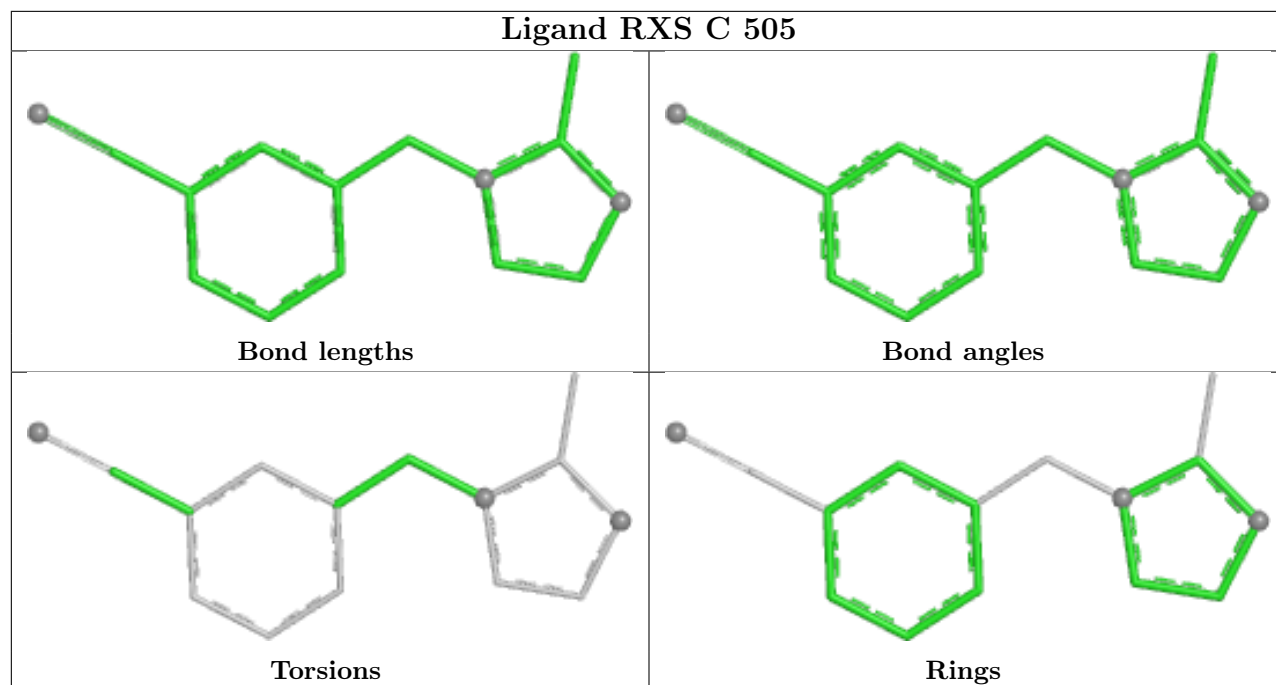


## Ligand FAD C 501



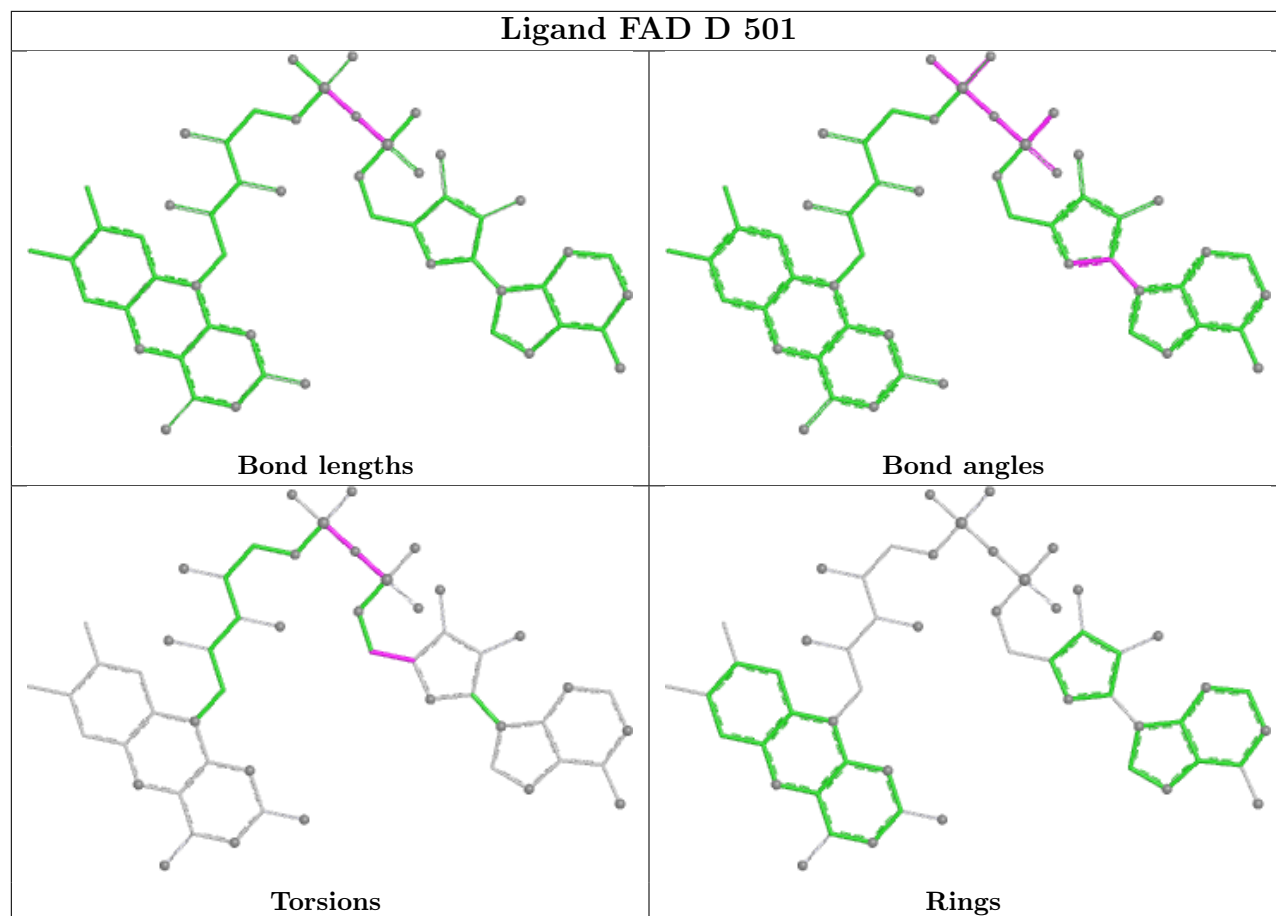
## Ligand RXS A 505



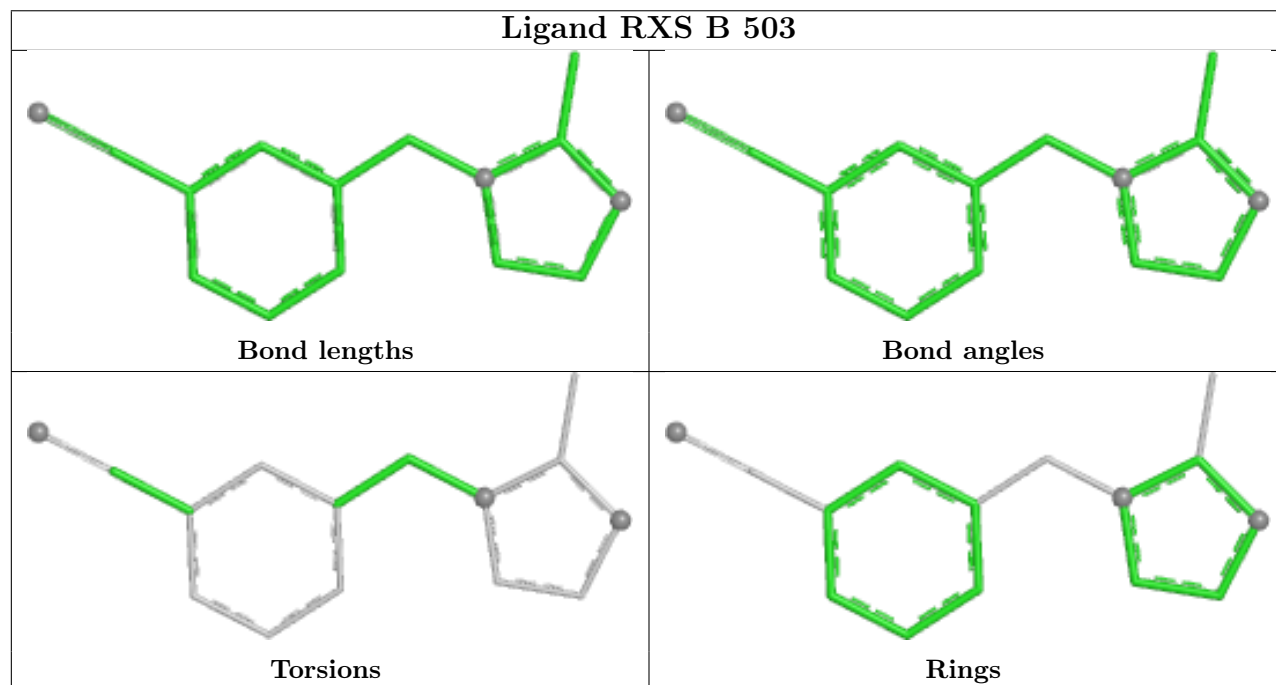


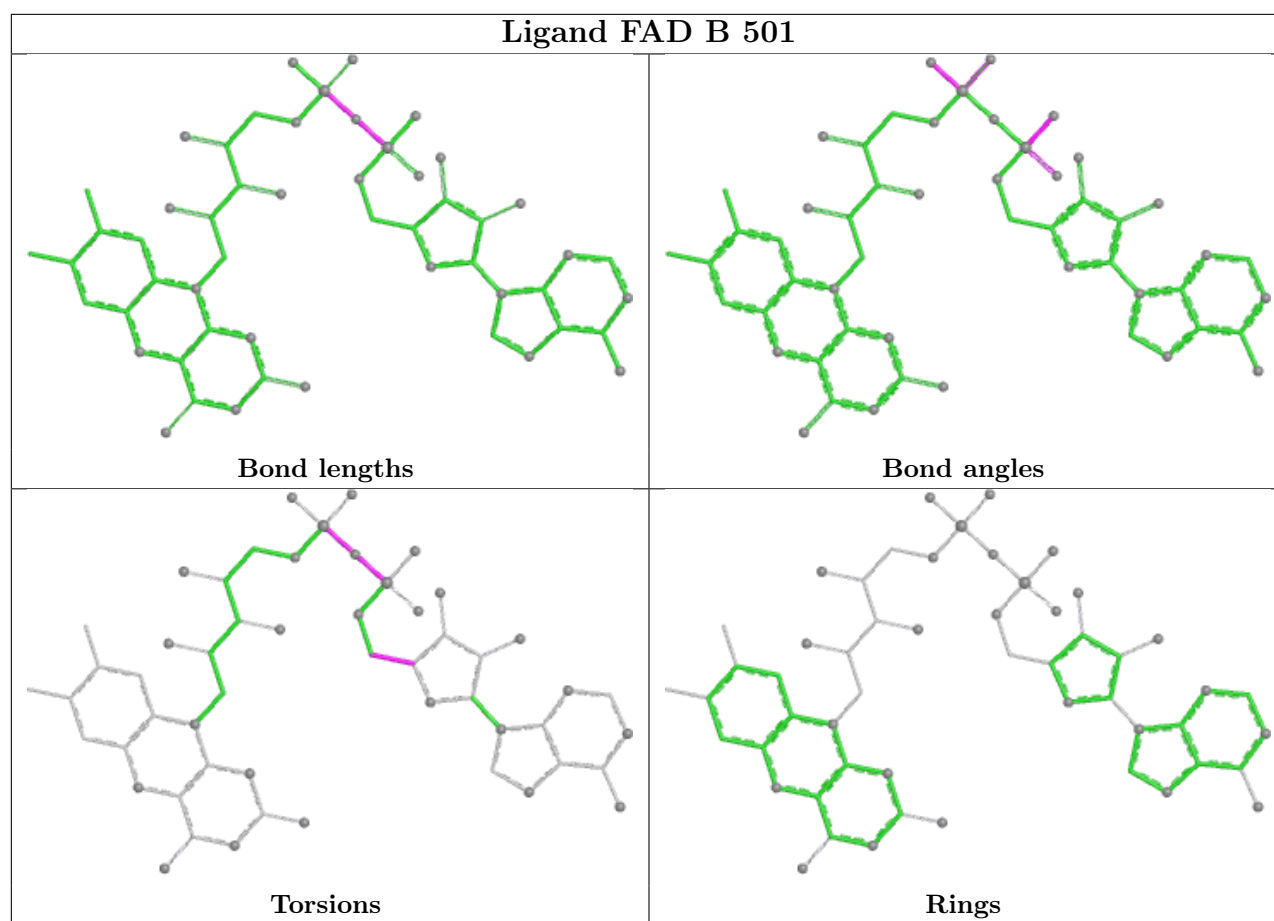


## Ligand FAD D 501



## Ligand RXS B 503





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	489/495 (98%)	0.12	11 (2%) 62 70	9, 32, 48, 77	6 (1%)
1	B	488/495 (98%)	0.54	37 (7%) 20 25	9, 36, 59, 91	6 (1%)
1	C	486/495 (98%)	0.39	23 (4%) 36 42	9, 34, 57, 89	7 (1%)
1	D	491/495 (99%)	0.18	9 (1%) 67 74	10, 32, 49, 71	5 (1%)
All	All	1954/1980 (98%)	0.31	80 (4%) 41 49	9, 34, 55, 91	24 (1%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0[A]	HIS	4.6
1	B	488	PRO	4.3
1	A	396	PHE	4.0
1	C	396	PHE	3.9
1	D	224[A]	ASN	3.9
1	B	455[A]	TYR	3.7
1	B	352	ASN	3.7
1	D	331[A]	ARG	3.5
1	B	4	ALA	3.4
1	B	446[A]	ARG	3.4
1	B	274[A]	LYS	3.3
1	A	488	PRO	3.3
1	A	331[A]	ARG	3.3
1	C	455[A]	TYR	3.2
1	D	488	PRO	3.2
1	B	124	LEU	3.2
1	A	352	ASN	3.1
1	B	147	VAL	3.1
1	B	487	LEU	3.0
1	B	146	ALA	3.0
1	B	30	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	34	VAL	2.8
1	C	305	PRO	2.8
1	B	2	SER	2.8
1	B	354	PRO	2.7
1	C	353	LYS	2.6
1	A	455[A]	TYR	2.6
1	B	153	ALA	2.6
1	C	488	PRO	2.6
1	B	319	VAL	2.5
1	D	30	ARG	2.5
1	C	321[A]	ASN	2.5
1	B	151	LEU	2.5
1	B	156	ILE	2.5
1	A	480	LYS	2.4
1	B	489	ASP	2.4
1	D	384	LYS	2.4
1	A	113[A]	MET	2.4
1	C	352	ASN	2.3
1	B	301	VAL	2.3
1	C	136	VAL	2.3
1	A	470	SER	2.3
1	C	351	GLY	2.3
1	A	320	PRO	2.3
1	C	3	LYS	2.3
1	B	5	PHE	2.3
1	B	123	PHE	2.3
1	B	353	LYS	2.3
1	B	113[A]	MET	2.3
1	D	213	PRO	2.3
1	C	331	ARG	2.3
1	C	349	VAL	2.3
1	C	354	PRO	2.2
1	C	4	ALA	2.2
1	B	448	ASN	2.2
1	C	350	PHE	2.2
1	C	152	GLN	2.2
1	B	31	VAL	2.2
1	B	396	PHE	2.2
1	C	30	ARG	2.2
1	B	355	ARG	2.2
1	B	8	VAL	2.1
1	B	134	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	135	VAL	2.1
1	A	399	LEU	2.1
1	D	411	PHE	2.1
1	B	322	ILE	2.1
1	D	455[A]	TYR	2.1
1	C	146	ALA	2.1
1	C	147	VAL	2.1
1	C	487	LEU	2.1
1	B	140	THR	2.1
1	C	110	TYR	2.1
1	B	28	GLY	2.0
1	C	299	VAL	2.0
1	D	399	LEU	2.0
1	B	305	PRO	2.0
1	C	485	GLU	2.0
1	B	114	PHE	2.0
1	B	132	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	IMD	A	506	5/5	0.62	0.24	61,62,66,68	0
5	RXS	A	505	15/15	0.63	0.38	34,41,47,49	15
5	RXS	C	505	15/15	0.67	0.33	40,45,51,54	15
3	IMD	D	502	5/5	0.69	0.26	61,65,75,82	0
5	RXS	D	504	15/15	0.70	0.24	26,33,40,40	15
3	IMD	C	506	5/5	0.72	0.20	54,60,68,73	0

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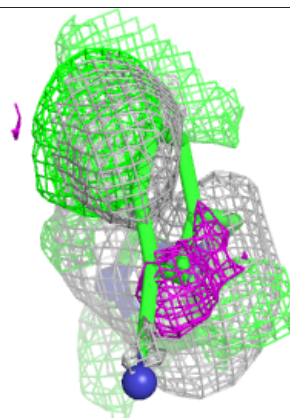
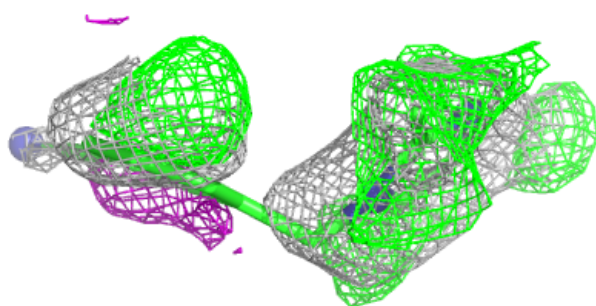
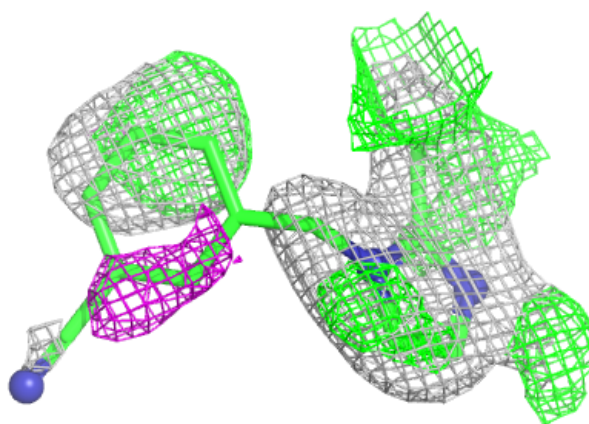
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	RXS	B	503	15/15	0.72	0.29	35,43,52,52	15
4	PEG	A	503	7/7	0.74	0.23	67,72,75,76	0
4	PEG	C	503	7/7	0.74	0.19	48,60,82,82	0
3	IMD	C	502	5/5	0.74	0.18	49,52,61,67	0
3	IMD	A	502	5/5	0.78	0.18	66,68,73,76	0
4	PEG	D	503	7/7	0.80	0.19	54,69,78,80	0
4	PEG	C	504	7/7	0.82	0.15	71,71,74,79	0
4	PEG	A	504	7/7	0.82	0.16	49,55,67,70	0
3	IMD	B	502	5/5	0.84	0.15	49,52,63,65	0
6	BR	A	508	1/1	0.86	0.26	103,103,103,103	0
4	PEG	B	504	7/7	0.91	0.13	23,34,46,53	0
6	BR	B	505	1/1	0.91	0.16	99,99,99,99	0
4	PEG	A	507	7/7	0.94	0.12	22,30,51,52	0
2	FAD	C	501	53/53	0.97	0.06	22,30,36,41	0
2	FAD	B	501	53/53	0.97	0.07	23,30,41,43	0
2	FAD	D	501	53/53	0.98	0.04	19,25,28,30	0
2	FAD	A	501	53/53	0.98	0.05	19,24,28,30	0
7	NA	D	505	1/1	0.98	0.10	30,30,30,30	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.

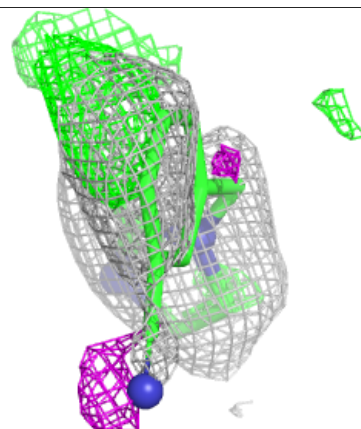
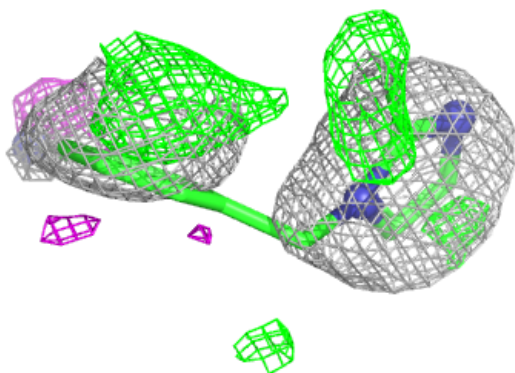
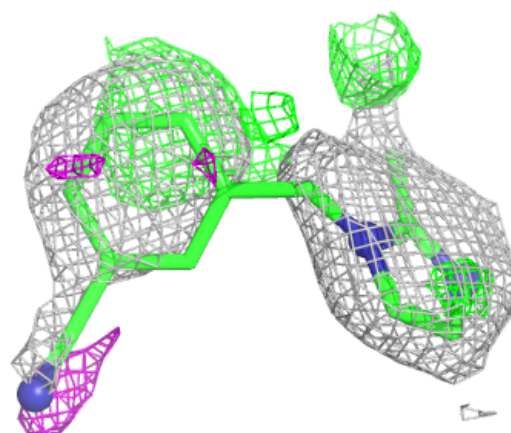
**Electron density around RXS A 505:**

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



**Electron density around RXS C 505:**

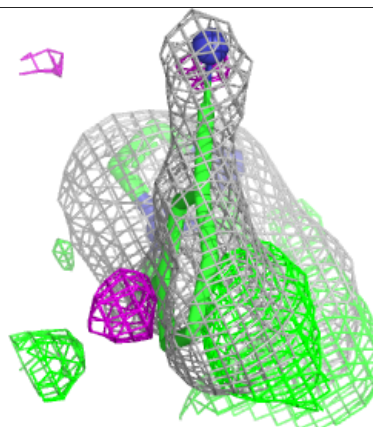
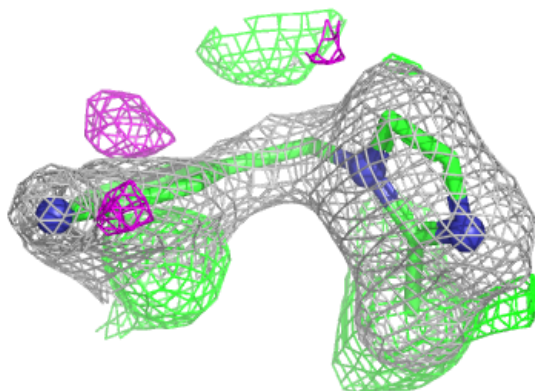
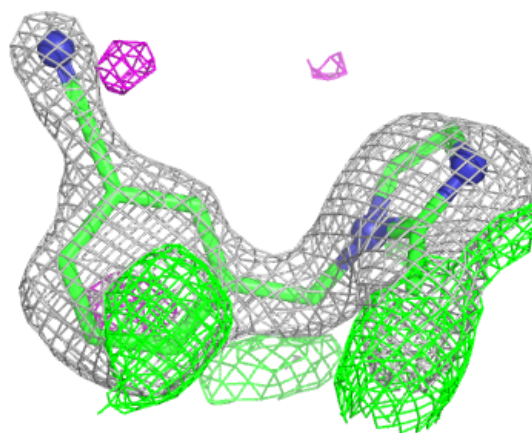
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





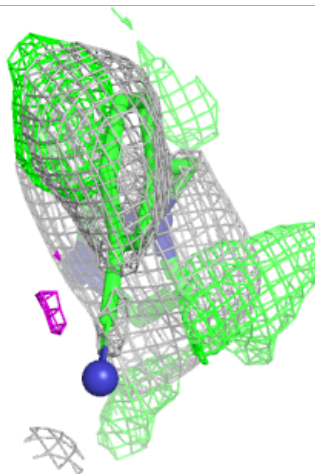
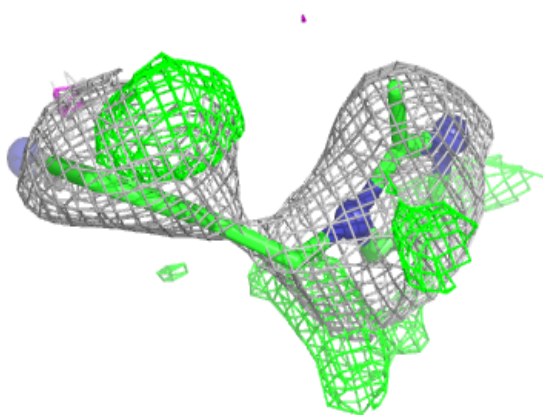
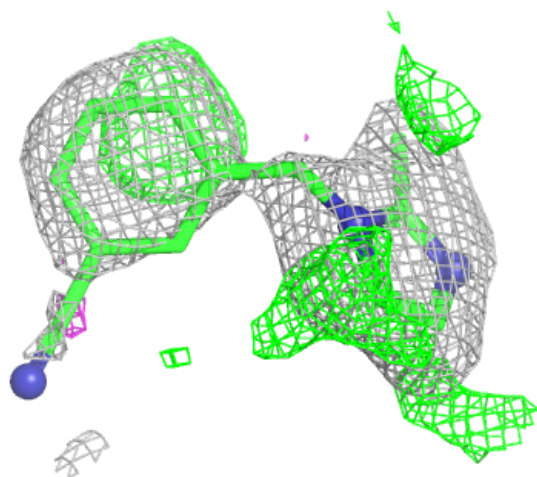
**Electron density around RXS D 504:**

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



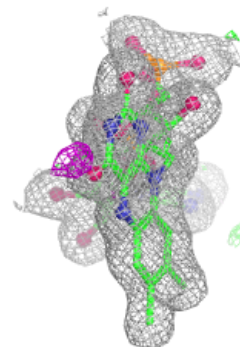
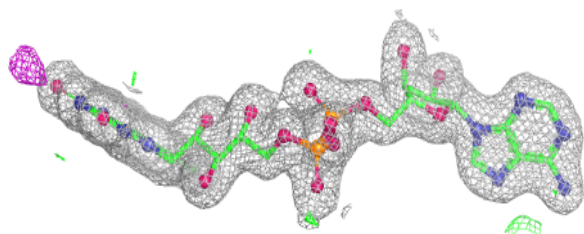
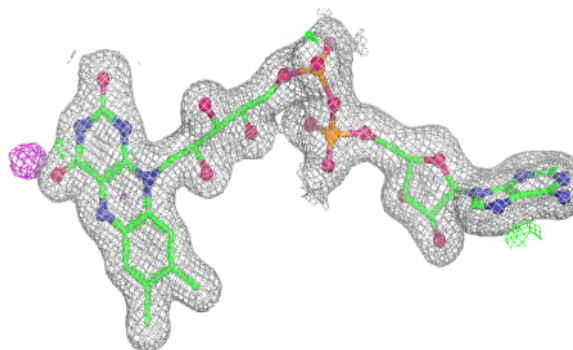
**Electron density around RXS B 503:**

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

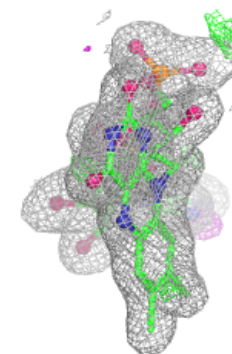
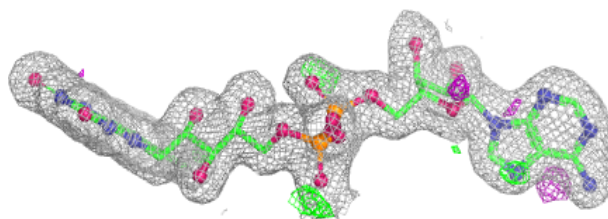
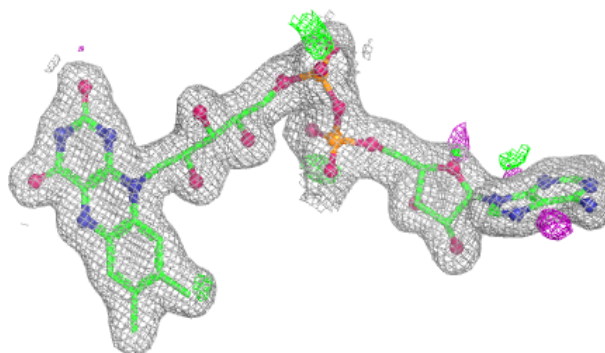


**Electron density around FAD C 501:**

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

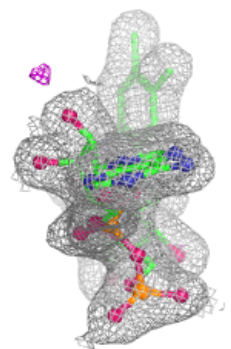
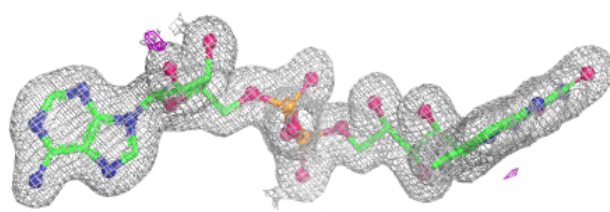
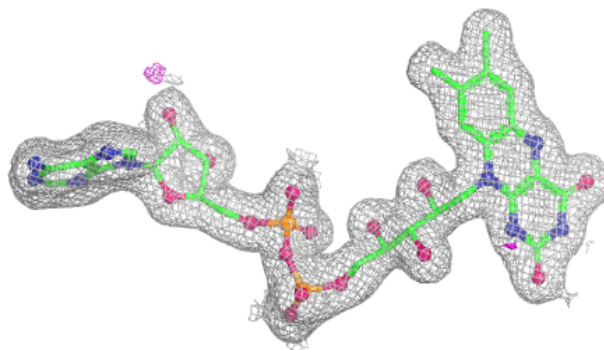
**Electron density around FAD B 501:**

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

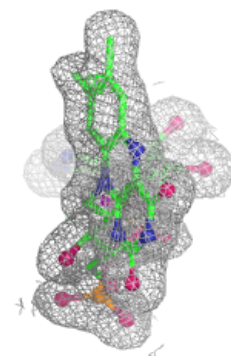
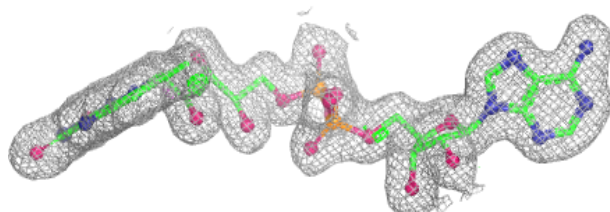
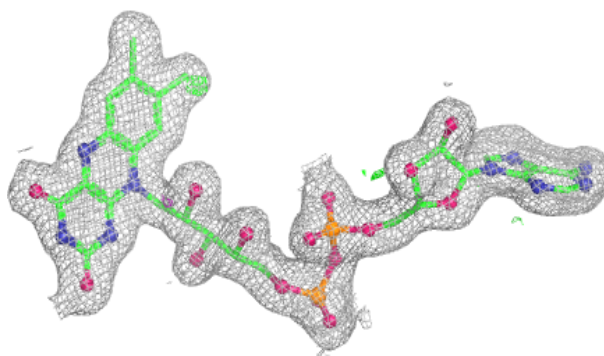


**Electron density around FAD D 501:**

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

**Electron density around 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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.