



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:58 pm BST

PDB ID : 6BU7  
Title : Crystal structure of Trypanothione Reductase from Trypanosoma brucei in complex with inhibitor RD130 1-[2-(Piperidin-4-yl)ethyl]-5-{5-[1-(pyrrolidin-1-yl)cyclohexyl]-1,3-thiazol-2-yl}-1H-indole  
Authors : Bryson, S.; De Gasparo, R.; Krauth-Siegel, R.L.; Diederich, F.; Pai, E.F.  
Deposited on : 2017-12-08  
Resolution : 2.73 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

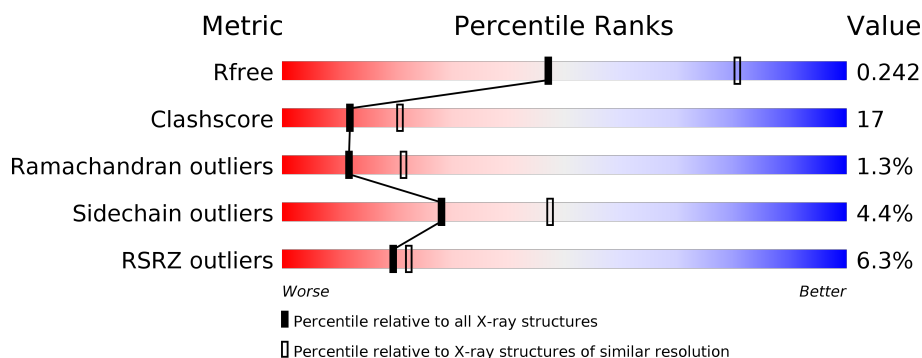
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 on 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	

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	RD0	A	505	-	-	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7791 atoms, of which 49 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.

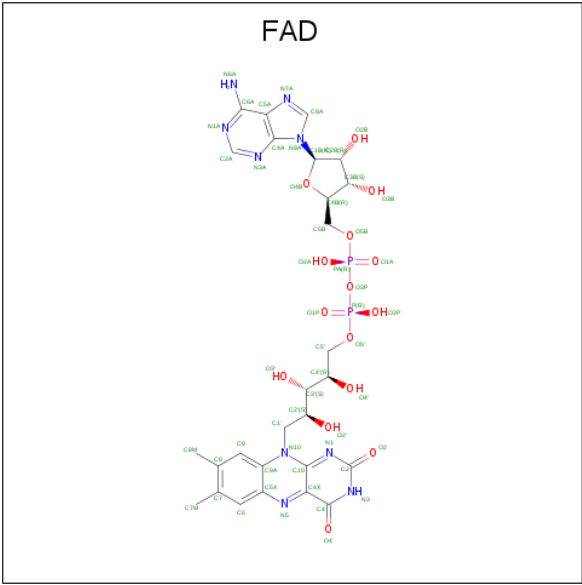
- Molecule 1 is a protein called Trypanothione reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3736	2375	634	707	20			
1	B	492	Total	C	N	O	S	0	0	0
			3736	2375	634	707	20			

There are 6 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

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



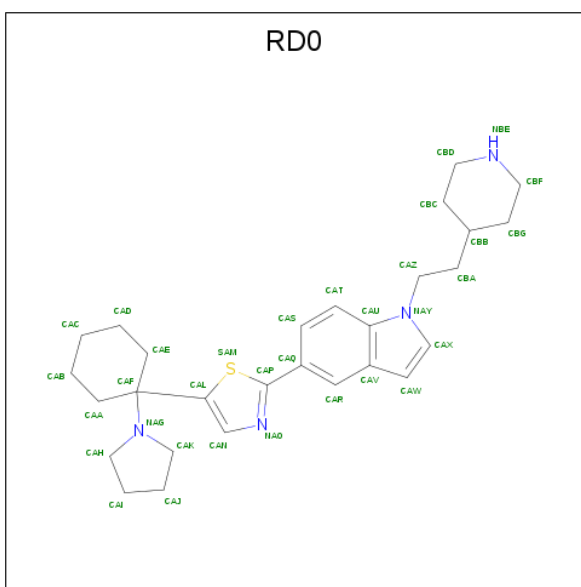
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



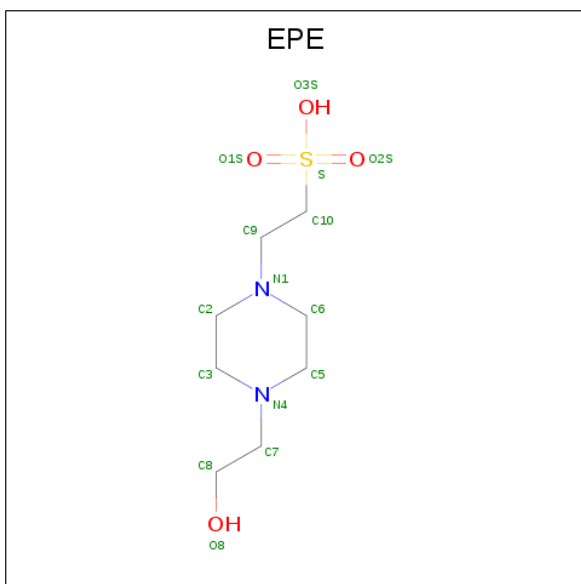
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1-[2-(piperidin-4-yl)ethyl]-5-{5-[1-(pyrrolidin-1-yl)cyclohexyl]-1,3-thiazol-2-yl}-1H-indole (three-letter code: RD0) (formula: C<sub>28</sub>H<sub>38</sub>N<sub>4</sub>S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			33	28	4	1		
4	B	1	Total	C	N	S	0	0
			33	28	4	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	S	
			32	8	17	2	4	1	
								0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O		
			14	3	8	3		
6	B	1	Total	C	H	O		
			14	3	8	3		
6	B	1	Total	C	H	O		
			14	3	8	3		
6	B	1	Total	C	H	O		
			14	3	8	3		

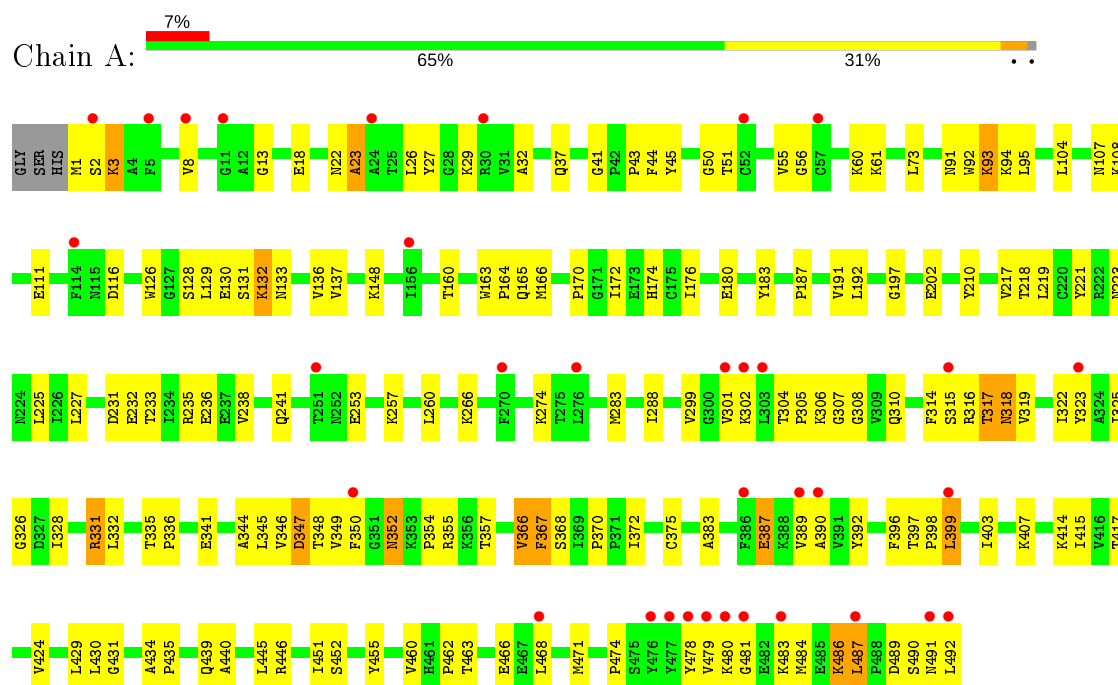
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	8	Total	O		
			8	8		
7	B	11	Total	O		
			11	11		

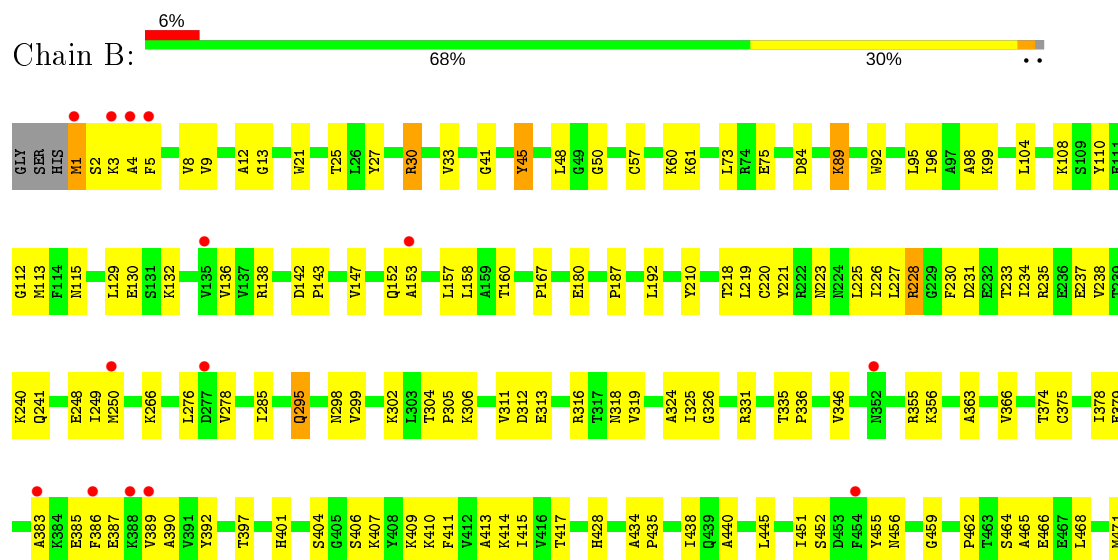
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

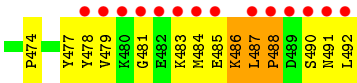
#### • Molecule 1: Trypanothione reductase



#### • Molecule 1: Trypanothione reductase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.28 Å 117.28 Å 224.53 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.50 – 2.73 47.52 – 2.73	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.50-2.73) 100.0 (47.52-2.73)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.73 Å)	Xtriage
Refinement program	PHENIX (1.12 _2829: ???)	Depositor
R, $R_{free}$	0.196 , 0.241 0.197 , 0.242	Depositor DCC
$R_{free}$ test set	2064 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.0	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7791	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EPE, RD0, FAD, SO4

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	0.28	0/3814	0.47	0/5174
1	B	0.29	0/3814	0.47	0/5174
All	All	0.28	0/7628	0.47	0/10348

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

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	3736	0	3746	145	0
1	B	3736	0	3746	125	0
2	A	53	0	31	4	0
2	B	53	0	31	1	0
3	A	20	0	0	1	0
3	B	5	0	0	0	0
4	A	33	0	0	3	0
4	B	33	0	0	0	0
5	B	30	17	35	0	0
6	B	24	32	32	3	0
7	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	11	0	0	0	0
All	All	7742	49	7621	264	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 17.

All (264) 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:487:LEU:HB3	1:B:488:PRO:CD	1.73	1.18
1:B:487:LEU:HB3	1:B:488:PRO:HD2	1.13	1.06
1:B:485:GLU:OE2	1:B:486:LYS:NZ	1.93	1.01
1:B:304:THR:HG22	1:B:306:LYS:H	1.27	0.95
1:A:348:THR:HG22	1:A:354:PRO:HA	1.48	0.94
1:A:370:PRO:HG2	1:A:430:LEU:HD11	1.52	0.89
1:B:486:LYS:H	1:B:486:LYS:HE2	1.44	0.82
1:B:484:MET:HE3	1:B:487:LEU:HA	1.61	0.82
1:A:93:LYS:H	1:A:93:LYS:HD2	1.45	0.81
1:B:392:TYR:HB3	1:B:471:MET:HE3	1.65	0.79
1:A:301:VAL:HG13	1:A:317:THR:HG21	1.65	0.79
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.20	0.77
1:A:392:TYR:CE1	1:A:451:ILE:HG12	2.20	0.76
1:A:348:THR:HG22	1:A:355:ARG:H	1.48	0.76
1:A:163:TRP:CG	1:A:164:PRO:HD2	2.23	0.74
1:B:486:LYS:HD2	1:B:486:LYS:O	1.87	0.74
1:B:355:ARG:NH1	6:B:507:GOL:O2	2.22	0.73
1:A:22:ASN:O	1:A:346:VAL:HG11	1.90	0.71
1:A:227:LEU:HD12	1:A:238:VAL:HG11	1.73	0.70
1:A:462:PRO:HG2	1:B:61:LYS:HG3	1.71	0.70
1:B:130:GLU:HB2	1:B:136:VAL:HG13	1.71	0.70
1:A:480:LYS:HE2	1:A:480:LYS:HA	1.73	0.69
1:B:392:TYR:CB	1:B:471:MET:HE3	2.21	0.69
1:B:304:THR:HG23	1:B:305:PRO:HD2	1.72	0.69
1:B:486:LYS:N	1:B:486:LYS:HE2	2.06	0.69
1:B:486:LYS:C	1:B:486:LYS:HD2	2.15	0.67
1:A:192:LEU:HD12	1:A:218:THR:O	1.94	0.67
1:B:487:LEU:CB	1:B:488:PRO:CD	2.56	0.67
1:B:4:ALA:HA	1:B:152:GLN:HB2	1.77	0.67
1:A:302:LYS:HD2	1:A:310:GLN:OE1	1.94	0.67
1:B:484:MET:CE	1:B:487:LEU:HA	2.25	0.66
1:A:165:GLN:HB2	1:A:288:ILE:HG23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLU:HB3	1:B:404:SER:HB2	1.77	0.66
1:A:29:LYS:HE2	1:A:350:PHE:HD1	1.59	0.66
1:A:392:TYR:HE1	1:A:451:ILE:HG12	1.58	0.66
1:B:452:SER:HA	1:B:455:TYR:CZ	2.30	0.66
1:B:95:LEU:HD22	1:B:210:TYR:CZ	2.29	0.66
1:A:8:VAL:HG12	1:A:32:ALA:HB3	1.78	0.65
1:A:366:VAL:O	1:A:368:SER:N	2.26	0.65
1:B:486:LYS:H	1:B:486:LYS:CE	2.09	0.65
1:B:304:THR:HG22	1:B:306:LYS:N	2.08	0.65
1:A:306:LYS:HD2	1:A:306:LYS:H	1.62	0.65
1:B:484:MET:HB2	1:B:486:LYS:HE3	1.79	0.65
1:A:93:LYS:H	1:A:93:LYS:CD	2.10	0.65
1:A:389:VAL:HB	1:A:478:TYR:HB2	1.77	0.64
1:A:221:TYR:CE2	1:A:223:ASN:HB2	2.32	0.64
1:B:485:GLU:HG2	1:B:486:LYS:HG3	1.80	0.64
1:B:295:GLN:HG2	1:B:298:ASN:ND2	2.14	0.63
1:A:29:LYS:HE2	1:A:350:PHE:CD1	2.34	0.63
1:B:4:ALA:O	1:B:30:ARG:NH1	2.31	0.63
1:A:163:TRP:CD2	1:A:164:PRO:HD2	2.34	0.63
1:B:110:TYR:O	1:B:113:MET:HB3	1.99	0.63
1:A:95:LEU:HD22	1:A:210:TYR:CZ	2.34	0.63
1:A:366:VAL:HB	1:A:372:ILE:HB	1.80	0.63
1:A:27:TYR:OH	1:A:347:ASP:HB3	1.98	0.62
1:B:234:ILE:O	1:B:238:VAL:HG12	1.99	0.62
1:B:302:LYS:HG3	1:B:318:ASN:ND2	2.16	0.61
1:B:485:GLU:CD	1:B:486:LYS:NZ	2.54	0.61
1:B:92:TRP:HB3	1:B:187:PRO:HD3	1.83	0.61
1:A:126:TRP:O	1:A:137:VAL:HA	2.01	0.61
1:A:317:THR:HG22	1:A:318:ASN:OD1	2.01	0.61
1:B:220:CYS:HA	1:B:250:MET:O	2.01	0.60
1:A:191:VAL:CG1	1:A:217:VAL:HG22	2.31	0.60
1:A:91:ASN:ND2	1:A:94:LYS:HB2	2.16	0.60
1:A:348:THR:HG22	1:A:355:ARG:N	2.17	0.60
1:A:344:ALA:O	1:A:348:THR:HG23	2.02	0.60
1:B:219:LEU:HD23	1:B:220:CYS:N	2.17	0.59
1:A:370:PRO:CG	1:A:430:LEU:HD11	2.31	0.59
1:A:348:THR:CG2	1:A:355:ARG:H	2.16	0.59
1:A:130:GLU:HB2	1:A:136:VAL:HG23	1.84	0.59
1:B:104:LEU:HG	1:B:108:LYS:HE3	1.85	0.58
1:A:392:TYR:HD2	1:A:474:PRO:HA	1.68	0.58
1:B:385:GLU:HG2	1:B:386:PHE:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HH11	1:A:446:ARG:HB3	1.68	0.57
1:A:61:LYS:HE3	1:A:367:PHE:CE2	2.38	0.57
1:B:167:PRO:HD3	1:B:285:ILE:CD1	2.34	0.57
1:B:379:GLU:OE1	1:B:414:LYS:NZ	2.36	0.57
1:A:446:ARG:HB3	1:A:446:ARG:NH1	2.19	0.57
1:B:378:ILE:HG22	1:B:428:HIS:CE1	2.40	0.57
1:A:396:PHE:CE2	1:A:398:PRO:HA	2.40	0.57
1:A:326:GLY:HA3	2:A:501:FAD:O2P	2.04	0.57
1:A:241:GLN:OE1	1:A:370:PRO:HG3	2.05	0.56
1:A:392:TYR:CD2	1:A:474:PRO:HA	2.39	0.56
1:A:37:GLN:HG3	1:A:44:PHE:HD2	1.71	0.56
1:B:167:PRO:HD3	1:B:285:ILE:HD13	1.87	0.56
1:A:392:TYR:HE2	1:A:474:PRO:HG3	1.71	0.56
1:B:130:GLU:HB2	1:B:136:VAL:CG1	2.37	0.55
1:B:389:VAL:HB	1:B:478:TYR:HB2	1.88	0.55
1:B:392:TYR:CZ	1:B:451:ILE:HG12	2.42	0.55
1:A:221:TYR:CZ	1:A:223:ASN:HB2	2.42	0.55
1:B:397:THR:OG1	1:B:410:LYS:HG2	2.06	0.55
1:B:13:GLY:HA2	1:B:50:GLY:CA	2.37	0.55
1:B:192:LEU:HA	1:B:218:THR:O	2.07	0.55
1:B:478:TYR:CE1	1:B:483:LYS:HB2	2.42	0.55
1:B:492:LEU:HD23	1:B:492:LEU:N	2.21	0.55
1:A:231:ASP:OD2	1:A:414:LYS:HD2	2.08	0.55
1:B:241:GLN:OE1	1:B:409:LYS:HA	2.07	0.55
1:B:226:ILE:HG13	1:B:227:LEU:HG	1.89	0.54
1:B:335:THR:HB	1:B:336:PRO:HD3	1.89	0.54
1:A:13:GLY:HA2	1:A:50:GLY:CA	2.36	0.54
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.89	0.54
1:A:160:THR:C	2:A:501:FAD:H52A	2.28	0.54
1:A:304:THR:HB	1:A:305:PRO:HD2	1.89	0.54
1:A:430:LEU:HD12	1:A:431:GLY:N	2.23	0.53
1:B:452:SER:HA	1:B:455:TYR:CE2	2.42	0.53
1:A:235:ARG:O	1:A:238:VAL:HG12	2.09	0.53
1:A:463:THR:O	1:A:466:GLU:HG2	2.08	0.53
4:A:505:RD0:CAK	4:A:505:RD0:CAN	2.86	0.53
1:A:104:LEU:HG	1:A:108:LYS:HE3	1.91	0.53
1:B:8:VAL:CG2	1:B:153:ALA:HB2	2.39	0.53
1:A:41:GLY:HA2	1:A:183:TYR:CZ	2.44	0.52
1:A:375:CYS:SG	1:A:445:LEU:HD22	2.49	0.52
1:A:92:TRP:HB3	1:A:187:PRO:HD3	1.90	0.52
1:A:108:LYS:O	1:A:111:GLU:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:GLN:HE22	1:B:459:GLY:HA2	1.73	0.52
1:A:415:ILE:HG13	1:A:471:MET:CE	2.40	0.52
1:A:417:THR:HG22	1:A:424:VAL:HA	1.92	0.51
1:A:348:THR:CG2	1:A:354:PRO:HA	2.31	0.51
1:B:276:LEU:HG	1:B:278:VAL:HG13	1.92	0.51
1:A:132:LYS:HG2	1:A:133:ASN:OD1	2.09	0.51
1:B:231:ASP:OD2	1:B:233:THR:OG1	2.28	0.51
1:B:387:GLU:CD	1:B:387:GLU:H	2.13	0.51
1:B:435:PRO:O	1:B:438:ILE:HG22	2.09	0.51
1:A:335:THR:HB	1:A:336:PRO:HD3	1.93	0.51
1:A:460:VAL:HG22	1:B:363:ALA:O	2.10	0.51
1:A:318:ASN:N	1:A:318:ASN:OD1	2.36	0.51
1:B:21:TRP:CE2	1:B:25:THR:HG21	2.46	0.51
1:B:411:PHE:HE2	1:B:413:ALA:HB2	1.74	0.51
1:A:61:LYS:HE3	1:A:367:PHE:CD2	2.47	0.50
1:B:411:PHE:CE1	1:B:464:SER:HB3	2.46	0.50
1:A:396:PHE:HE2	1:A:398:PRO:HA	1.77	0.50
1:B:462:PRO:HA	1:B:466:GLU:OE2	2.11	0.50
1:B:415:ILE:HD12	1:B:471:MET:HE2	1.94	0.50
1:A:37:GLN:OE1	1:A:43:PRO:HD2	2.12	0.49
1:A:130:GLU:HG3	1:A:136:VAL:HG21	1.94	0.49
1:A:403:ILE:HD12	1:B:98:ALA:HB1	1.93	0.49
1:B:225:LEU:HD23	1:B:235:ARG:CZ	2.42	0.49
1:A:392:TYR:HE2	1:A:474:PRO:CG	2.26	0.49
1:B:89:LYS:NZ	1:B:89:LYS:HB2	2.28	0.49
1:A:486:LYS:HA	1:A:486:LYS:HD3	1.41	0.49
1:A:129:LEU:HD21	1:A:322:ILE:HD13	1.94	0.49
1:A:266:LYS:HD2	1:A:266:LYS:N	2.28	0.48
1:A:415:ILE:HG13	1:A:471:MET:HE1	1.93	0.48
1:B:233:THR:OG1	1:B:414:LYS:HE3	2.13	0.48
1:A:13:GLY:HA2	1:A:50:GLY:HA3	1.94	0.48
1:A:60:LYS:HG2	1:A:61:LYS:N	2.29	0.48
1:B:112:GLY:HA2	1:B:115:ASN:HB2	1.96	0.48
1:B:266:LYS:N	1:B:266:LYS:HD2	2.27	0.48
1:B:313:GLU:OE1	1:B:356:LYS:HD2	2.14	0.48
1:A:197:GLY:HA3	3:A:502:SO4:O1	2.13	0.48
1:A:383:ALA:HB1	1:A:481:GLY:HA2	1.96	0.48
1:A:60:LYS:HD2	1:A:202:GLU:OE1	2.14	0.48
1:B:8:VAL:HG21	1:B:153:ALA:HB2	1.96	0.48
1:A:479:VAL:HG22	1:A:480:LYS:HG2	1.96	0.48
1:B:227:LEU:HD12	1:B:238:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ILE:HD12	1:B:428:HIS:HB3	1.96	0.48
1:A:91:ASN:OD1	1:A:93:LYS:HD2	2.14	0.47
1:A:130:GLU:HB2	1:A:136:VAL:CG2	2.44	0.47
1:A:233:THR:OG1	1:A:414:LYS:HE3	2.14	0.47
1:A:478:TYR:OH	1:A:483:LYS:HD2	2.15	0.47
1:A:478:TYR:CE1	1:A:483:LYS:HB2	2.49	0.47
1:B:492:LEU:HG	1:B:492:LEU:O	2.14	0.47
1:A:22:ASN:O	1:A:23:ALA:HB2	2.15	0.47
1:A:392:TYR:CE2	1:A:474:PRO:HG3	2.49	0.47
1:B:415:ILE:HD11	1:B:468:LEU:HD22	1.97	0.47
1:A:18:GLU:OE2	1:A:22:ASN:ND2	2.48	0.47
1:B:225:LEU:HB3	6:B:509:GOL:O3	2.14	0.47
1:B:248:GLU:C	1:B:249:ILE:HD12	2.35	0.47
1:B:41:GLY:O	1:B:45:TYR:N	2.42	0.47
1:A:331:ARG:HB3	1:A:332:LEU:H	1.56	0.46
1:A:108:LYS:HA	1:A:111:GLU:HB3	1.97	0.46
1:B:383:ALA:HB1	1:B:481:GLY:HA2	1.97	0.46
1:B:138:ARG:NH1	1:B:147:VAL:HG23	2.30	0.46
1:B:228:ARG:NH1	6:B:509:GOL:O2	2.48	0.46
1:B:5:PHE:N	1:B:5:PHE:CD1	2.83	0.46
1:A:219:LEU:HD23	1:A:219:LEU:C	2.35	0.46
1:B:304:THR:HG23	1:B:305:PRO:CD	2.44	0.46
1:B:474:PRO:HG2	1:B:477:TYR:CZ	2.51	0.46
1:A:316:ARG:HG2	1:A:323:TYR:CE1	2.51	0.46
1:A:452:SER:HA	1:A:455:TYR:CZ	2.50	0.46
1:B:12:ALA:HB1	1:B:48:LEU:HD12	1.98	0.46
1:A:174:HIS:CD2	1:A:260:LEU:HG	2.51	0.46
1:B:219:LEU:HD23	1:B:219:LEU:C	2.36	0.45
1:A:306:LYS:O	1:A:308:GLY:N	2.49	0.45
1:B:392:TYR:HB2	1:B:415:ILE:HB	1.98	0.45
1:A:29:LYS:HG2	1:A:350:PHE:CD1	2.52	0.45
1:A:176:ILE:HB	1:A:180:GLU:HB2	1.98	0.45
1:A:345:LEU:O	1:A:349:VAL:HG23	2.17	0.45
1:A:487:LEU:CD2	1:A:487:LEU:C	2.85	0.45
1:B:487:LEU:HD22	1:B:488:PRO:HD3	1.98	0.45
1:A:341:GLU:HA	1:A:357:THR:HG21	1.99	0.45
1:B:237:GLU:OE1	1:B:240:LYS:HD2	2.17	0.45
1:B:142:ASP:OD1	1:B:143:PRO:HD2	2.17	0.44
1:B:434:ALA:HB3	1:B:435:PRO:HD3	1.99	0.44
1:A:104:LEU:HD12	1:A:107:ASN:HB2	1.99	0.44
1:A:225:LEU:HB3	1:A:235:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:TYR:CZ	1:B:223:ASN:HB2	2.52	0.44
1:A:22:ASN:HB3	1:A:26:LEU:HD12	1.99	0.44
1:A:390:ALA:HB3	1:A:417:THR:OG1	2.17	0.44
1:A:129:LEU:HA	1:A:129:LEU:HD12	1.84	0.44
1:A:480:LYS:HE2	1:A:480:LYS:CA	2.46	0.44
1:A:299:VAL:HG12	1:A:319:VAL:HG21	1.99	0.43
1:A:306:LYS:C	1:A:308:GLY:H	2.21	0.43
1:A:325:ILE:O	1:A:328:ILE:HG22	2.17	0.43
1:B:92:TRP:CZ2	1:B:96:ILE:HD11	2.53	0.43
1:A:392:TYR:HE1	1:A:451:ILE:CG1	2.29	0.43
2:A:501:FAD:H1'1	2:A:501:FAD:H9	1.83	0.43
1:A:61:LYS:HG3	1:B:462:PRO:HG2	2.01	0.43
1:A:166:MET:HE3	1:A:172:ILE:HD11	1.98	0.43
1:A:60:LYS:NZ	2:A:501:FAD:O4	2.42	0.43
1:A:166:MET:HE1	1:A:283:MET:HG3	2.00	0.43
1:A:170:PRO:HG2	1:A:257:LYS:CB	2.47	0.43
1:A:368:SER:OG	1:A:370:PRO:O	2.30	0.43
1:A:446:ARG:HH21	1:B:456:ASN:HB3	1.84	0.43
1:A:348:THR:HG22	1:A:354:PRO:CA	2.34	0.43
4:A:505:RD0:CAH	4:A:505:RD0:CAN	2.95	0.43
1:B:390:ALA:HB3	1:B:417:THR:HB	2.00	0.43
1:A:253:GLU:OE2	1:A:274:LYS:NZ	2.34	0.43
1:A:352:ASN:C	1:A:354:PRO:HD3	2.39	0.43
1:B:9:VAL:HB	1:B:33:VAL:HG22	2.00	0.43
1:B:192:LEU:HD11	1:B:220:CYS:SG	2.58	0.43
1:A:3:LYS:HE2	1:A:3:LYS:CA	2.47	0.43
1:B:326:GLY:HA3	2:B:501:FAD:O2P	2.19	0.43
1:A:304:THR:HB	1:A:305:PRO:CD	2.49	0.42
1:A:439:GLN:HG2	1:B:465:ALA:HB1	2.01	0.42
1:B:249:ILE:N	1:B:249:ILE:HD12	2.34	0.42
1:A:316:ARG:HG2	1:A:323:TYR:CD1	2.54	0.42
1:A:429:LEU:HD21	1:A:468:LEU:HD21	2.00	0.42
1:A:116:ASP:OD2	4:A:505:RD0:CAX	2.68	0.42
1:A:56:GLY:O	1:A:60:LYS:HB3	2.20	0.42
1:B:1:MET:HE2	1:B:2:SER:N	2.34	0.42
1:A:95:LEU:HD22	1:A:210:TYR:CE2	2.54	0.42
1:B:231:ASP:O	1:B:235:ARG:HG3	2.20	0.42
1:A:315:SER:O	1:A:323:TYR:HB3	2.20	0.42
1:A:434:ALA:HB3	1:A:435:PRO:HD3	2.02	0.41
1:A:3:LYS:HE2	1:A:3:LYS:HA	2.01	0.41
1:A:73:LEU:CD2	1:B:73:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:VAL:HB	1:A:478:TYR:CB	2.48	0.41
1:B:385:GLU:HG2	1:B:386:PHE:CD2	2.56	0.41
1:B:45:TYR:OH	1:B:180:GLU:HG3	2.19	0.41
1:A:130:GLU:HB3	1:A:131:SER:H	1.62	0.41
1:A:29:LYS:HG2	1:A:350:PHE:CE1	2.55	0.41
1:B:129:LEU:HD11	1:B:158:LEU:HD21	2.01	0.41
1:B:157:LEU:HD11	1:B:325:ILE:HG12	2.02	0.41
1:B:12:ALA:HB2	1:B:33:VAL:CG1	2.50	0.41
1:A:137:VAL:HG12	1:A:148:LYS:HG3	2.03	0.41
1:B:3:LYS:N	1:B:30:ARG:HH22	2.18	0.41
1:B:95:LEU:HD22	1:B:210:TYR:CE2	2.56	0.41
1:B:299:VAL:HG12	1:B:319:VAL:HG21	2.01	0.41
1:B:3:LYS:O	1:B:3:LYS:HG3	2.21	0.41
1:B:401:HIS:HB3	1:B:406:SER:O	2.21	0.41
1:B:407:LYS:HE3	1:B:407:LYS:HB2	1.68	0.40
1:A:344:ALA:HB1	1:A:355:ARG:O	2.20	0.40
1:A:417:THR:HG21	1:A:451:ILE:HB	2.02	0.40
1:B:312:ASP:OD2	1:B:316:ARG:HB2	2.21	0.40
1:B:375:CYS:SG	1:B:445:LEU:HD22	2.61	0.40
1:A:51:THR:HG23	1:A:55:VAL:HG23	2.03	0.40
1:A:399:LEU:HG	1:A:399:LEU:H	1.41	0.40
1:B:27:TYR:CE2	1:B:346:VAL:HG12	2.57	0.40
1:B:311:VAL:HG11	1:B:324:ALA:HB3	2.02	0.40
1:B:230:PHE:CZ	1:B:366:VAL:HG21	2.57	0.40
1:B:479:VAL:CG1	1:B:484:MET:HE2	2.52	0.40
1:B:486:LYS:N	1:B:486:LYS:CE	2.77	0.40
1:A:314:PHE:O	1:A:315:SER:HB2	2.21	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	490/495 (99%)	440 (90%)	42 (9%)	8 (2%)	9	17
1	B	490/495 (99%)	462 (94%)	23 (5%)	5 (1%)	15	28
All	All	980/990 (99%)	902 (92%)	65 (7%)	13 (1%)	12	21

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	SER
1	A	23	ALA
1	A	367	PHE
1	B	488	PRO
1	A	387	GLU
1	B	84	ASP
1	A	45	TYR
1	A	307	GLY
1	B	45	TYR
1	B	490	SER
1	B	487	LEU
1	A	352	ASN
1	A	366	VAL

### 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	405/407 (100%)	383 (95%)	22 (5%)	22	38
1	B	405/407 (100%)	391 (96%)	14 (4%)	36	57
All	All	810/814 (100%)	774 (96%)	36 (4%)	28	47

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	SER
1	A	3	LYS

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Mol	Chain	Res	Type
1	A	93	LYS
1	A	128	SER
1	A	132	LYS
1	A	232	GLU
1	A	236	GLU
1	A	317	THR
1	A	318	ASN
1	A	331	ARG
1	A	347	ASP
1	A	387	GLU
1	A	397	THR
1	A	399	LEU
1	A	407	LYS
1	A	484	MET
1	A	486	LYS
1	A	487	LEU
1	A	489	ASP
1	A	491	ASN
1	A	492	LEU
1	B	1	MET
1	B	30	ARG
1	B	57	CYS
1	B	60	LYS
1	B	89	LYS
1	B	99	LYS
1	B	132	LYS
1	B	160	THR
1	B	228	ARG
1	B	295	GLN
1	B	331	ARG
1	B	374	THR
1	B	486	LYS
1	B	491	ASN

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

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

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$
2	FAD	A	501	-	51,58,58	1.21	5 (9%)	60,89,89	2.23	7 (11%)
3	SO4	B	502	-	4,4,4	0.13	0	6,6,6	0.08	0
5	EPE	B	503	-	15,15,15	0.85	1 (6%)	18,20,20	1.73	5 (27%)
6	GOL	B	508	-	5,5,5	0.94	0	5,5,5	0.93	0
6	GOL	B	509	-	5,5,5	0.89	0	5,5,5	0.99	0
4	RD0	A	505	-	34,38,38	1.99	8 (23%)	35,54,54	1.16	4 (11%)
2	FAD	B	501	-	51,58,58	1.21	5 (9%)	60,89,89	2.25	8 (13%)
3	SO4	A	504	-	4,4,4	0.13	0	6,6,6	0.07	0
3	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.07	0
5	EPE	B	505	-	15,15,15	2.04	1 (6%)	18,20,20	1.11	3 (16%)
6	GOL	B	506	-	5,5,5	0.92	0	5,5,5	0.98	0
3	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.06	0
4	RD0	B	504	-	34,38,38	2.00	9 (26%)	35,54,54	1.17	4 (11%)
6	GOL	B	507	-	5,5,5	0.88	0	5,5,5	1.02	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
5	EPE	B	503	-	-	6/9/19/19	0/1/1/1
6	GOL	B	508	-	-	1/4/4/4	-
4	RD0	A	505	-	-	6/15/46/46	0/6/6/6
2	FAD	B	501	-	-	8/30/50/50	0/6/6/6
2	FAD	A	501	-	-	7/30/50/50	0/6/6/6
6	GOL	B	509	-	-	2/4/4/4	-
5	EPE	B	505	-	-	4/9/19/19	0/1/1/1
6	GOL	B	506	-	-	1/4/4/4	-
4	RD0	B	504	-	-	5/15/46/46	0/6/6/6
6	GOL	B	507	-	-	0/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	505	EPE	C10-S	-7.66	1.66	1.77
2	A	501	FAD	C4X-C10	5.50	1.44	1.38
2	B	501	FAD	C4X-C10	5.47	1.44	1.38
4	A	505	RD0	CAP-SAM	-5.03	1.66	1.73
4	B	504	RD0	CAP-SAM	-5.01	1.66	1.73
4	B	504	RD0	CAU-NAY	-4.91	1.33	1.39
4	A	505	RD0	CAU-NAY	-4.90	1.33	1.39
4	B	504	RD0	CAL-SAM	-3.98	1.66	1.74
4	A	505	RD0	CAL-SAM	-3.94	1.66	1.74
4	B	504	RD0	CAT-CAU	-3.72	1.33	1.41
4	A	505	RD0	CAT-CAU	-3.71	1.33	1.41
4	B	504	RD0	CAR-CAV	-3.67	1.33	1.42
4	A	505	RD0	CAR-CAV	-3.66	1.33	1.42
4	A	505	RD0	CAV-CAU	-3.42	1.33	1.41
4	B	504	RD0	CAV-CAU	-3.39	1.34	1.41
2	B	501	FAD	C4-N3	3.35	1.38	1.33
4	B	504	RD0	CAX-NAY	-3.35	1.33	1.38
4	A	505	RD0	CAX-NAY	-3.33	1.33	1.38
2	A	501	FAD	C4-N3	3.13	1.38	1.33
5	B	503	EPE	C10-S	2.87	1.81	1.77
2	B	501	FAD	C4-C4X	2.46	1.45	1.41
2	A	501	FAD	C4-C4X	2.39	1.45	1.41
2	A	501	FAD	C5X-N5	2.33	1.39	1.35
2	B	501	FAD	C5X-N5	2.28	1.39	1.35
2	B	501	FAD	C9A-N10	2.05	1.41	1.38
4	B	504	RD0	CAA-CAF	-2.05	1.52	1.54
4	A	505	RD0	CAA-CAF	-2.02	1.52	1.54
4	B	504	RD0	CAE-CAF	-2.01	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C9A-N10	2.01	1.41	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FAD	C4-N3-C2	13.19	126.28	115.14
2	A	501	FAD	C4-N3-C2	13.11	126.21	115.14
2	B	501	FAD	C4X-C4-N3	-7.17	113.62	123.43
2	A	501	FAD	C4X-C4-N3	-7.10	113.72	123.43
2	B	501	FAD	C10-C4X-N5	4.56	124.41	121.26
2	A	501	FAD	C10-C4X-N5	4.54	124.40	121.26
2	A	501	FAD	C4-C4X-C10	-3.86	117.40	119.95
2	B	501	FAD	C4-C4X-C10	-3.84	117.41	119.95
5	B	503	EPE	C5-N4-C3	3.52	116.74	108.83
2	A	501	FAD	C4X-C10-N10	-3.48	116.72	120.30
2	B	501	FAD	C4X-C10-N10	-3.44	116.77	120.30
5	B	503	EPE	O1S-S-C10	3.26	110.84	106.92
5	B	503	EPE	C7-N4-C3	3.12	119.20	111.23
2	B	501	FAD	C1'-N10-C9A	3.00	120.66	118.29
2	A	501	FAD	C1'-N10-C9A	2.84	120.53	118.29
4	B	504	RD0	CAZ-CBA-CBB	-2.43	109.53	115.07
4	A	505	RD0	CAZ-CBA-CBB	-2.43	109.53	115.07
5	B	503	EPE	C7-N4-C5	2.36	117.27	111.23
2	B	501	FAD	P-O3P-PA	-2.34	124.81	132.83
5	B	503	EPE	O2S-S-C10	2.33	109.72	106.92
2	B	501	FAD	C5A-C6A-N6A	2.33	123.89	120.35
5	B	505	EPE	O3S-S-C10	2.28	109.46	105.77
2	A	501	FAD	C5A-C6A-N6A	2.28	123.81	120.35
4	B	504	RD0	CAD-CAE-CAF	-2.18	109.46	113.15
4	B	504	RD0	CAB-CAA-CAF	-2.18	109.47	113.15
4	A	505	RD0	CAB-CAA-CAF	-2.17	109.47	113.15
4	A	505	RD0	CAD-CAE-CAF	-2.17	109.48	113.15
5	B	505	EPE	O2S-S-C10	2.15	109.50	106.92
5	B	505	EPE	O1S-S-C10	2.11	109.46	106.92
4	A	505	RD0	CAN-CAL-SAM	-2.03	109.98	112.00
4	B	504	RD0	CAN-CAL-SAM	-2.02	109.99	112.00

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	B	503	EPE	C8-C7-N4-C3
5	B	503	EPE	C9-C10-S-O2S
5	B	503	EPE	C9-C10-S-O3S
6	B	509	GOL	O1-C1-C2-O2
4	A	505	RD0	CAL-CAF-NAG-CAH
4	A	505	RD0	CBA-CAZ-NAY-CAU
4	A	505	RD0	CBA-CAZ-NAY-CAX
2	B	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	C1'-C2'-C3'-C4'
5	B	505	EPE	C9-C10-S-O1S
4	B	504	RD0	CBA-CAZ-NAY-CAU
4	B	504	RD0	CBA-CAZ-NAY-CAX
2	A	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	C3B-C4B-C5B-O5B
6	B	509	GOL	O1-C1-C2-C3
4	B	504	RD0	NAY-CAZ-CBA-CBB
5	B	505	EPE	C9-C10-S-O3S
4	A	505	RD0	NAY-CAZ-CBA-CBB
5	B	503	EPE	C10-C9-N1-C6
2	B	501	FAD	O2'-C2'-C3'-O3'
2	B	501	FAD	O2'-C2'-C3'-C4'
5	B	505	EPE	N4-C7-C8-O8
2	A	501	FAD	C5B-O5B-PA-O3P
2	A	501	FAD	C5B-O5B-PA-O2A
5	B	503	EPE	C9-C10-S-O1S
5	B	505	EPE	C9-C10-S-O2S
4	A	505	RD0	CAZ-CBA-CBB-CBG
4	B	504	RD0	CAZ-CBA-CBB-CBC
5	B	503	EPE	C10-C9-N1-C2
2	B	501	FAD	P-O3P-PA-O1A
2	A	501	FAD	O3'-C3'-C4'-C5'
2	A	501	FAD	C2'-C3'-C4'-C5'
6	B	508	GOL	O1-C1-C2-C3
4	A	505	RD0	CAZ-CBA-CBB-CBC
4	B	504	RD0	CAZ-CBA-CBB-CBG
2	B	501	FAD	C1'-C2'-C3'-O3'
6	B	506	GOL	O1-C1-C2-O2
2	B	501	FAD	O4'-C4'-C5'-O5'

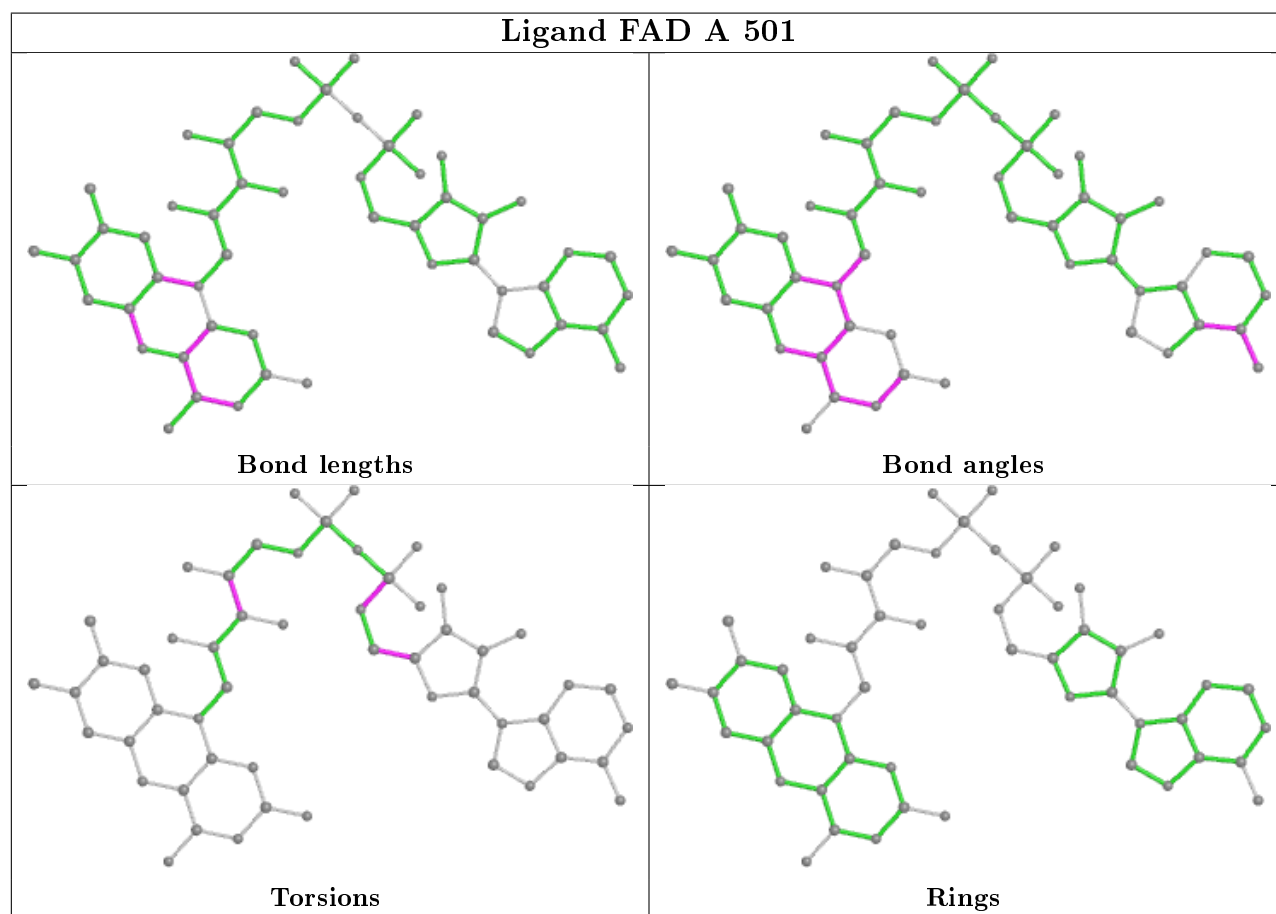
There are no ring outliers.

6 monomers are involved in 12 short contacts:

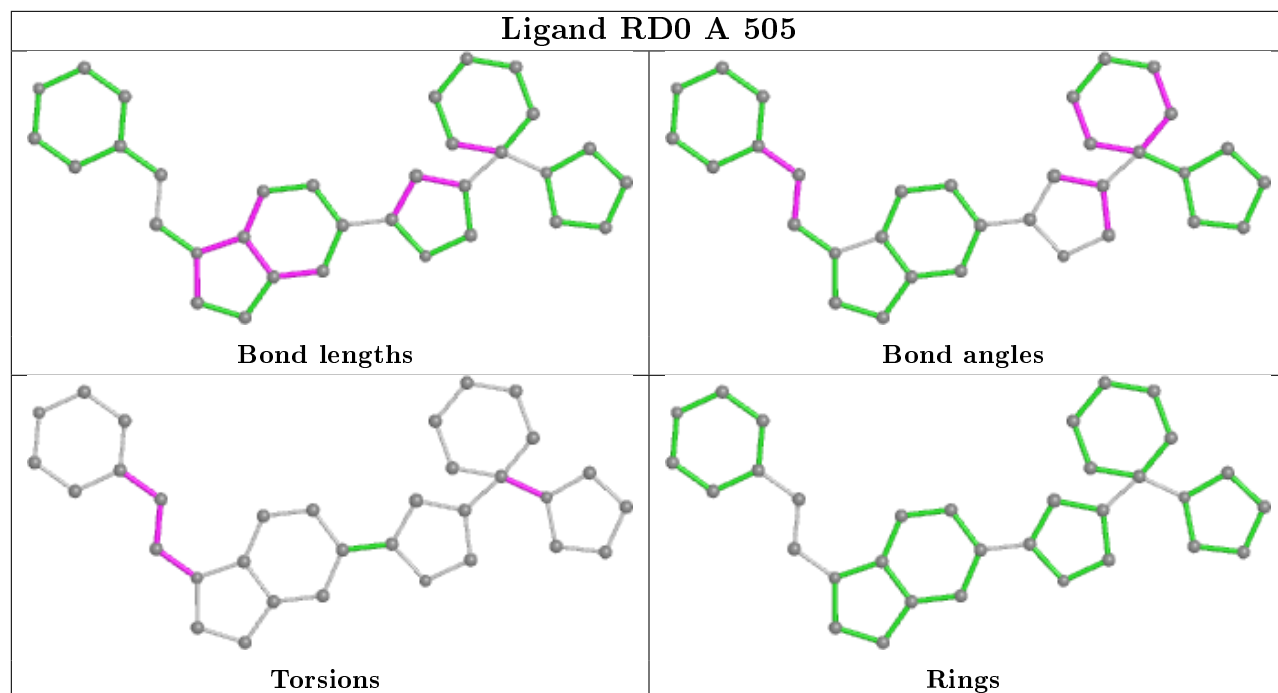


Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	4	0
6	B	509	GOL	2	0
4	A	505	RD0	3	0
2	B	501	FAD	1	0
3	A	502	SO4	1	0
6	B	507	GOL	1	0

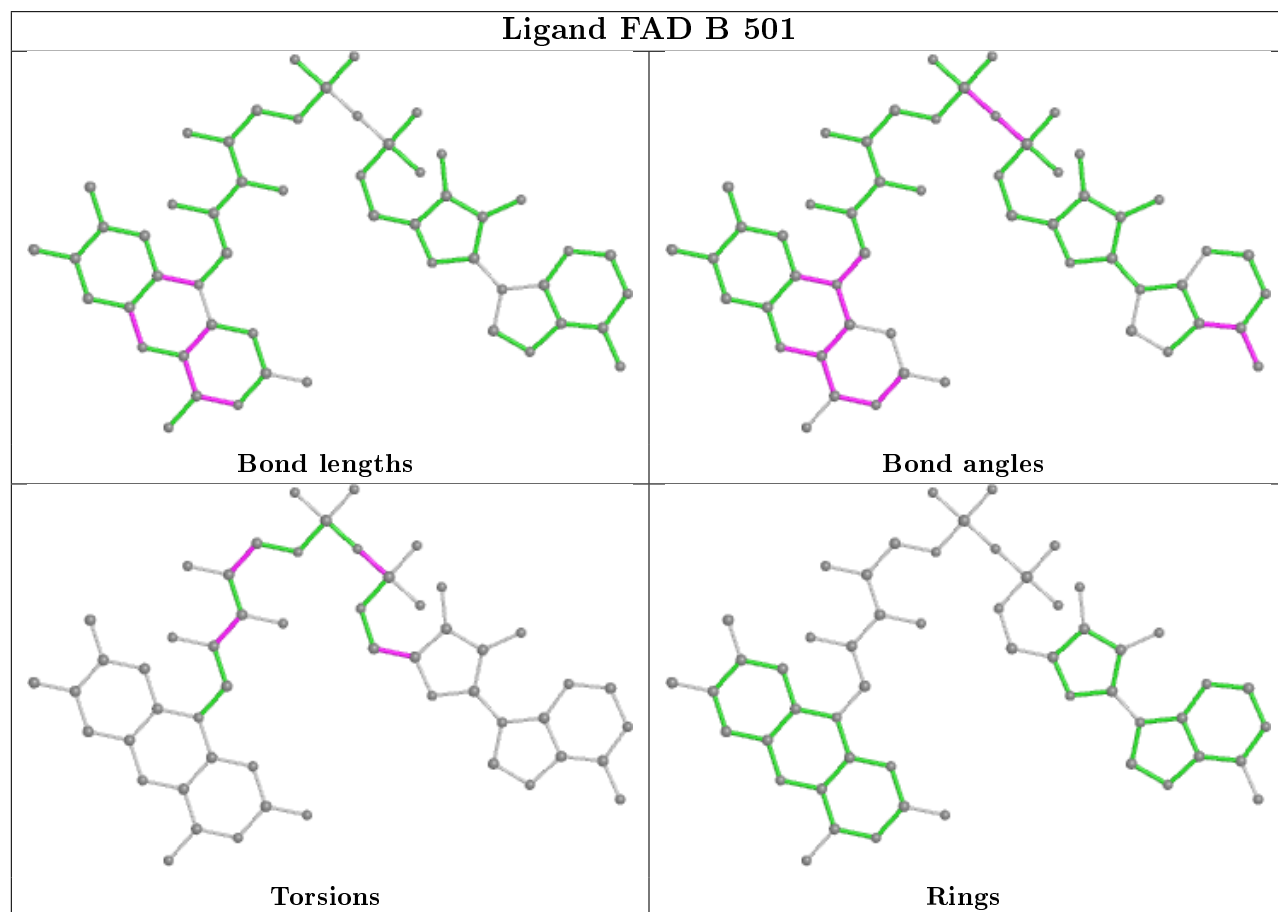
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

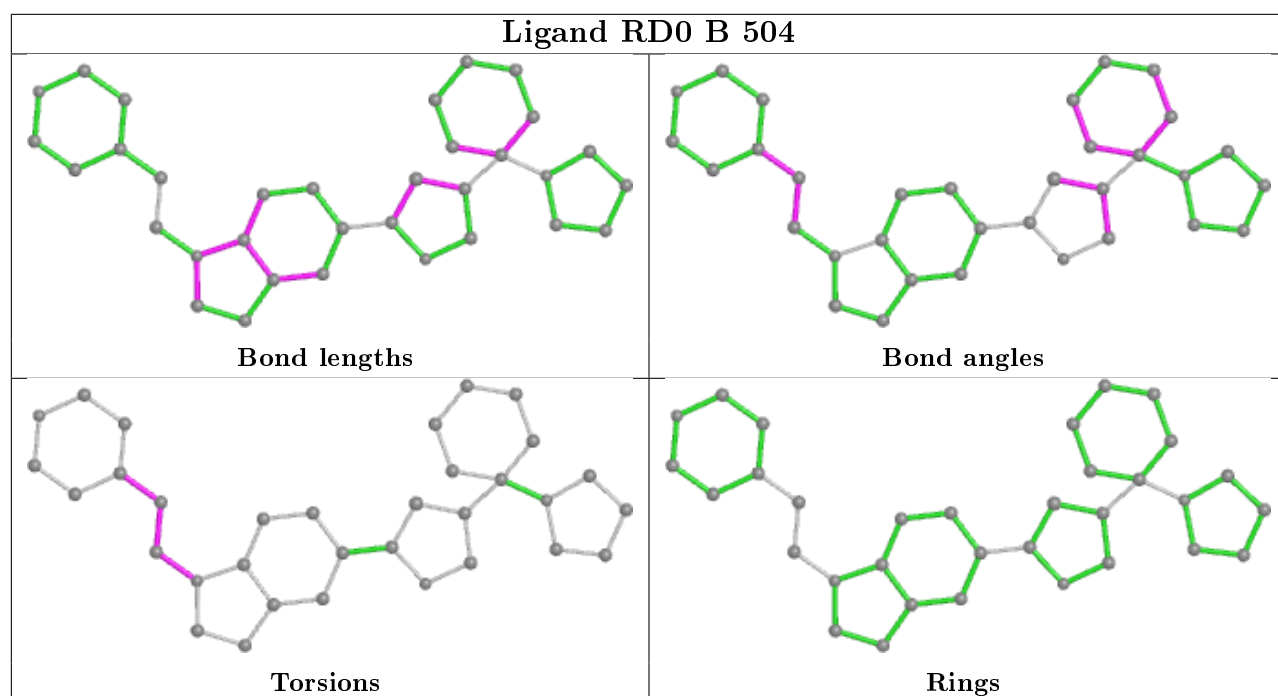


## Ligand RD0 A 505



## Ligand FAD B 501





## 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	492/495 (99%)	0.31	34 (6%) 16 18	52, 83, 124, 220	0
1	B	492/495 (99%)	0.36	28 (5%) 23 26	47, 75, 119, 210	0
All	All	984/990 (99%)	0.33	62 (6%) 20 22	47, 79, 122, 220	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	LEU	8.1
1	A	491	ASN	7.9
1	B	491	ASN	6.0
1	A	5	PHE	5.4
1	A	2	SER	5.0
1	B	479	VAL	4.9
1	B	488	PRO	4.4
1	B	483	LYS	4.3
1	A	301	VAL	4.2
1	B	492	LEU	4.2
1	A	30	ARG	4.1
1	B	490	SER	3.8
1	B	478	TYR	3.7
1	B	489	ASP	3.7
1	B	389	VAL	3.6
1	B	481	GLY	3.4
1	B	482	GLU	3.4
1	B	454	PHE	3.3
1	B	3	LYS	3.3
1	A	276	LEU	3.2
1	A	8	VAL	3.0
1	A	480	LYS	2.9
1	A	483	LYS	2.9
1	A	386	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	156	ILE	2.9
1	A	479	VAL	2.9
1	A	114	PHE	2.8
1	B	1	MET	2.8
1	B	388	LYS	2.8
1	B	386	PHE	2.7
1	B	4	ALA	2.7
1	A	302	LYS	2.7
1	A	303	LEU	2.7
1	B	383	ALA	2.6
1	A	481	GLY	2.6
1	B	352	ASN	2.5
1	A	52	CYS	2.5
1	B	484	MET	2.5
1	A	24	ALA	2.5
1	B	153	ALA	2.4
1	A	476	TYR	2.4
1	B	277	ASP	2.4
1	A	57	CYS	2.4
1	B	480	LYS	2.4
1	A	350	PHE	2.3
1	B	487	LEU	2.3
1	A	468	LEU	2.3
1	A	399	LEU	2.3
1	A	478	TYR	2.3
1	B	5	PHE	2.3
1	B	250	MET	2.2
1	A	477	TYR	2.2
1	B	135	VAL	2.2
1	A	270	PHE	2.2
1	A	323	TYR	2.1
1	A	390	ALA	2.1
1	A	11	GLY	2.1
1	B	485	GLU	2.1
1	A	315	SER	2.1
1	A	487	LEU	2.1
1	A	389	VAL	2.1
1	A	251	THR	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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

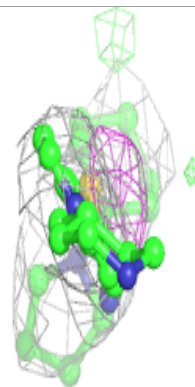
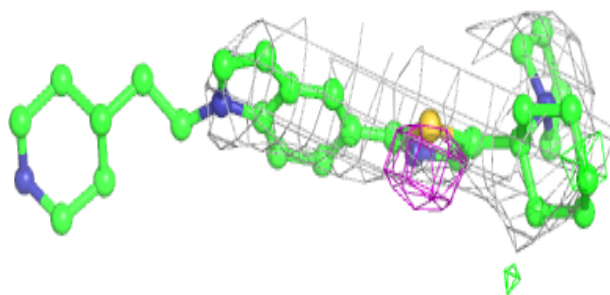
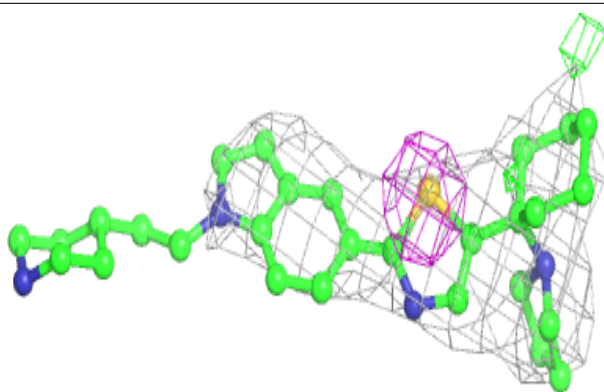
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	RD0	A	505	33/33	0.63	0.43	138,146,166,167	0
5	EPE	B	505	15/15	0.71	0.29	119,148,175,176	0
3	SO4	A	504	5/5	0.72	0.17	169,171,174,177	0
6	GOL	B	509	6/6	0.74	0.21	101,127,149,152	0
6	GOL	B	508	6/6	0.74	0.22	127,153,164,168	0
3	SO4	B	502	5/5	0.79	0.35	170,172,175,176	0
6	GOL	B	507	6/6	0.86	0.20	112,135,140,140	0
6	GOL	B	506	6/6	0.88	0.17	100,120,136,137	0
3	SO4	A	506	5/5	0.89	0.21	141,141,145,147	0
4	RD0	B	504	33/33	0.91	0.35	93,109,127,128	0
3	SO4	A	503	5/5	0.92	0.10	121,122,125,126	0
3	SO4	A	502	5/5	0.93	0.25	123,123,133,135	0
5	EPE	B	503	15/15	0.95	0.18	72,85,89,92	0
2	FAD	A	501	53/53	0.95	0.20	49,72,83,91	0
2	FAD	B	501	53/53	0.96	0.20	42,58,73,80	0

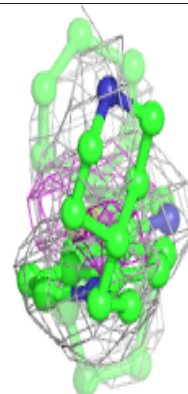
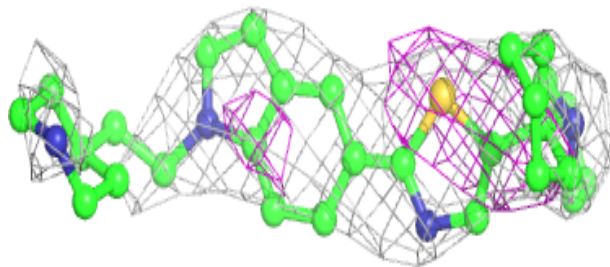
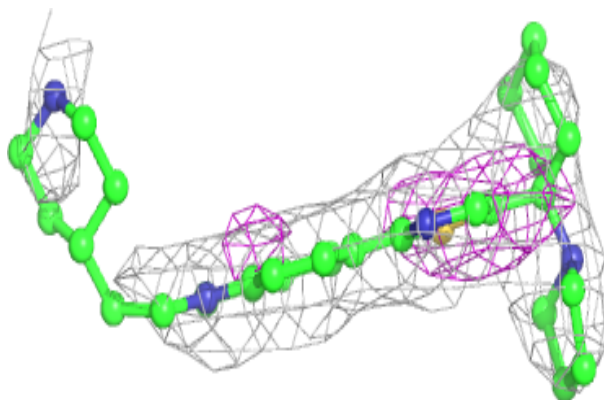
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around RD0 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)

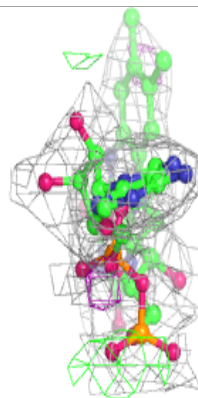
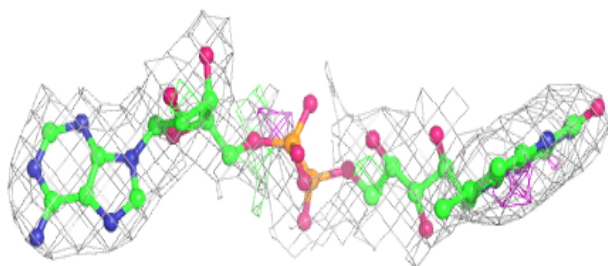
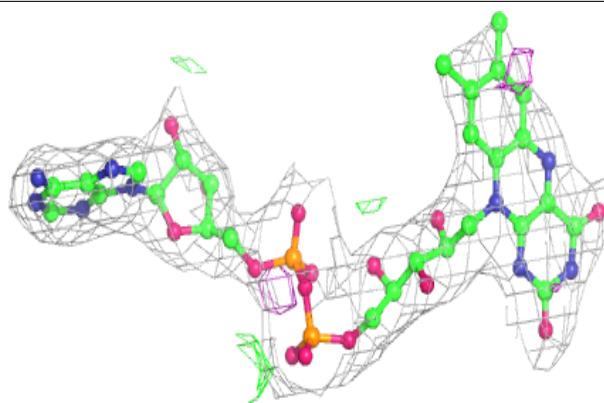
**Electron density around RD0 B 504:**

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

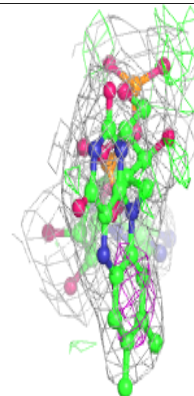
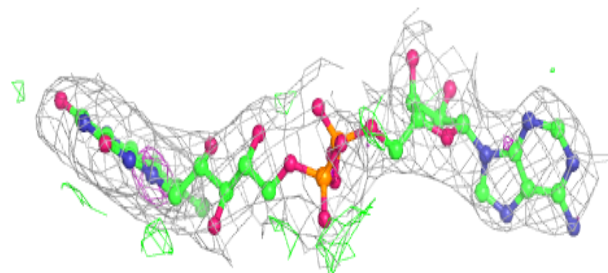
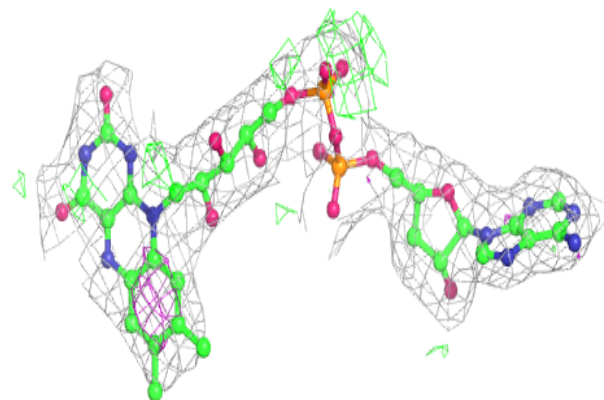


**Electron density around FAD A 501:**

$2mF_o-DF_c$  (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

There are no such residues in this entry.