



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:41 PM UTC

PDB ID : 7PUT / pdb\_00007put  
Title : Crystal structure of Thioredoxin Reductase from Brugia Malayi in complex with NADP(H)  
Authors : Fata, F.; Ardini, M.; Silvestri, I.; Gabriele, F.; Ippoliti, R.; Gencheva, R.; Cheng, Q.; Arner, E.S.J.; Angelucci, F.; Williams, D.L.  
Deposited on : 2021-09-30  
Resolution : 2.80 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)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

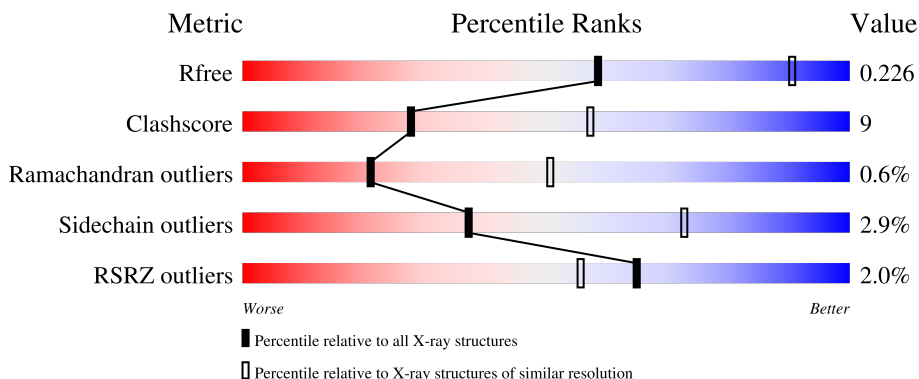
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

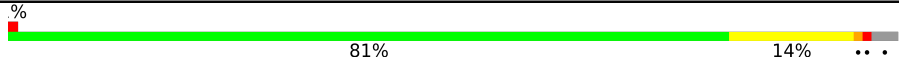
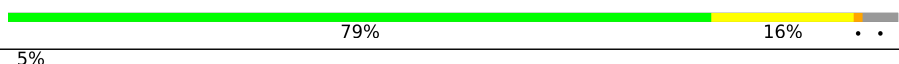
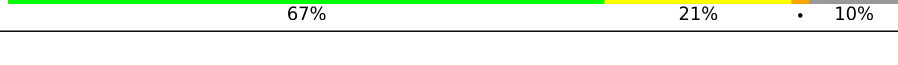
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	598	 81% 14% 5%
1	B	598	 79% 16% 5%
2	C	598	 67% 21% 10% 5%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13432 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.

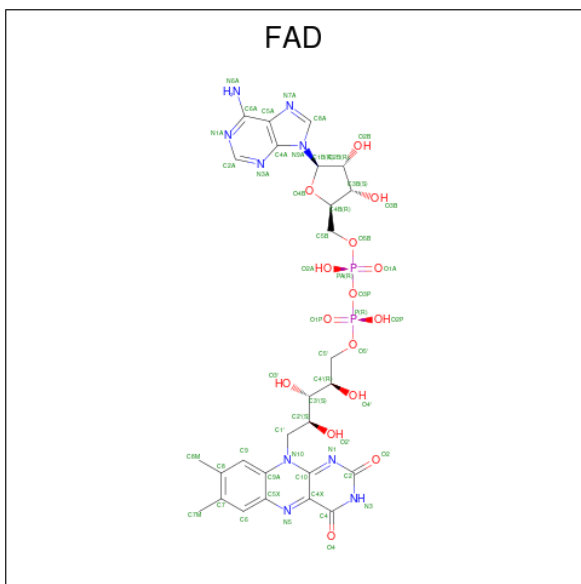
- Molecule 1 is a protein called Glutaredoxin domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	578	Total	C	N	O	S	0	0	0
			4492	2864	753	846	29			
1	B	575	Total	C	N	O	S	0	0	0
			4474	2855	750	840	29			

- Molecule 2 is a protein called Glutaredoxin domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	540	Total	C	N	O	S	0	0	0
			4210	2690	710	783	27			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



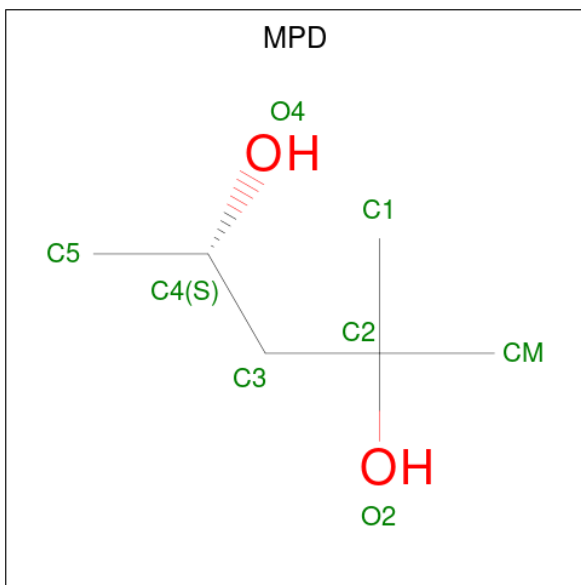
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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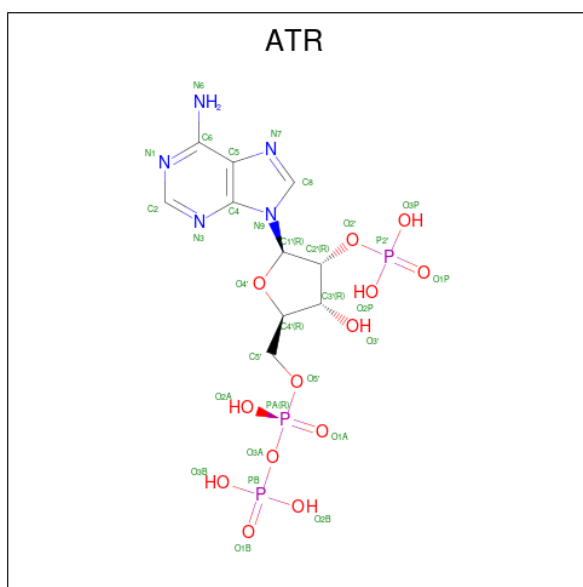
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is 2'-MONOPHOSPHOADENOSINE-5'-DIPHOSPHATE (CCD ID: ATR) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	31	10	5	13	3	0	0

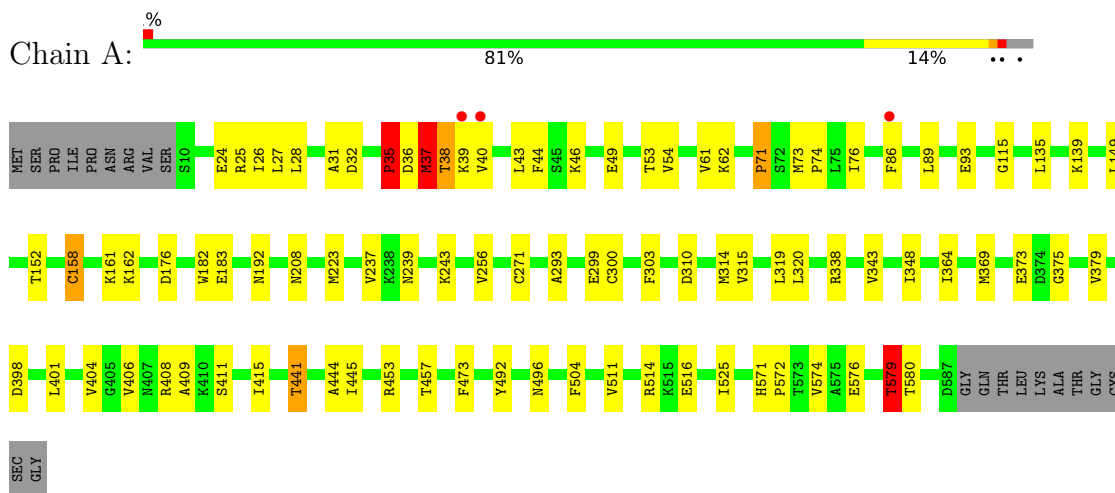
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total O 6 6	0	0
6	B	4	Total O 4 4	0	0

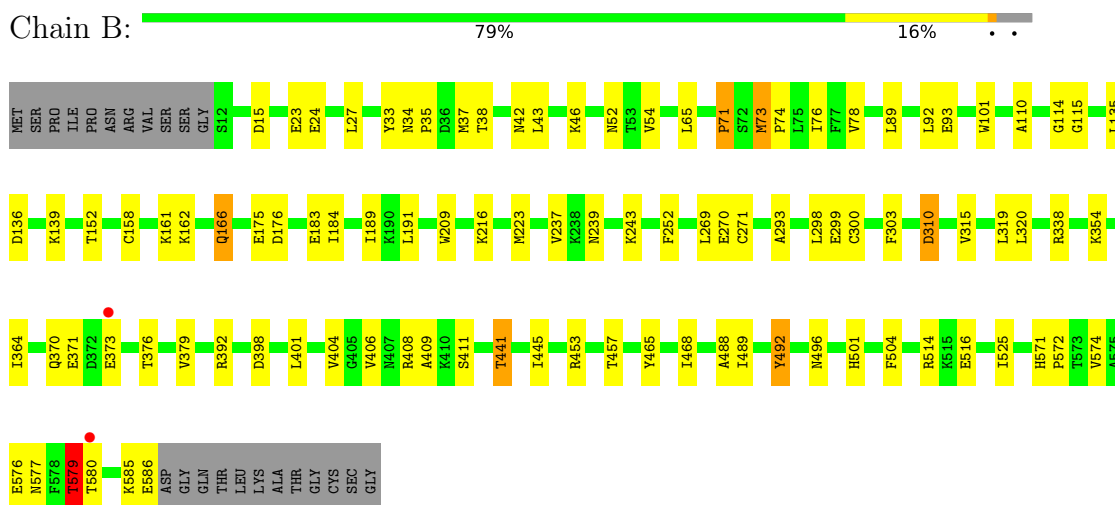
### 3 Residue-property plots [i](#)

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: Glutaredoxin domain-containing protein

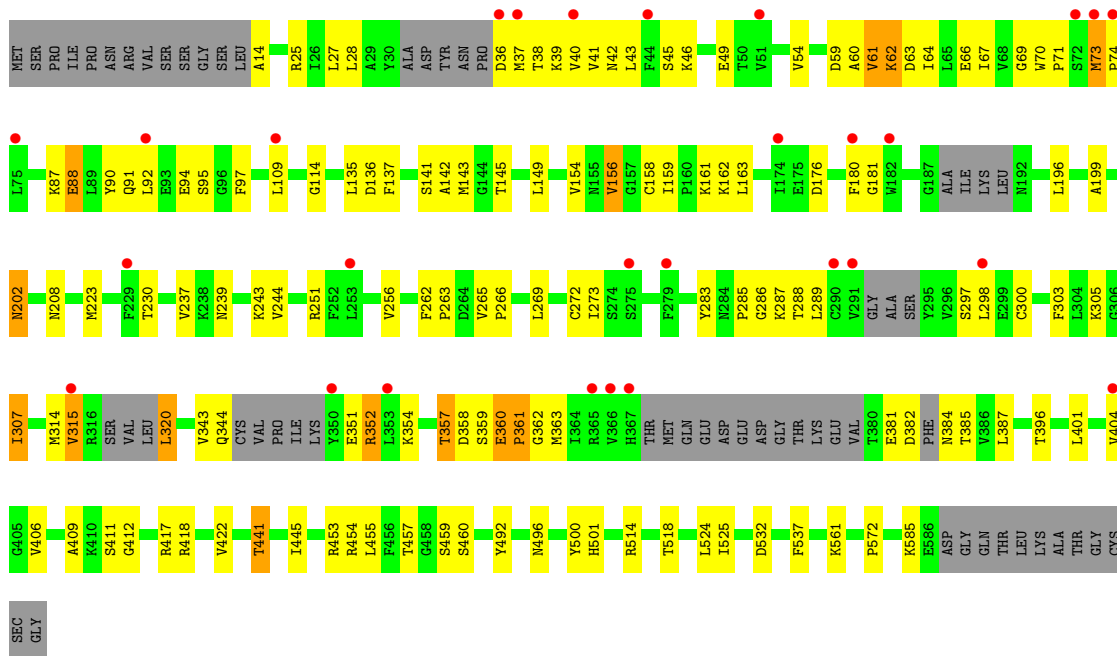


- Molecule 1: Glutaredoxin domain-containing protein



- Molecule 2: Glutaredoxin domain-containing protein





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.39Å 260.29Å 130.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 2.80 49.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.13-2.80) 99.9 (49.13-2.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.196 , 0.229 (Not available) , 0.226	Depositor DCC
$R_{free}$ test set	3054 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.7	Xtrriage
Anisotropy	0.080	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.015 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: MPD, FAD, ATR, 2CO

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	1.14	3/4572 (0.1%)	1.43	12/6179 (0.2%)
1	B	1.13	3/4554 (0.1%)	1.41	5/6155 (0.1%)
2	C	1.12	1/4288 (0.0%)	1.45	10/5784 (0.2%)
All	All	1.13	7/13414 (0.1%)	1.43	27/18118 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	GLY	C-O	6.87	1.30	1.24
1	A	415	ILE	C-O	5.68	1.30	1.24
1	A	444	ALA	C-O	5.45	1.30	1.24
1	B	115	GLY	C-O	5.44	1.29	1.24
1	B	488	ALA	C-O	5.34	1.30	1.24
1	B	92	LEU	C-O	5.04	1.30	1.24
2	C	196	LEU	C-O	5.03	1.29	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	351	GLU	N-CA-C	-15.57	77.64	110.80
1	A	38	THR	N-CA-C	-12.11	97.98	113.12
1	B	71	PRO	CB-CA-C	-10.64	94.01	111.56
1	A	37	MET	CB-CA-C	-9.12	92.26	110.42
1	A	71	PRO	CB-CA-C	-8.63	97.32	111.56
1	B	492	TYR	CA-C-O	-8.55	110.18	121.73
2	C	352	ARG	N-CA-C	-8.50	92.69	110.80
1	A	35	PRO	CB-CA-C	-8.23	97.97	111.56
1	B	492	TYR	N-CA-C	-8.03	98.39	109.95
1	A	375	GLY	CA-C-O	-7.17	115.96	120.91
1	A	152	THR	CA-CB-OG1	-6.61	99.68	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	PRO	N-CA-C	6.41	125.68	112.47
2	C	307	ILE	N-CA-C	-6.25	103.24	110.05
1	A	71	PRO	N-CA-C	5.85	124.53	112.47
2	C	181	GLY	CA-C-O	-5.70	116.02	121.38
2	C	202	ASN	CB-CA-C	5.63	120.42	110.85
1	A	24	GLU	CA-C-N	5.54	127.70	120.28
1	A	24	GLU	C-N-CA	5.54	127.70	120.28
2	C	352	ARG	CB-CA-C	-5.43	99.61	110.42
1	A	579	THR	CA-CB-OG1	-5.33	101.60	109.60
2	C	180	PHE	CA-C-O	-5.29	113.41	119.60
1	B	579	THR	CA-CB-OG1	-5.26	101.71	109.60
2	C	88	GLU	CA-C-O	-5.26	115.30	120.82
2	C	307	ILE	CA-C-O	-5.17	115.72	121.98
2	C	572	PRO	N-CD-CG	-5.16	97.61	103.80
1	A	93	GLU	CA-C-N	5.11	127.13	120.28
1	A	93	GLU	C-N-CA	5.11	127.13	120.28

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	4492	0	4516	55	0
1	B	4474	0	4504	68	0
2	C	4210	0	4236	119	0
3	A	53	0	31	2	0
3	B	53	0	31	3	0
3	C	53	0	31	3	0
4	A	32	0	56	6	0
4	B	24	0	42	3	0
5	A	31	0	11	1	0
6	A	6	0	0	0	0
6	B	4	0	0	0	0
All	All	13432	0	13458	242	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 9.

All (242) 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)
2:C:363:MET:HE2	2:C:382:ASP:HB3	1.20	1.15
2:C:501:HIS:CD2	2:C:585:LYS:HB2	1.87	1.09
1:B:501:HIS:CD2	1:B:585:LYS:HB2	1.90	1.05
2:C:363:MET:CE	2:C:382:ASP:HB3	1.87	1.04
1:A:37:MET:HG3	1:A:37:MET:O	1.31	1.04
1:A:37:MET:O	1:A:37:MET:CG	2.01	1.03
2:C:66:GLU:O	2:C:418:ARG:NH2	1.91	1.02
1:B:24:GLU:OE1	1:B:52:ASN:ND2	1.92	1.02
1:B:501:HIS:HD2	1:B:585:LYS:HB2	1.30	0.93
2:C:91:GLN:O	2:C:95:SER:N	2.04	0.89
2:C:501:HIS:HD2	2:C:585:LYS:HB2	1.30	0.88
2:C:352:ARG:HD2	2:C:352:ARG:O	1.72	0.88
2:C:362:GLY:O	2:C:384:ASN:O	1.91	0.88
2:C:396:THR:HG21	2:C:412:GLY:O	1.75	0.87
2:C:417:ARG:HG2	2:C:422:VAL:HG23	1.57	0.85
1:A:579:THR:HG22	1:A:580:THR:HG23	1.65	0.78
1:B:161:LYS:HD2	1:B:299:GLU:OE1	1.84	0.78
1:A:161:LYS:HD2	1:A:299:GLU:OE1	1.84	0.78
2:C:285:PRO:HB2	2:C:385:THR:HG21	1.65	0.77
1:A:25:ARG:NH1	1:A:49:GLU:OE2	2.18	0.76
1:B:209:TRP:CD1	2:C:39:LYS:HZ3	2.02	0.76
2:C:363:MET:CE	2:C:382:ASP:CB	2.63	0.75
2:C:401:LEU:HD22	2:C:406:VAL:HB	1.69	0.75
4:B:604:MPD:O4	4:B:604:MPD:O2	2.04	0.74
1:B:209:TRP:CH2	2:C:87:LYS:HA	2.23	0.73
2:C:363:MET:HA	2:C:384:ASN:HA	1.71	0.71
1:B:43:LEU:HD21	1:B:93:GLU:HG3	1.70	0.71
1:A:43:LEU:O	1:A:46:LYS:HB3	1.90	0.71
1:A:576:GLU:O	1:A:579:THR:HB	1.91	0.71
2:C:352:ARG:O	2:C:352:ARG:CD	2.38	0.71
1:B:38:THR:HG22	1:B:42:ASN:HD21	1.54	0.71
1:A:27:LEU:HD11	1:A:54:VAL:HG23	1.73	0.71
1:B:27:LEU:HD11	1:B:54:VAL:HG23	1.72	0.71
1:B:34:ASN:H	1:B:37:MET:CE	2.04	0.70
1:B:576:GLU:O	1:B:579:THR:HB	1.91	0.70
2:C:27:LEU:HD11	2:C:54:VAL:HG23	1.73	0.70
2:C:357:THR:N	2:C:360:GLU:O	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:TRP:CZ3	2:C:87:LYS:HA	2.27	0.69
2:C:73:MET:HB2	2:C:74:PRO:HD3	1.74	0.69
2:C:73:MET:CB	2:C:74:PRO:HD3	2.23	0.69
1:B:166:GLN:HE21	1:B:166:GLN:HA	1.59	0.67
1:B:315:VAL:HG21	1:B:319:LEU:CD2	2.25	0.67
1:B:453:ARG:O	1:B:457:THR:HB	1.93	0.67
1:A:453:ARG:O	1:A:457:THR:HB	1.95	0.66
2:C:453:ARG:O	2:C:457:THR:HB	1.95	0.66
2:C:141:SER:HB3	2:C:145:THR:CG2	2.26	0.66
1:B:401:LEU:HD12	1:B:408:ARG:HD3	1.78	0.65
2:C:454:ARG:HG3	2:C:459:SER:O	1.97	0.65
2:C:352:ARG:O	2:C:352:ARG:CG	2.44	0.64
1:A:36:ASP:O	1:A:38:THR:N	2.31	0.64
1:B:161:LYS:NZ	3:B:601:FAD:O4	2.30	0.64
4:A:603:MPD:HM1	4:A:603:MPD:H52	1.78	0.63
2:C:70:TRP:HB2	2:C:71:PRO:HD2	1.79	0.63
1:B:43:LEU:O	1:B:46:LYS:HB3	1.98	0.63
2:C:239:ASN:HD21	2:C:243:LYS:HE3	1.62	0.63
2:C:404:VAL:HG13	2:C:406:VAL:HG23	1.80	0.63
1:B:76:ILE:HD13	1:B:89:LEU:HD22	1.80	0.62
1:B:293:ALA:HB2	1:B:315:VAL:HG13	1.81	0.62
4:B:602:MPD:H52	4:B:602:MPD:H11	1.81	0.61
2:C:92:LEU:O	2:C:97:PHE:N	2.34	0.61
1:A:76:ILE:HD13	1:A:89:LEU:HD22	1.83	0.60
1:B:34:ASN:H	1:B:37:MET:HE3	1.65	0.60
2:C:156:VAL:CG1	2:C:156:VAL:O	2.49	0.60
1:A:404:VAL:HG13	1:A:406:VAL:HG23	1.84	0.59
4:A:605:MPD:HM2	4:A:605:MPD:H52	1.82	0.59
2:C:70:TRP:HB2	2:C:71:PRO:CD	2.32	0.59
2:C:298:LEU:N	2:C:298:LEU:HD12	2.17	0.59
1:A:271:CYS:HB3	1:A:364:ILE:HG12	1.85	0.59
1:B:38:THR:O	1:B:42:ASN:ND2	2.34	0.59
2:C:273:ILE:O	2:C:387:LEU:HD12	2.02	0.59
2:C:67:ILE:HD13	2:C:460:SER:HB3	1.84	0.59
1:B:371:GLU:OE2	1:B:376:THR:HG22	2.02	0.58
1:B:404:VAL:HG13	1:B:406:VAL:HG23	1.84	0.58
2:C:320:LEU:HD12	2:C:320:LEU:N	2.18	0.58
1:A:314:MET:HG2	1:A:343:VAL:HG23	1.86	0.58
1:A:182:TRP:CZ3	4:A:602:MPD:H12	2.38	0.58
1:B:33:TYR:HA	1:B:37:MET:HE1	1.86	0.58
1:A:315:VAL:HG11	1:A:319:LEU:CD2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:602:MPD:O4	4:A:602:MPD:H13	2.03	0.58
2:C:305:LYS:O	2:C:307:ILE:O	2.22	0.58
1:B:33:TYR:HA	1:B:37:MET:CE	2.34	0.57
2:C:273:ILE:O	2:C:387:LEU:CD1	2.52	0.57
2:C:43:LEU:O	2:C:46:LYS:HB3	2.05	0.56
2:C:88:GLU:O	2:C:91:GLN:HB3	2.06	0.56
2:C:251:ARG:NH1	2:C:455:LEU:HB3	2.21	0.56
2:C:28:LEU:CD1	2:C:40:VAL:HG11	2.37	0.55
1:A:183:GLU:O	1:B:189:ILE:HG23	2.06	0.55
2:C:42:ASN:O	2:C:45:SER:OG	2.22	0.55
4:A:603:MPD:HM1	4:A:603:MPD:C5	2.36	0.55
2:C:161:LYS:NZ	3:C:601:FAD:O4	2.38	0.55
2:C:297:SER:HB3	2:C:298:LEU:HD12	1.89	0.55
2:C:359:SER:C	2:C:360:GLU:HG2	2.31	0.55
2:C:92:LEU:HB3	2:C:97:PHE:HB2	1.88	0.54
1:A:40:VAL:O	1:A:43:LEU:HB3	2.07	0.54
2:C:315:VAL:O	2:C:344:GLN:C	2.51	0.54
2:C:500:TYR:OH	2:C:532:ASP:OD2	2.22	0.54
1:B:34:ASN:OD1	1:B:35:PRO:HD2	2.08	0.53
1:A:161:LYS:NZ	3:A:601:FAD:O4	2.41	0.53
1:A:314:MET:HG2	1:A:343:VAL:CG2	2.39	0.53
2:C:298:LEU:HD12	2:C:298:LEU:H	1.74	0.52
1:B:166:GLN:HA	1:B:166:GLN:NE2	2.24	0.52
2:C:25:ARG:NH2	2:C:49:GLU:OE2	2.43	0.52
1:A:293:ALA:HB1	1:A:319:LEU:HA	1.91	0.52
1:B:338:ARG:NH1	1:B:516:GLU:OE2	2.42	0.52
1:B:135:LEU:HD23	1:B:223:MET:HB2	1.92	0.51
1:A:135:LEU:HD23	1:A:223:MET:HB2	1.91	0.51
1:B:293:ALA:HB1	1:B:319:LEU:HA	1.93	0.51
1:A:310:ASP:OD1	1:A:310:ASP:C	2.53	0.51
1:B:271:CYS:HB3	1:B:364:ILE:HD12	1.93	0.51
1:B:43:LEU:O	1:B:43:LEU:HD23	2.10	0.51
2:C:269:LEU:O	2:C:272:CYS:HB2	2.10	0.51
1:B:310:ASP:OD1	1:B:310:ASP:C	2.54	0.50
2:C:357:THR:HB	2:C:360:GLU:HB2	1.93	0.50
2:C:69:GLY:CA	2:C:70:TRP:CE3	2.95	0.50
1:A:35:PRO:O	1:A:37:MET:HB3	2.10	0.50
2:C:289:LEU:HD11	2:C:314:MET:HG3	1.93	0.50
2:C:69:GLY:HA2	2:C:70:TRP:CE3	2.47	0.50
1:B:34:ASN:H	1:B:37:MET:HE2	1.77	0.50
2:C:28:LEU:HD12	2:C:40:VAL:HG11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:288:THR:HG23	2:C:385:THR:HG23	1.93	0.50
2:C:36:ASP:O	2:C:38:THR:N	2.45	0.50
1:B:43:LEU:HD23	1:B:43:LEU:C	2.37	0.49
2:C:199:ALA:O	2:C:202:ASN:OD1	2.30	0.49
1:B:34:ASN:OD1	1:B:35:PRO:CD	2.60	0.49
1:B:409:ALA:O	1:B:411:SER:O	2.31	0.49
2:C:36:ASP:C	2:C:38:THR:H	2.19	0.49
2:C:59:ASP:C	2:C:61:VAL:H	2.21	0.49
1:A:409:ALA:O	1:A:411:SER:O	2.30	0.49
1:B:139:LYS:NZ	1:B:398:ASP:OD2	2.45	0.49
2:C:90:TYR:CE2	2:C:94:GLU:HB2	2.48	0.48
2:C:263:PRO:HG2	2:C:266:PRO:CG	2.42	0.48
2:C:409:ALA:O	2:C:411:SER:O	2.31	0.48
2:C:92:LEU:HD22	2:C:97:PHE:CD2	2.48	0.48
1:B:176:ASP:OD2	1:B:514:ARG:NH1	2.46	0.48
1:B:489:ILE:O	1:B:492:TYR:O	2.31	0.48
2:C:396:THR:CG2	2:C:412:GLY:HA3	2.44	0.48
2:C:287:LYS:H	2:C:384:ASN:ND2	2.11	0.48
2:C:285:PRO:CB	2:C:385:THR:HG21	2.41	0.48
1:B:73:MET:O	1:B:74:PRO:C	2.57	0.48
2:C:36:ASP:C	2:C:38:THR:N	2.72	0.47
4:A:602:MPD:HM1	1:B:175:GLU:OE2	2.15	0.47
1:A:31:ALA:O	1:A:32:ASP:C	2.57	0.47
2:C:256:VAL:HG13	3:C:601:FAD:N7A	2.28	0.47
2:C:492:TYR:O	2:C:496:ASN:ND2	2.48	0.47
1:B:152:THR:OG1	3:B:601:FAD:O1A	2.32	0.46
2:C:91:GLN:O	2:C:95:SER:HB2	2.15	0.46
1:B:209:TRP:CD1	2:C:39:LYS:NZ	2.80	0.46
2:C:320:LEU:N	2:C:320:LEU:CD1	2.78	0.46
1:A:139:LYS:NZ	1:A:398:ASP:OD2	2.49	0.46
2:C:135:LEU:HD23	2:C:223:MET:HB2	1.97	0.46
2:C:262:PHE:HZ	2:C:272:CYS:HG	1.59	0.46
2:C:73:MET:CB	2:C:74:PRO:CD	2.94	0.46
1:A:192:ASN:HB2	1:B:183:GLU:OE2	2.16	0.46
2:C:141:SER:OG	2:C:142:ALA:N	2.48	0.46
2:C:298:LEU:CD2	2:C:320:LEU:HD11	2.46	0.46
2:C:269:LEU:CB	2:C:272:CYS:HB2	2.46	0.45
2:C:518:THR:HG22	2:C:518:THR:O	2.16	0.45
2:C:298:LEU:HD21	2:C:320:LEU:HD11	1.96	0.45
2:C:501:HIS:CD2	2:C:585:LYS:CB	2.78	0.45
2:C:524:LEU:HD12	2:C:537:PHE:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LEU:HD23	1:B:65:LEU:HA	1.81	0.45
2:C:357:THR:CG2	2:C:358:ASP:N	2.80	0.45
1:A:239:ASN:ND2	1:A:243:LYS:HB3	2.32	0.45
1:B:571:HIS:HA	1:B:572:PRO:HA	1.82	0.45
1:A:293:ALA:HB2	1:A:315:VAL:HG12	1.99	0.45
1:A:293:ALA:HB3	5:A:606:ATR:O3'	2.17	0.45
2:C:137:PHE:O	3:C:601:FAD:H1B	2.16	0.45
2:C:154:VAL:HA	2:C:159:ILE:HG13	1.99	0.45
1:B:216:LYS:NZ	2:C:90:TYR:CE1	2.85	0.45
2:C:273:ILE:O	2:C:273:ILE:HG22	2.16	0.45
1:A:348:ILE:HD13	1:A:369:MET:HG2	1.98	0.45
2:C:263:PRO:HG2	2:C:266:PRO:CD	2.47	0.45
1:B:501:HIS:CD2	1:B:585:LYS:CB	2.82	0.44
2:C:135:LEU:HD21	2:C:223:MET:HE2	1.98	0.44
2:C:518:THR:O	2:C:518:THR:CG2	2.65	0.44
1:A:73:MET:O	1:A:74:PRO:C	2.59	0.44
1:A:158:CYS:HB3	3:A:601:FAD:C4	2.47	0.44
1:A:86:PHE:CD1	1:A:86:PHE:N	2.85	0.44
1:B:161:LYS:CD	1:B:299:GLU:OE1	2.61	0.44
1:B:392:ARG:N	4:B:604:MPD:H12	2.33	0.44
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.83	0.44
2:C:135:LEU:HD21	2:C:223:MET:CE	2.47	0.44
2:C:143:MET:O	2:C:145:THR:HG22	2.18	0.44
2:C:396:THR:HG22	2:C:412:GLY:HA3	2.00	0.44
1:A:161:LYS:CD	1:A:299:GLU:OE1	2.61	0.44
1:A:492:TYR:O	1:A:496:ASN:ND2	2.50	0.44
2:C:286:GLY:HA3	2:C:384:ASN:HD22	1.83	0.43
1:B:315:VAL:HG21	1:B:319:LEU:HD23	1.99	0.43
2:C:500:TYR:CG	2:C:561:LYS:HE3	2.53	0.43
1:A:338:ARG:NH1	1:A:516:GLU:OE2	2.50	0.43
2:C:244:VAL:HG13	2:C:244:VAL:O	2.17	0.43
1:A:61:VAL:HG13	1:A:62:LYS:N	2.34	0.43
1:A:441:THR:O	1:A:445:ILE:HG13	2.18	0.43
2:C:70:TRP:HE3	2:C:417:ARG:HG3	1.84	0.43
1:A:571:HIS:HA	1:A:572:PRO:HA	1.82	0.43
1:B:300:CYS:HA	1:B:303:PHE:CE2	2.53	0.43
1:B:577:ASN:O	1:B:580:THR:HG22	2.18	0.43
2:C:314:MET:HG2	2:C:343:VAL:CG2	2.48	0.43
2:C:300:CYS:HA	2:C:303:PHE:CE2	2.53	0.43
1:A:35:PRO:HG2	1:A:86:PHE:CZ	2.54	0.42
1:A:401:LEU:HD12	1:A:408:ARG:HD3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:LYS:HG3	2:C:63:ASP:N	2.34	0.42
2:C:363:MET:HE2	2:C:363:MET:HB3	1.72	0.42
1:B:239:ASN:ND2	1:B:243:LYS:HB3	2.34	0.42
2:C:14:ALA:HA	2:C:64:ILE:HD11	2.01	0.42
2:C:441:THR:O	2:C:445:ILE:HG13	2.19	0.42
1:A:31:ALA:CB	1:A:73:MET:SD	3.08	0.42
1:B:270:GLU:OE1	1:B:270:GLU:N	2.53	0.42
2:C:91:GLN:O	2:C:95:SER:CB	2.67	0.42
2:C:354:LYS:HB2	2:C:362:GLY:HA2	2.01	0.42
1:B:504:PHE:CE1	1:B:574:VAL:HG13	2.54	0.42
2:C:176:ASP:OD2	2:C:514:ARG:NH1	2.51	0.42
2:C:41:VAL:O	2:C:45:SER:CB	2.68	0.41
2:C:114:GLY:HA3	2:C:136:ASP:HB2	2.01	0.41
1:B:298:LEU:HD12	1:B:320:LEU:HD21	2.01	0.41
1:A:36:ASP:C	1:A:38:THR:N	2.78	0.41
1:A:300:CYS:HA	1:A:303:PHE:CE2	2.55	0.41
1:B:78:VAL:HB	1:B:101:TRP:CH2	2.56	0.41
1:B:465:TYR:HA	1:B:468:ILE:HD11	2.02	0.41
1:B:441:THR:O	1:B:445:ILE:HG13	2.20	0.41
1:B:585:LYS:O	1:B:586:GLU:C	2.63	0.41
1:A:26:ILE:HD13	1:A:44:PHE:CE1	2.55	0.41
1:A:504:PHE:CE1	1:A:574:VAL:HG13	2.55	0.41
1:A:176:ASP:OD2	1:A:514:ARG:NH1	2.51	0.41
1:B:34:ASN:OD1	1:B:35:PRO:N	2.54	0.41
2:C:163:LEU:HD23	2:C:163:LEU:HA	1.93	0.41
1:A:28:LEU:O	1:A:53:THR:HA	2.21	0.41
3:B:601:FAD:H9	3:B:601:FAD:H1'1	1.90	0.41
2:C:41:VAL:O	2:C:45:SER:HB3	2.21	0.41
2:C:230:THR:O	2:C:230:THR:HG22	2.21	0.41
1:A:162:LYS:HE3	1:A:473:PHE:CE1	2.55	0.41
1:A:149:LEU:O	1:A:208:ASN:ND2	2.52	0.40
1:A:319:LEU:O	1:A:320:LEU:C	2.64	0.40
1:B:114:GLY:HA3	1:B:136:ASP:HB2	2.03	0.40
2:C:363:MET:HE1	2:C:382:ASP:CB	2.48	0.40
1:A:36:ASP:C	1:A:38:THR:H	2.28	0.40
2:C:283:TYR:CE1	2:C:361:PRO:HB3	2.56	0.40
1:A:239:ASN:HD21	1:A:243:LYS:HB3	1.86	0.40
2:C:149:LEU:O	2:C:208:ASN:ND2	2.54	0.40
2:C:352:ARG:O	2:C:352:ARG:HG3	2.20	0.40
1:B:110:ALA:O	1:B:252:PHE:HA	2.21	0.40
2:C:59:ASP:C	2:C:61:VAL:N	2.79	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/598 (96%)	547 (95%)	25 (4%)	3 (0%)	24	55
1	B	572/598 (96%)	550 (96%)	21 (4%)	1 (0%)	43	72
2	C	524/598 (88%)	488 (93%)	30 (6%)	6 (1%)	11	36
All	All	1671/1794 (93%)	1585 (95%)	76 (4%)	10 (1%)	21	51

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	MET
2	C	60	ALA
2	C	37	MET
2	C	73	MET
2	C	61	VAL
2	C	361	PRO
1	A	71	PRO
2	C	62	LYS
1	A	35	PRO
1	B	71	PRO

### 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	488/503 (97%)	478 (98%)	10 (2%)	48	80
1	B	486/503 (97%)	468 (96%)	18 (4%)	30	65
2	C	457/504 (91%)	444 (97%)	13 (3%)	38	73
All	All	1431/1510 (95%)	1390 (97%)	41 (3%)	37	73

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	158	CYS
1	A	237	VAL
1	A	256	VAL
1	A	373	GLU
1	A	379	VAL
1	A	441	THR
1	A	511	VAL
1	A	525	ILE
1	A	579	THR
1	B	15	ASP
1	B	23	GLU
1	B	73	MET
1	B	158	CYS
1	B	162	LYS
1	B	166	GLN
1	B	184	ILE
1	B	191	LEU
1	B	237	VAL
1	B	310	ASP
1	B	354	LYS
1	B	370	GLN
1	B	373	GLU
1	B	379	VAL
1	B	441	THR
1	B	496	ASN
1	B	525	ILE
1	B	579	THR
2	C	109	LEU
2	C	156	VAL
2	C	158	CYS
2	C	162	LYS
2	C	237	VAL
2	C	265	VAL

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Mol	Chain	Res	Type
2	C	315	VAL
2	C	320	LEU
2	C	357	THR
2	C	360	GLU
2	C	381	GLU
2	C	441	THR
2	C	525	ILE

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	52	ASN
1	A	99	ASN
1	A	309	ASN
1	A	344	GLN
1	A	529	ASN
1	B	42	ASN
1	B	99	ASN
1	B	166	GLN
1	B	203	HIS
1	B	224	ASN
1	B	367	HIS
1	B	384	ASN
1	B	490	GLN
1	B	529	ASN
2	C	58	ASN
2	C	208	ASN
2	C	384	ASN
2	C	529	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](#)

2 non-standard protein/DNA/RNA residues 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
1	2CO	B	345	1	3,7,8	0.77	0	1,7,9	0.42	0
1	2CO	A	345	1	3,7,8	1.03	0	1,7,9	0.36	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
1	2CO	B	345	1	-	1/1/6/8	-
1	2CO	A	345	1	-	1/1/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	2CO	N-CA-CB-SG
1	B	345	2CO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

11 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
4	MPD	B	603	-	7,7,7	0.21	0	9,10,10	0.67	0
3	FAD	C	601	-	58,58,58	0.55	0	85,89,89	0.64	1 (1%)
4	MPD	B	604	-	7,7,7	0.29	0	9,10,10	0.38	0
3	FAD	B	601	-	58,58,58	0.71	1 (1%)	85,89,89	0.70	1 (1%)
4	MPD	A	605	-	7,7,7	0.11	0	9,10,10	0.50	0
4	MPD	A	604	-	7,7,7	0.12	0	9,10,10	0.33	0
4	MPD	B	602	-	7,7,7	0.13	0	9,10,10	0.53	0
5	ATR	A	606	-	32,33,33	1.51	4 (12%)	50,52,52	1.91	12 (24%)
3	FAD	A	601	-	58,58,58	0.67	0	85,89,89	0.68	0
4	MPD	A	602	-	7,7,7	0.11	0	9,10,10	0.34	0
4	MPD	A	603	-	7,7,7	0.16	0	9,10,10	0.78	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	MPD	B	603	-	-	1/5/5/5	-
3	FAD	C	601	-	-	12/34/50/50	0/6/6/6
4	MPD	B	604	-	-	3/5/5/5	-
3	FAD	B	601	-	-	5/34/50/50	0/6/6/6
4	MPD	A	605	-	-	3/5/5/5	-
4	MPD	A	604	-	-	0/5/5/5	-
4	MPD	B	602	-	-	3/5/5/5	-
5	ATR	A	606	-	-	2/21/37/37	0/3/3/3
3	FAD	A	601	-	-	3/34/50/50	0/6/6/6
4	MPD	A	602	-	-	0/5/5/5	-
4	MPD	A	603	-	-	0/5/5/5	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	606	ATR	C5-C4	5.01	1.48	1.39
5	A	606	ATR	PA-O3A	3.18	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	606	ATR	C5-C6	3.08	1.49	1.41
3	B	601	FAD	C1'-C2'	-2.74	1.48	1.52
5	A	606	ATR	C8-N7	2.42	1.36	1.31

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606	ATR	C5-C4-N3	-5.09	119.70	126.72
5	A	606	ATR	N3-C4-N9	4.30	134.48	127.17
5	A	606	ATR	N3-C2-N1	-4.22	122.19	128.58
5	A	606	ATR	C2-N3-C4	3.85	121.24	111.83
5	A	606	ATR	C4-N9-C8	3.34	109.25	105.74
5	A	606	ATR	C4-C5-N7	-3.21	106.91	110.58
5	A	606	ATR	C2-N1-C6	2.66	123.09	118.73
5	A	606	ATR	C5-N7-C8	2.58	107.51	103.45
5	A	606	ATR	C6-C5-N7	2.58	137.06	132.09
5	A	606	ATR	N9-C8-N7	-2.41	110.52	113.94
5	A	606	ATR	O2'-P2'-O1P	-2.25	101.31	109.33
5	A	606	ATR	O3'-C3'-C4'	-2.15	104.91	111.08
3	B	601	FAD	C4X-C4-N3	2.10	118.60	113.25
3	C	601	FAD	C4-N3-C2	-2.04	122.02	125.64

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	FAD	PA-O3P-P-O5'
3	C	601	FAD	C5B-O5B-PA-O1A
4	A	605	MPD	C2-C3-C4-O4
4	A	605	MPD	C2-C3-C4-C5
4	B	602	MPD	C2-C3-C4-O4
4	B	602	MPD	C2-C3-C4-C5
5	A	606	ATR	PA-O3A-PB-O2B
5	A	606	ATR	PA-O3A-PB-O3B
3	A	601	FAD	O4B-C4B-C5B-O5B
3	C	601	FAD	O4B-C4B-C5B-O5B
3	C	601	FAD	C3B-C4B-C5B-O5B
3	A	601	FAD	C3B-C4B-C5B-O5B
3	B	601	FAD	O4B-C4B-C5B-O5B
3	B	601	FAD	C3B-C4B-C5B-O5B
3	C	601	FAD	PA-O3P-P-O5'
3	C	601	FAD	C2B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
3	A	601	FAD	C2B-C1B-N9A-C8A
3	C	601	FAD	P-O3P-PA-O1A
4	A	605	MPD	O2-C2-C3-C4
4	B	602	MPD	O2-C2-C3-C4
3	C	601	FAD	C5B-O5B-PA-O2A
3	C	601	FAD	C5B-O5B-PA-O3P
4	B	603	MPD	C2-C3-C4-C5
3	C	601	FAD	P-O3P-PA-O2A
3	C	601	FAD	C2B-C1B-N9A-C4A
3	B	601	FAD	P-O3P-PA-O1A
3	C	601	FAD	O4B-C1B-N9A-C8A
4	B	604	MPD	C2-C3-C4-O4
4	B	604	MPD	C1-C2-C3-C4
4	B	604	MPD	CM-C2-C3-C4
3	B	601	FAD	P-O3P-PA-O2A
3	C	601	FAD	PA-O3P-P-O2P

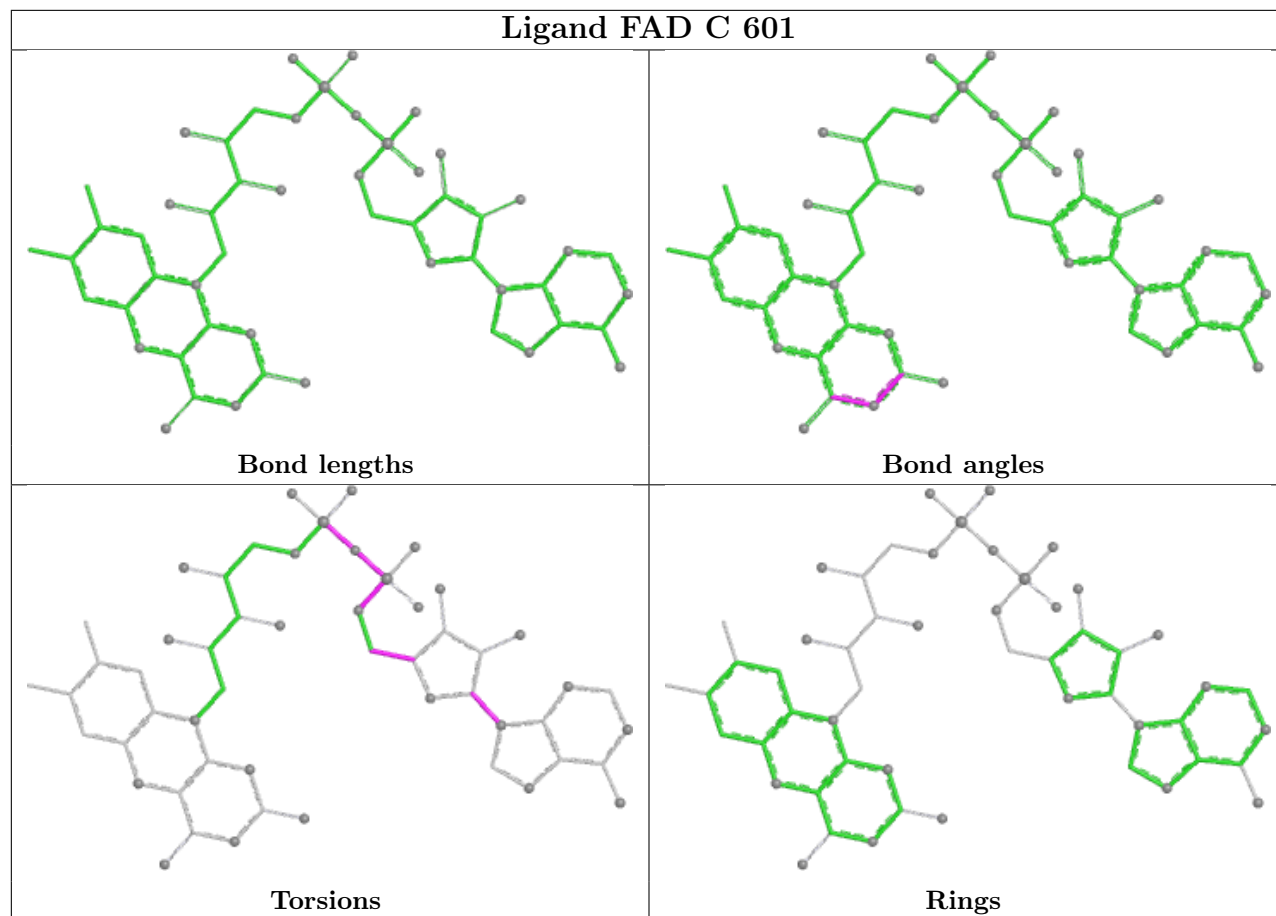
There are no ring outliers.

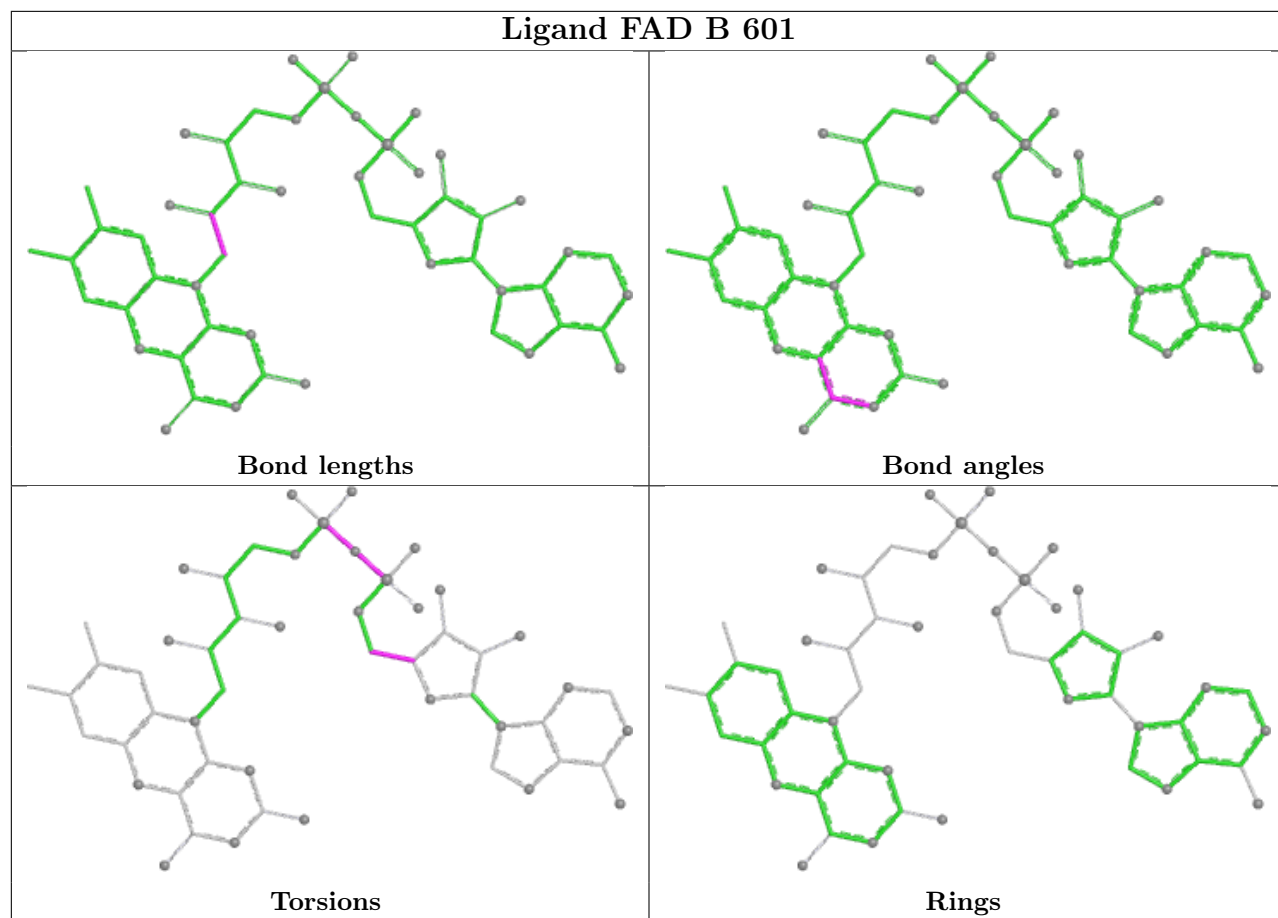
9 monomers are involved in 18 short contacts:

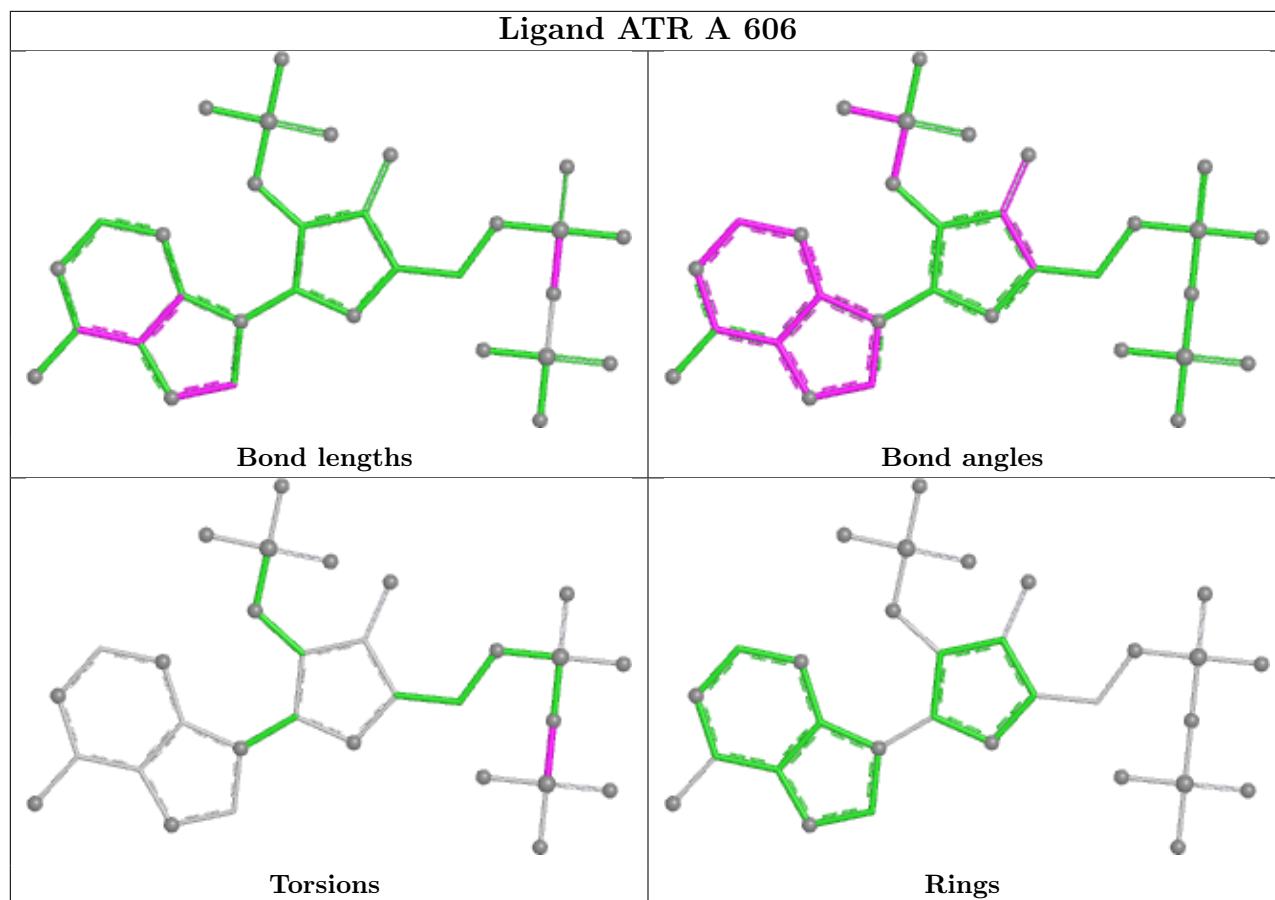
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	FAD	3	0
4	B	604	MPD	2	0
3	B	601	FAD	3	0
4	A	605	MPD	1	0
4	B	602	MPD	1	0
5	A	606	ATR	1	0
3	A	601	FAD	2	0
4	A	602	MPD	3	0
4	A	603	MPD	2	0

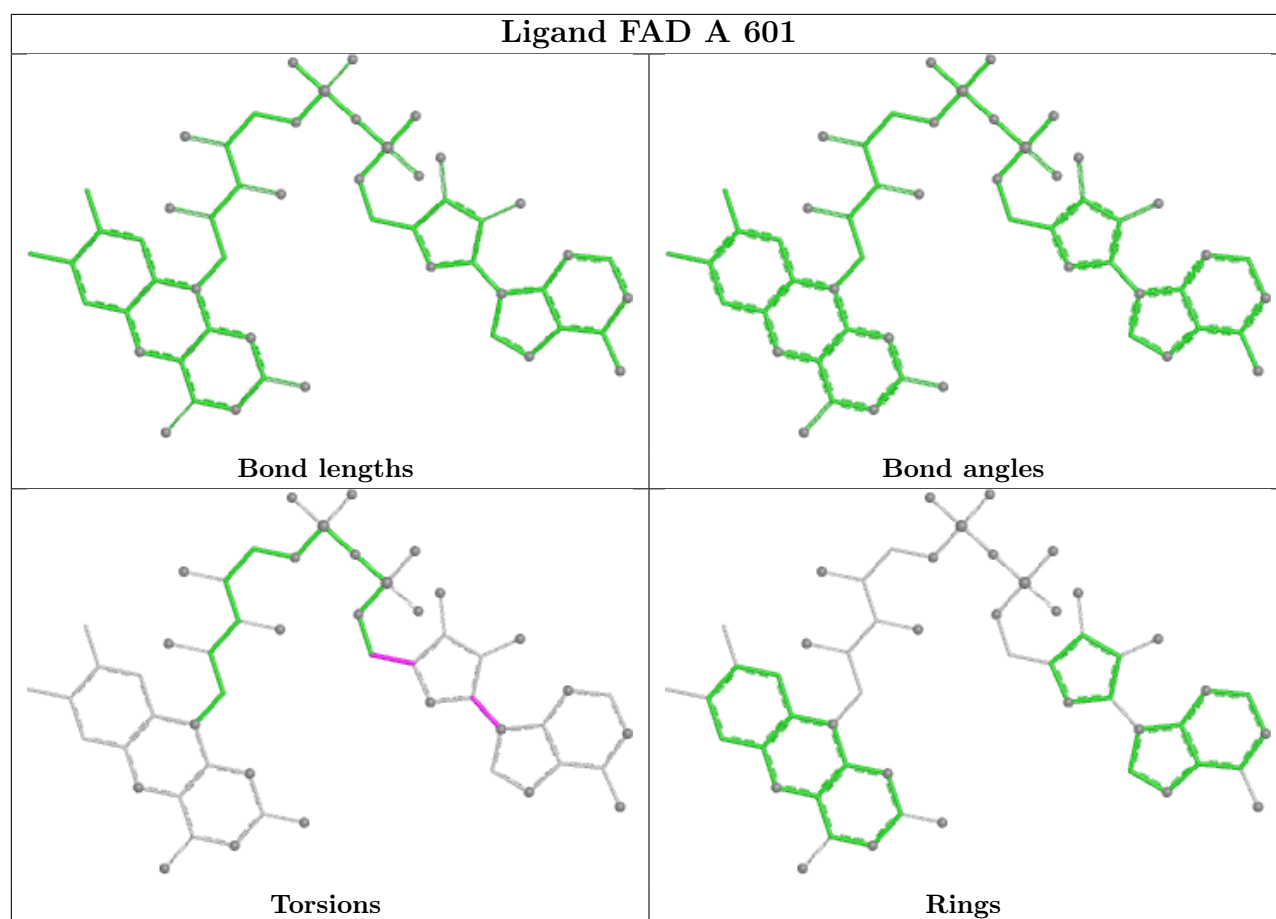
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









## 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	577/598 (96%)	-0.44	3 (0%) 87 82	52, 83, 150, 228	1 (0%)
1	B	574/598 (95%)	-0.45	2 (0%) 90 86	36, 86, 138, 190	2 (0%)
2	C	540/598 (90%)	0.43	28 (5%) 33 25	76, 150, 250, 287	1 (0%)
All	All	1691/1794 (94%)	-0.17	33 (1%) 65 56	36, 98, 201, 287	4 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	290	CYS	4.3
2	C	275	SER	4.2
1	B	580	THR	3.4
2	C	75	LEU	3.1
2	C	350	TYR	3.0
2	C	72	SER	2.9
1	A	39	LYS	2.8
2	C	44	PHE	2.7
2	C	74	PRO	2.7
1	A	40	VAL	2.7
2	C	182	TRP	2.5
2	C	366	VAL	2.5
2	C	229	PHE	2.5
2	C	279	PHE	2.4
2	C	73	MET	2.4
2	C	298	LEU	2.4
2	C	180	PHE	2.3
1	B	373	GLU	2.3
2	C	51	VAL	2.3
2	C	40	VAL	2.3
2	C	37	MET	2.2
2	C	353	LEU	2.2
2	C	365	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	36	ASP	2.2
2	C	404	VAL	2.2
1	A	86	PHE	2.2
2	C	253	LEU	2.2
2	C	109	LEU	2.1
2	C	367	HIS	2.0
2	C	291	VAL	2.0
2	C	92	LEU	2.0
2	C	174	ILE	2.0
2	C	315	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	2CO	A	345	8/9	0.81	0.10	91,100,130,132	0
1	2CO	B	345	8/9	0.90	0.08	92,102,133,135	0

## 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.

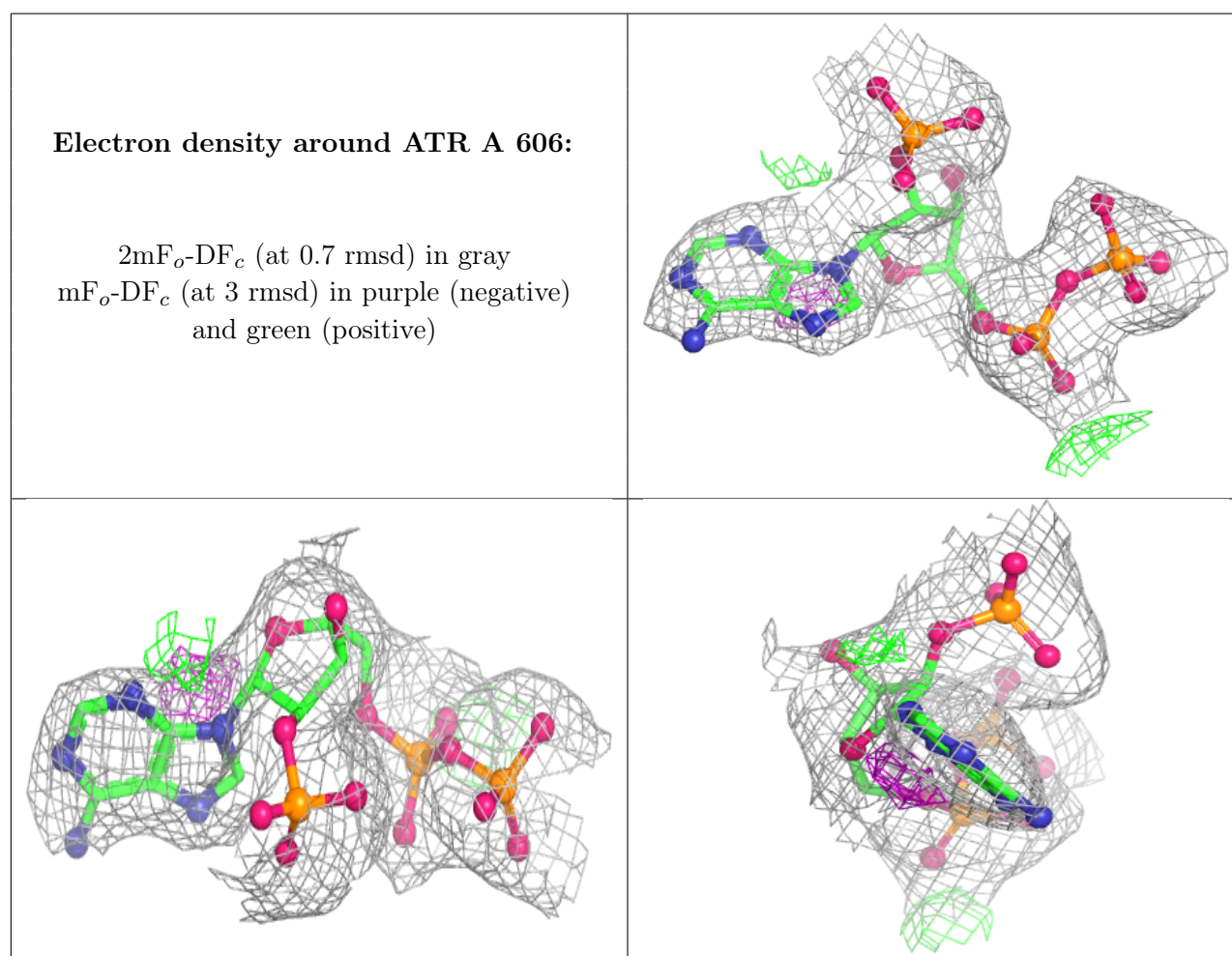
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MPD	B	604	8/8	0.79	0.23	76,88,101,108	8
4	MPD	A	605	8/8	0.84	0.16	131,147,151,151	0
5	ATR	A	606	31/31	0.86	0.10	76,86,99,103	31
4	MPD	A	604	8/8	0.87	0.23	121,131,138,138	0
4	MPD	A	603	8/8	0.88	0.23	98,101,117,118	0
4	MPD	B	603	8/8	0.88	0.24	103,113,117,118	0

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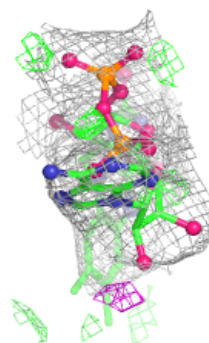
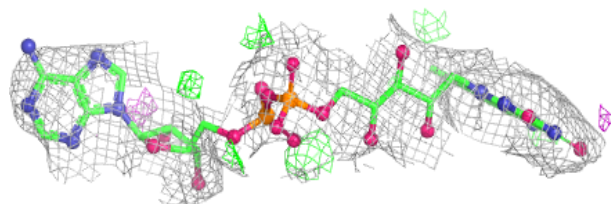
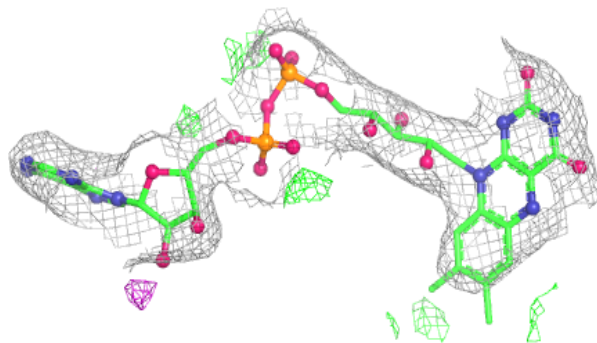
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MPD	A	602	8/8	0.89	0.15	102,118,125,131	0
4	MPD	B	602	8/8	0.90	0.20	90,109,121,127	0
3	FAD	C	601	53/53	0.92	0.10	98,126,141,148	0
3	FAD	B	601	53/53	0.96	0.06	54,68,88,90	0
3	FAD	A	601	53/53	0.97	0.07	55,66,81,86	0

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.

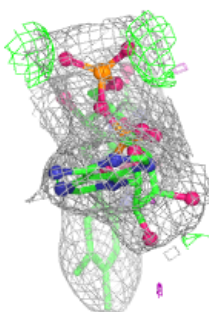
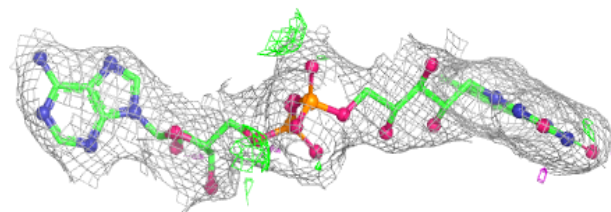
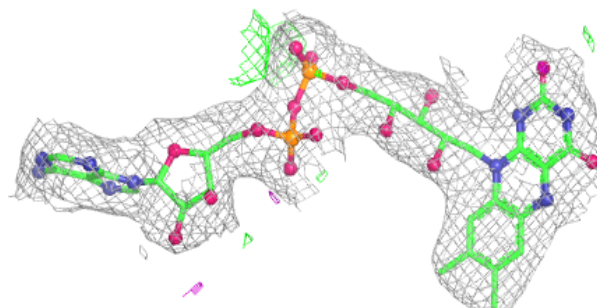


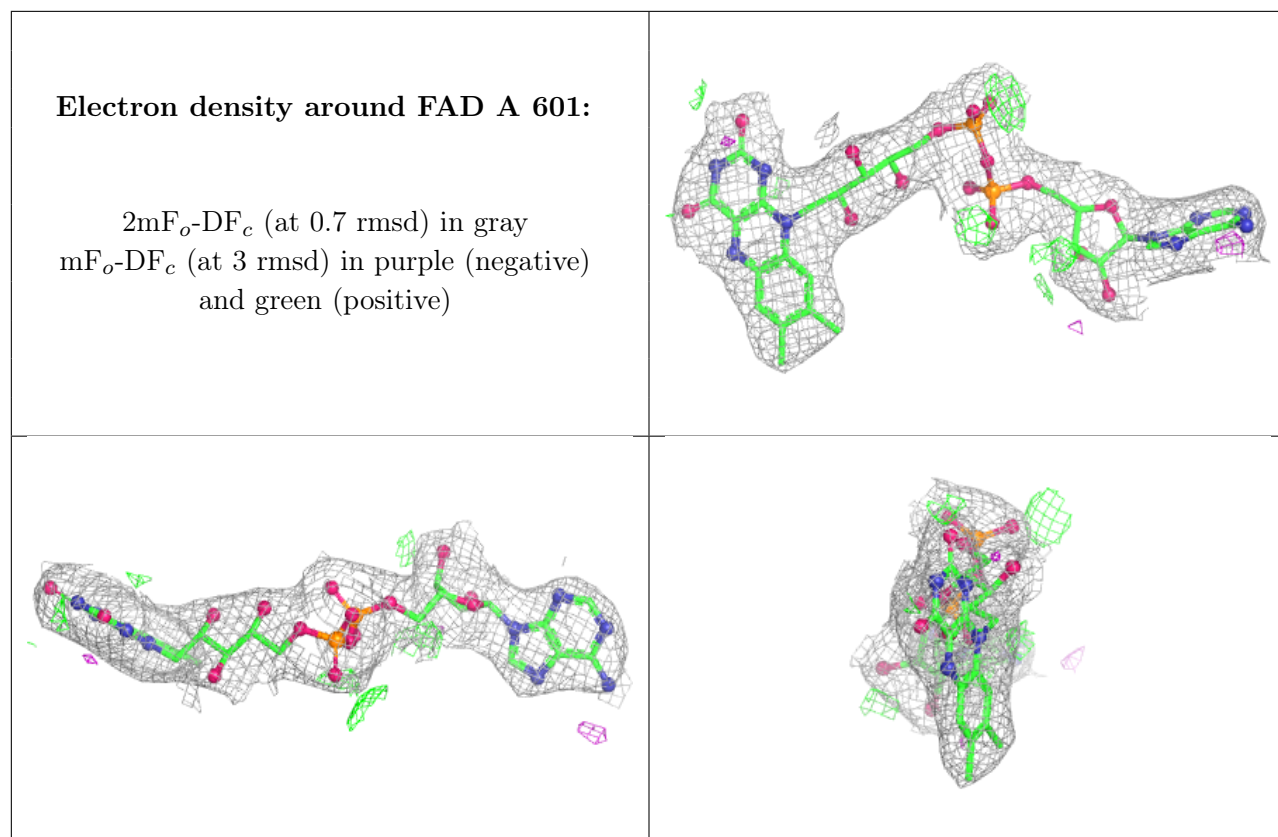
**Electron density around FAD C 601:**

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

**Electron density around FAD B 601:**

$2mF_o-DF_c$  (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.