Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2022 – 04:20 pm BST

PDB ID	:	7PUT
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

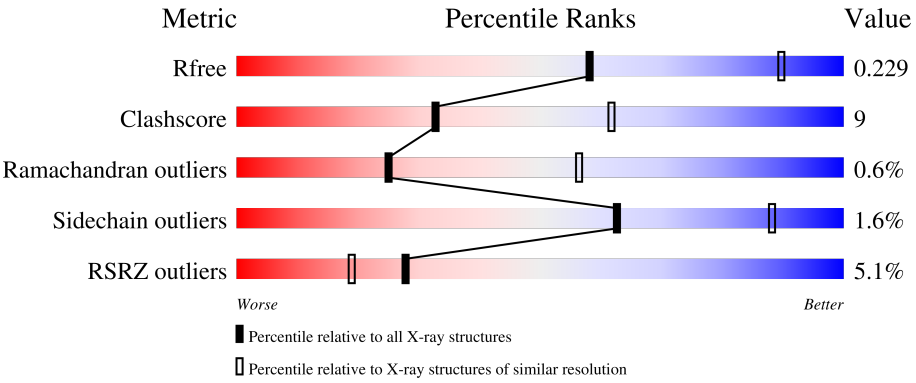
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 >=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 <=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	2% 84% 12%
1	B	598	% 81% 14%
2	C	598	12% 68% 20% 10%

2 Entry composition

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.

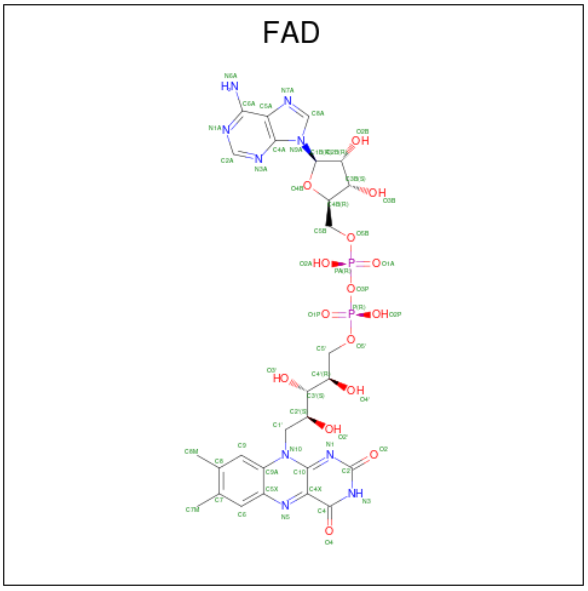
- Molecule 1 is a protein called Glutaredoxin domain-containing protein.

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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

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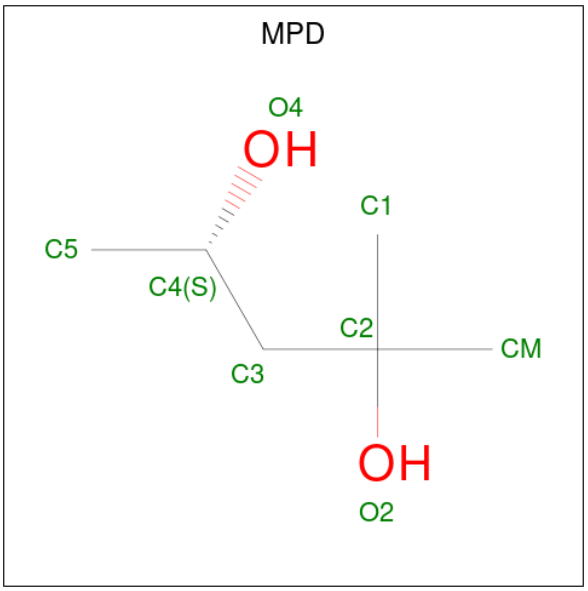
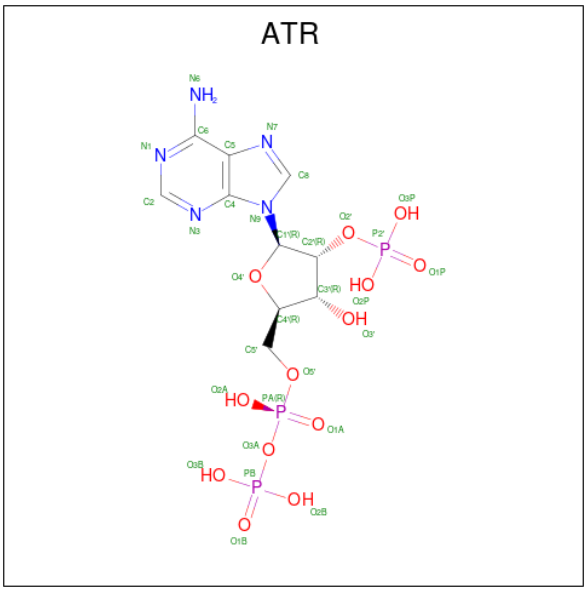
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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 (three-letter code: ATR) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is water.

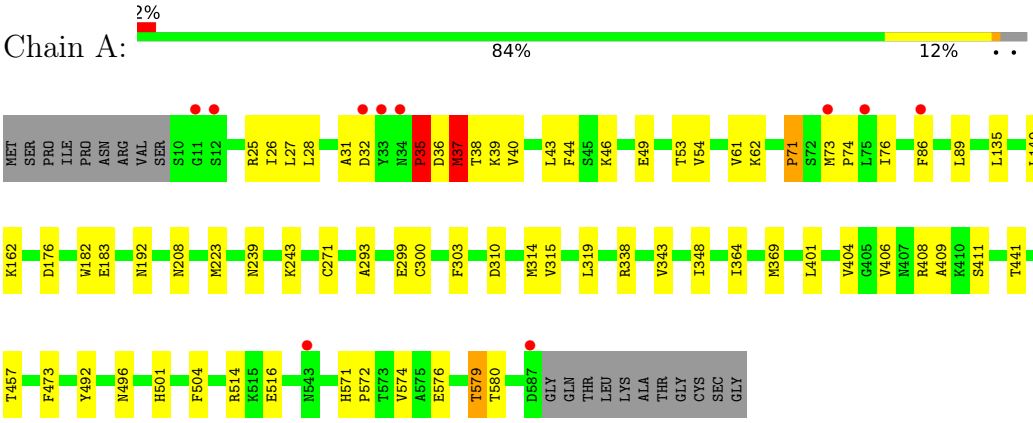
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	4	Total	O	0	0
			4	4		

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.

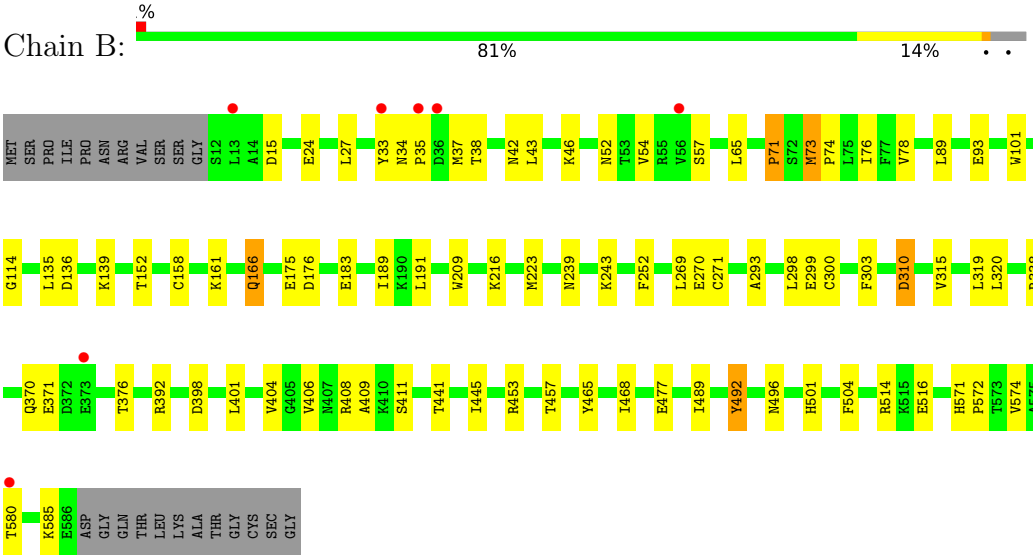
• Molecule 1: Glutaredoxin domain-containing protein

Chain A:



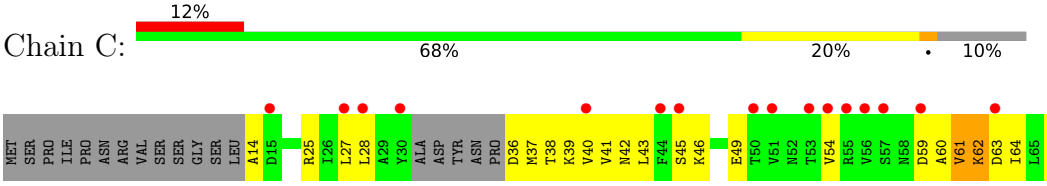
• Molecule 1: Glutaredoxin domain-containing protein

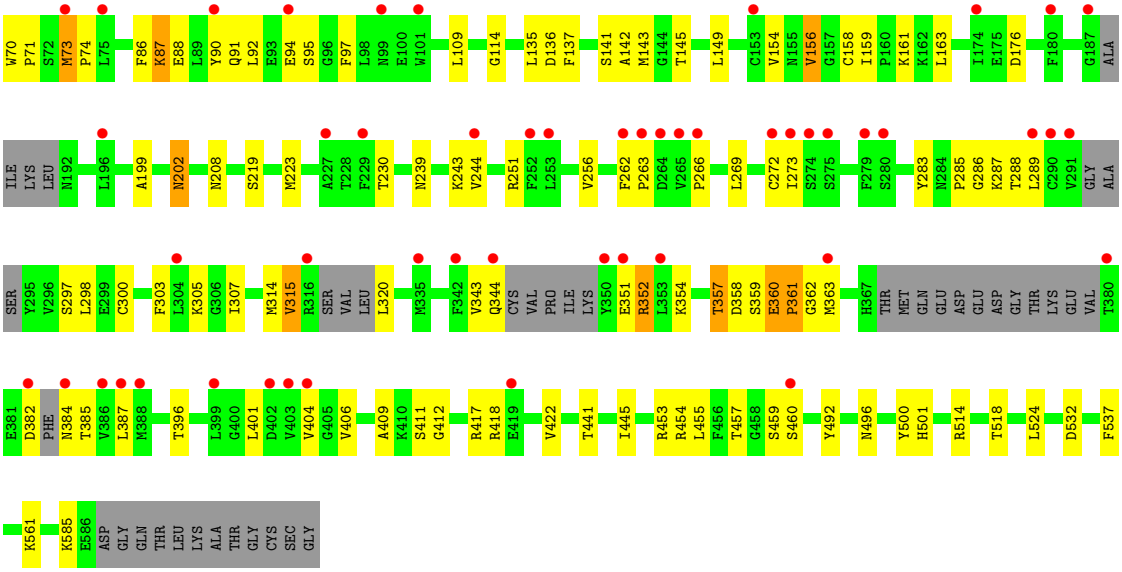
Chain B:



• Molecule 2: Glutaredoxin domain-containing protein

Chain C:




W70 P71 S72 M73 P74 L75 F86 K87 E88 L89 Y90 Q91 L92 E93 E94 S95 G96 F97 L98 N99 E100 W101 L109 G114 L135 D136 F137 S141 A142 M143 G144 T145 L149 C153 V154 N155 V156 G157 C158 I159 P160 K161 K162 L163 I174 E175 D176 F180 G187 A188
ILE LYS LEU N192 L196 A199 N202 N208 S219 M223 A227 T228 F229 T230 N239 K243 V244 R251 P252 L253 V256 F262 P263 D264 V265 P266 L269 C272 I273 S274 S275 P279 S280 Y283 N284 P285 G286 K287 T288 L289 C290 V291 GLY ALA
SER Y295 V296 S297 L298 E299 C300 F303 L304 K305 G306 I307 M314 V315 R316 SER VAL LEU L320 M335 F342 V343 Q344 CYS VAL PRO ILE LYS Y350 E351 R352 L353 K354 T357 D358 S359 E360 P361 G362 M363 H367 THR MET GLN GLU ASP GLU ASP GLY THR LYS GLU VAL T380
E381 D382 PHE N384 T385 V386 L387 M388 T396 L399 G400 L401 D402 V403 V404 G405 V406 A409 K410 S411 G412 R417 R418 E419 V422 T441 I445 R453 R454 L455 F456 T457 G458 S459 S460 Y492 N496 Y500 H501 R514 T518 L524 D532 F537
K561 K585 E586 ASP GLY GLN THR LEU LYS ALA THR GLY CYS SEC GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	147.39Å 260.29Å 130.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 2.80 49.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.13-2.80) 99.9 (49.09-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.196 , 0.229 0.196 , 0.229	Depositor DCC
R_{free} test set	3054 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	85.7	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
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	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13432	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ATR, 2CO, FAD, MPD

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	0.79	0/4572	0.90	3/6179 (0.0%)
1	B	0.79	2/4554 (0.0%)	0.89	3/6155 (0.0%)
2	C	0.76	0/4288	0.89	4/5784 (0.1%)
All	All	0.78	2/13414 (0.0%)	0.90	10/18118 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	GLU	CD-OE1	5.33	1.31	1.25
1	B	477	GLU	CD-OE1	5.16	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	351	GLU	N-CA-C	-12.36	77.64	111.00
1	A	37	MET	CB-CA-C	-9.07	92.26	110.40
1	B	71	PRO	CB-CA-C	-7.20	94.01	112.00
2	C	352	ARG	N-CA-C	-6.78	92.69	111.00
1	A	71	PRO	CB-CA-C	-5.87	97.32	112.00
1	B	492	TYR	CA-C-N	5.86	127.91	116.20
1	A	35	PRO	CB-CA-C	-5.61	97.97	112.00
2	C	352	ARG	CB-CA-C	-5.39	99.61	110.40
1	B	71	PRO	N-CA-C	5.22	125.68	112.10
2	C	202	ASN	CB-CA-C	5.01	120.42	110.40

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	4492	0	4515	51	0
1	B	4474	0	4503	66	0
2	C	4210	0	4236	115	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	4	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	13456	234	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 (234) 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	1.24	1.12
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:363:MET:HE2	2:C:382:ASP:CB	2.04	0.86
2:C:417:ARG:HG2	2:C:422:VAL:HG23	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:B:604:MPD:HO2	4:B:604:MPD:HO4	1.48	0.58
1:A:315:VAL:HG11	1:A:319:LEU:CD2	2.34	0.58
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
1:B:34:ASN:H	1:B:37:MET:HE3	1.68	0.57
2:C:273:ILE:O	2:C:387:LEU:CD1	2.52	0.57
1:B:33:TYR:HA	1:B:37:MET:HE1	1.87	0.56
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: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: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:B:34:ASN:H	1:B:37:MET:HE2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:359:SER:C	2:C:360:GLU:HG2	2.31	0.50
2:C:69:GLY:HA2	2:C:70:TRP:CE3	2.47	0.50
2:C:28:LEU:HD12	2:C:40:VAL:HG11	1.94	0.50
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
2:C:315:VAL:O	2:C:344:GLN:C	2.51	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
1:A:409:ALA:O	1:A:411:SER:O	2.30	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
4:A:602:MPD:HM1	1:B:175:GLU:OE2	2.15	0.47
2:C:141:SER:OG	2:C:142:ALA:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:310:ASP:OD1	1:A:310:ASP:C	2.53	0.46
2:C:135:LEU:HD23	2:C:223:MET:HB2	1.97	0.46
1:B:310:ASP:OD1	1:B:310:ASP:C	2.54	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: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:273:ILE:O	2:C:273:ILE:HG22	2.16	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
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:36:ASP:C	2:C:38:THR:H	2.19	0.45
1:A:348:ILE:HD13	1:A:369:MET:HG2	1.98	0.45
1:B:43:LEU:HD23	1:B:43:LEU:C	2.37	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:518:THR:O	2:C:518:THR:CG2	2.65	0.44
1:A:158:CYS:HB3	3:A:601:FAD:C4	2.47	0.44
2:C:59:ASP:C	2:C:61:VAL:H	2.21	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
1:B:139:LYS:NZ	1:B:398:ASP:OD2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:73:MET:O	1:B:74:PRO:C	2.57	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
2:C:36:ASP:C	2:C:38:THR:N	2.72	0.42
2:C:62:LYS:HG3	2:C:63:ASP:N	2.34	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:O	1:A:32:ASP:C	2.57	0.42
1:A:31:ALA:CB	1:A:73:MET:SD	3.08	0.42
2:C:262:PHE:HZ	2:C:272:CYS:HG	1.65	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: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:A:26:ILE:HD13	1:A:44:PHE:CE1	2.55	0.41
1:A:73:MET:O	1:A:74:PRO:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:114:GLY:HA3	1:B:136:ASP:HB2	2.03	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

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%)	29	61
1	B	572/598 (96%)	550 (96%)	21 (4%)	1 (0%)	47	78
2	C	524/598 (88%)	488 (93%)	30 (6%)	6 (1%)	14	41
All	All	1671/1794 (93%)	1585 (95%)	76 (4%)	10 (1%)	25	56

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

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Mol	Chain	Res	Type
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%)	484 (99%)	4 (1%)	81 94
1	B	486/503 (97%)	476 (98%)	10 (2%)	53 84
2	C	457/504 (91%)	448 (98%)	9 (2%)	55 84
All	All	1431/1510 (95%)	1408 (98%)	23 (2%)	62 88

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	158	CYS
1	A	501	HIS
1	A	579	THR
1	B	15	ASP
1	B	57	SER
1	B	73	MET
1	B	158	CYS
1	B	166	GLN
1	B	191	LEU
1	B	310	ASP
1	B	370	GLN
1	B	496	ASN
1	B	579	THR
2	C	86	PHE
2	C	87	LYS

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Mol	Chain	Res	Type
2	C	109	LEU
2	C	156	VAL
2	C	158	CYS
2	C	219	SER
2	C	315	VAL
2	C	357	THR
2	C	360	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	ASN
1	B	155	ASN
1	B	166	GLN
1	B	208	ASN
1	B	367	HIS
2	C	58	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	0.74	0	1,7,9	0.29	0
1	2CO	A	345	1	3,7,8	0.99	0	1,7,9	0.38	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 monosaccharides 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	$\#\|Z\| > 2$
3	FAD	B	601	-	51,58,58	1.04	2 (3%)	60,89,89	1.86	6 (10%)
4	MPD	B	603	-	7,7,7	0.19	0	9,10,10	0.69	0
4	MPD	A	603	-	7,7,7	0.15	0	9,10,10	0.76	0
4	MPD	A	604	-	7,7,7	0.11	0	9,10,10	0.35	0
4	MPD	A	605	-	7,7,7	0.10	0	9,10,10	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MPD	A	602	-	7,7,7	0.10	0	9,10,10	0.36	0
3	FAD	A	601	-	51,58,58	1.14	2 (3%)	60,89,89	1.90	5 (8%)
4	MPD	B	604	-	7,7,7	0.27	0	9,10,10	0.42	0
5	ATR	A	606	-	27,33,33	1.16	3 (11%)	35,52,52	1.52	5 (14%)
4	MPD	B	602	-	7,7,7	0.11	0	9,10,10	0.54	0
3	FAD	C	601	-	51,58,58	1.11	2 (3%)	60,89,89	1.75	7 (11%)

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	FAD	B	601	-	-	5/30/50/50	0/6/6/6
4	MPD	B	603	-	-	1/5/5/5	-
4	MPD	A	603	-	-	1/5/5/5	-
4	MPD	A	604	-	-	0/5/5/5	-
4	MPD	A	605	-	-	1/5/5/5	-
4	MPD	A	602	-	-	0/5/5/5	-
3	FAD	A	601	-	-	2/30/50/50	0/6/6/6
4	MPD	B	604	-	-	2/5/5/5	-
5	ATR	A	606	-	-	2/17/37/37	0/3/3/3
4	MPD	B	602	-	-	1/5/5/5	-
3	FAD	C	601	-	-	8/30/50/50	0/6/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	FAD	C4X-C10	5.85	1.44	1.38
3	C	601	FAD	C4X-C10	5.77	1.44	1.38
3	B	601	FAD	C4X-C10	4.92	1.43	1.38
5	A	606	ATR	O4'-C1'	3.29	1.45	1.41
3	C	601	FAD	C4-N3	2.77	1.37	1.33
5	A	606	ATR	C5-C4	2.68	1.48	1.40
3	B	601	FAD	C4-N3	2.58	1.37	1.33
3	A	601	FAD	C4-N3	2.54	1.37	1.33
5	A	606	ATR	C2-N3	2.09	1.35	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	FAD	C2-N3-C4	8.70	122.49	115.14
3	B	601	FAD	C2-N3-C4	8.40	122.24	115.14
3	C	601	FAD	C2-N3-C4	8.14	122.02	115.14
3	A	601	FAD	C10-C4X-C4	-7.27	115.14	119.95
3	B	601	FAD	C10-C4X-C4	-6.90	115.38	119.95
3	C	601	FAD	C10-C4X-C4	-5.49	116.32	119.95
3	B	601	FAD	C10-C4X-N5	5.32	124.94	121.26
3	A	601	FAD	C10-C4X-N5	5.20	124.86	121.26
3	C	601	FAD	C10-C4X-N5	4.95	124.68	121.26
3	C	601	FAD	C4X-C4-N3	-4.19	117.70	123.43
5	A	606	ATR	N3-C2-N1	-4.15	122.19	128.68
3	B	601	FAD	C4X-C10-N10	-4.11	116.08	120.30
3	A	601	FAD	C4X-C4-N3	-3.79	118.25	123.43
3	C	601	FAD	C4X-C10-N10	-3.53	116.67	120.30
3	B	601	FAD	C4X-C4-N3	-3.53	118.60	123.43
3	A	601	FAD	C4X-C10-N10	-3.50	116.70	120.30
3	C	601	FAD	C1'-N10-C9A	2.77	120.47	118.29
5	A	606	ATR	C2-N1-C6	2.54	123.09	118.75
5	A	606	ATR	C4-C5-N7	-2.39	106.91	109.40
3	C	601	FAD	C5A-C6A-N6A	2.28	123.82	120.35
3	B	601	FAD	C5A-C6A-N6A	2.25	123.78	120.35
5	A	606	ATR	O3'-C3'-C4'	-2.12	104.91	111.05
5	A	606	ATR	O2'-P2'-O1P	-2.10	101.31	109.39

There are no chirality outliers.

All (23) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	B	603	MPD	C2-C3-C4-C5
3	C	601	FAD	C5B-O5B-PA-O2A
3	C	601	FAD	P-O3P-PA-O2A
3	B	601	FAD	P-O3P-PA-O1A
4	B	604	MPD	O2-C2-C3-C4
4	A	603	MPD	C2-C3-C4-C5
3	B	601	FAD	C5'-O5'-P-O1P
4	B	604	MPD	C2-C3-C4-O4

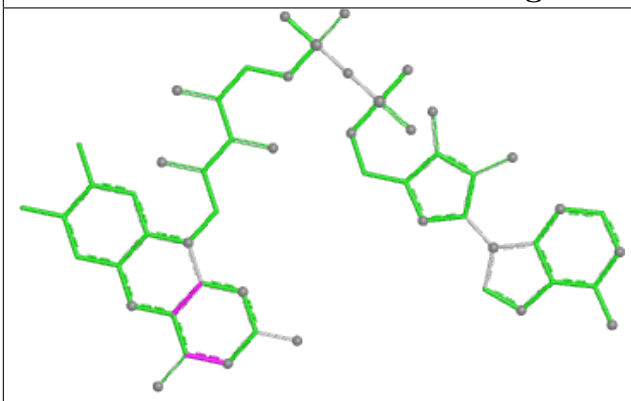
There are no ring outliers.

9 monomers are involved in 19 short contacts:

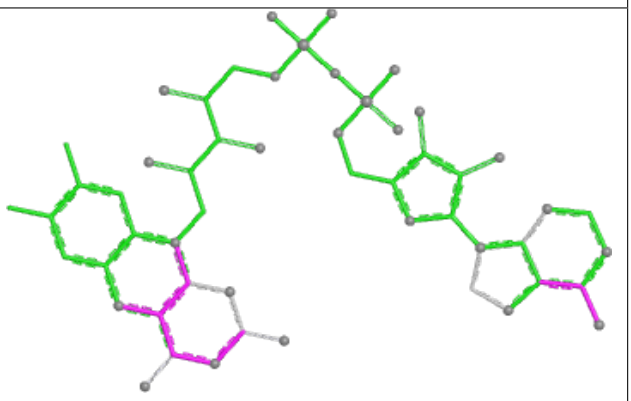
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	FAD	3	0
4	A	603	MPD	2	0
4	A	605	MPD	1	0
4	A	602	MPD	3	0
3	A	601	FAD	2	0
4	B	604	MPD	3	0
5	A	606	ATR	1	0
4	B	602	MPD	1	0
3	C	601	FAD	3	0

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 then 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.

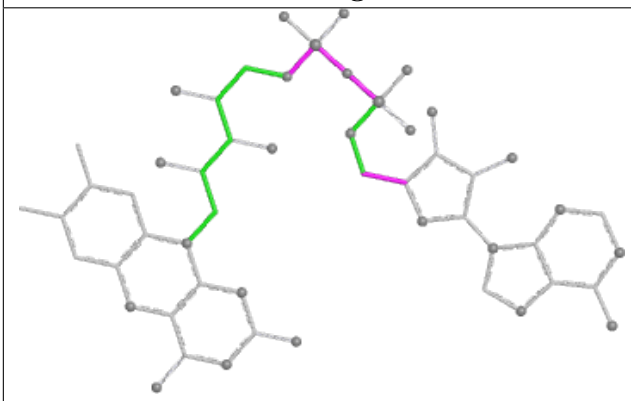
Ligand FAD B 601



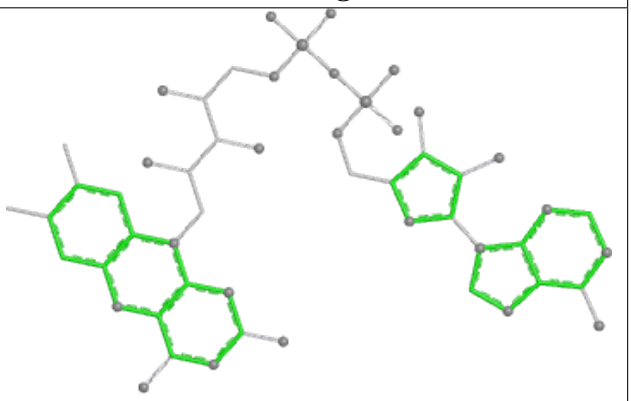
Bond lengths



Bond angles

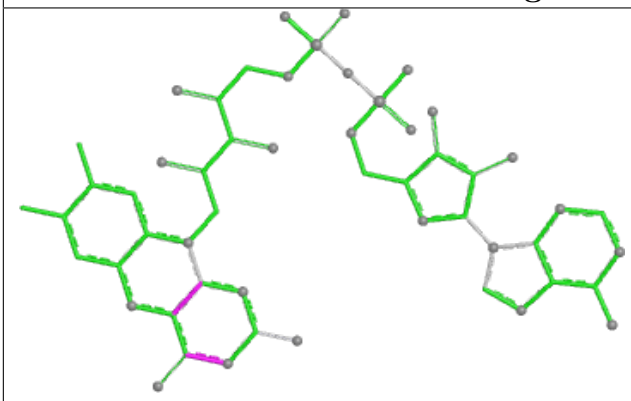


Torsions

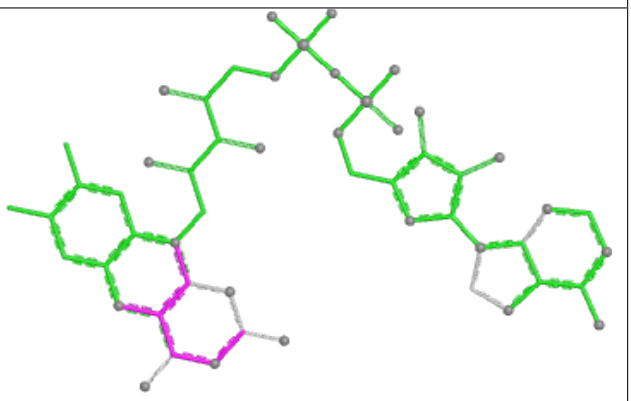


Rings

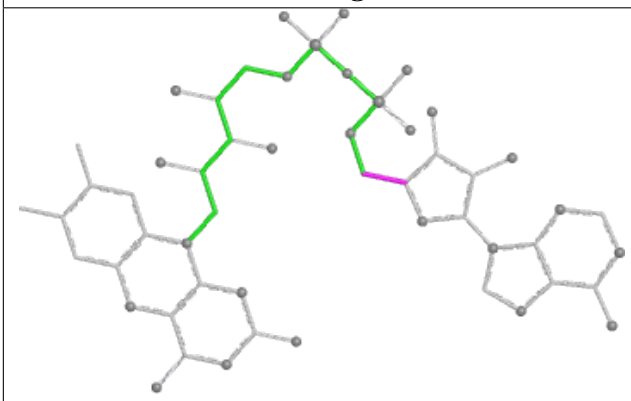
Ligand FAD A 601



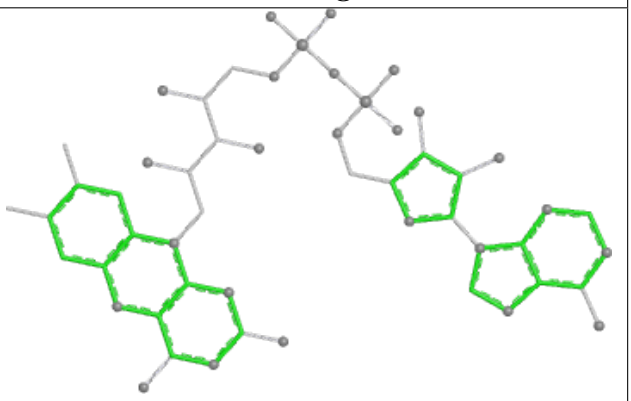
Bond lengths



Bond angles

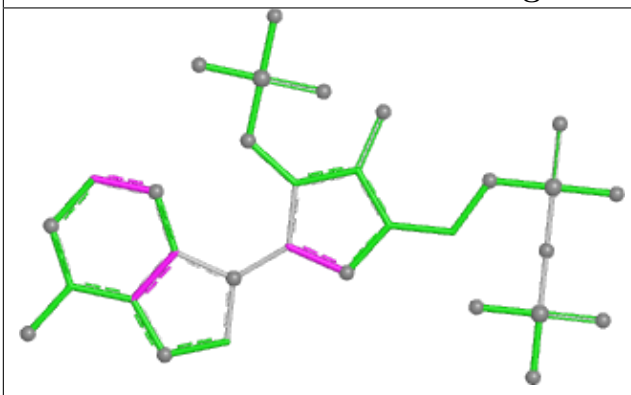


Torsions

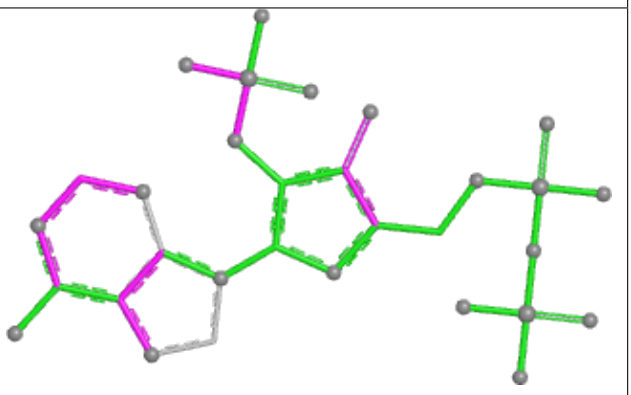


Rings

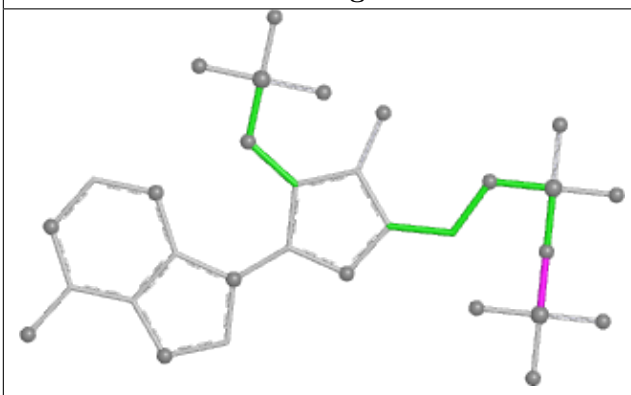
Ligand ATR A 606



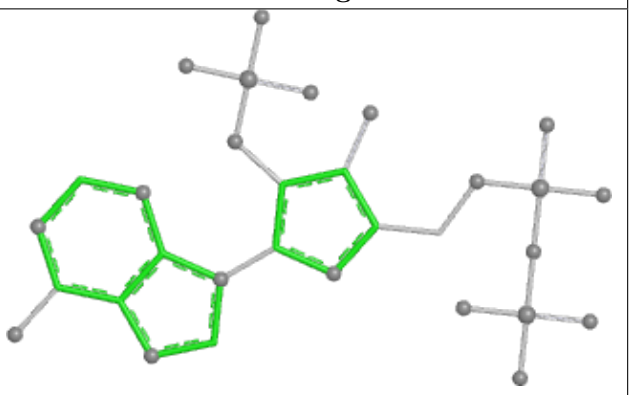
Bond lengths



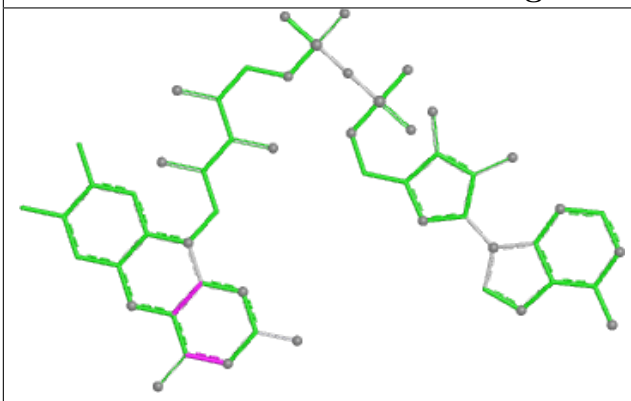
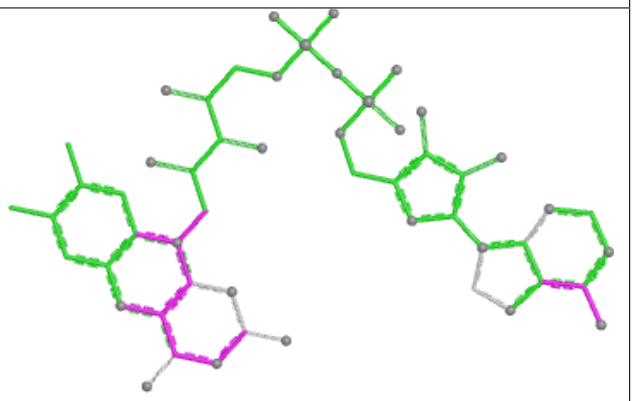
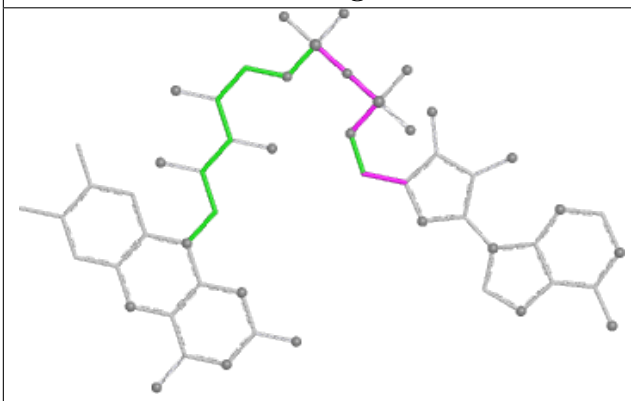
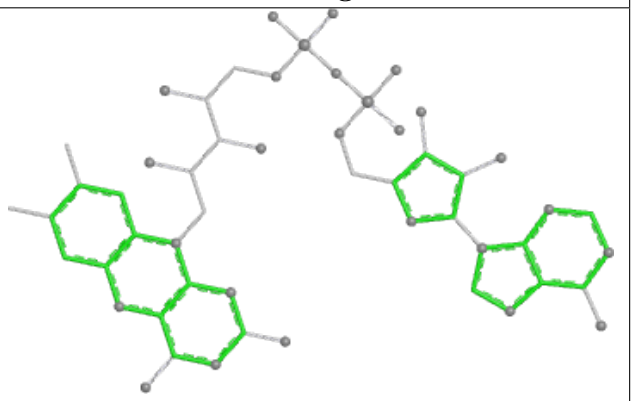
Bond angles



Torsions



Rings

Ligand FAD C 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	577/598 (96%)	-0.18	10 (1%) 70 63	52, 83, 150, 228	1 (0%)
1	B	574/598 (95%)	-0.23	8 (1%) 75 70	51, 86, 139, 190	2 (0%)
2	C	540/598 (90%)	0.61	69 (12%) 3 2	76, 150, 250, 287	1 (0%)
All	All	1691/1794 (94%)	0.06	87 (5%) 28 19	51, 98, 201, 287	4 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	55	ARG	7.6
2	C	290	CYS	7.0
2	C	275	SER	6.8
1	A	33	TYR	6.5
2	C	229	PHE	6.3
2	C	272	CYS	6.1
2	C	54	VAL	5.6
2	C	387	LEU	5.2
2	C	353	LEU	5.0
2	C	273	ILE	5.0
2	C	388	MET	4.9
2	C	404	VAL	4.6
2	C	386	VAL	4.5
2	C	90	TYR	4.5
1	A	587	ASP	4.2
2	C	263	PRO	4.2
2	C	50	THR	4.1
2	C	57	SER	4.1
2	C	40	VAL	4.1
2	C	289	LEU	4.1
1	B	33	TYR	4.0
2	C	402	ASP	4.0
2	C	265	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
2	C	264	ASP	3.9
2	C	51	VAL	3.9
2	C	227	ALA	3.8
2	C	342	PHE	3.8
2	C	344	GLN	3.7
2	C	351	GLU	3.7
2	C	280	SER	3.7
2	C	266	PRO	3.6
1	A	32	ASP	3.6
2	C	45	SER	3.6
2	C	59	ASP	3.6
2	C	15	ASP	3.5
2	C	75	LEU	3.5
2	C	279	PHE	3.5
2	C	460	SER	3.5
1	B	36	ASP	3.4
2	C	291	VAL	3.3
2	C	44	PHE	3.3
2	C	252	PHE	3.2
2	C	63	ASP	3.1
2	C	187	GLY	3.0
2	C	73	MET	3.0
2	C	27	LEU	3.0
2	C	68	VAL	2.9
2	C	262	PHE	2.9
2	C	350	TYR	2.9
2	C	382	ASP	2.9
2	C	316	ARG	2.8
2	C	384	ASN	2.8
1	B	373	GLU	2.8
1	B	344	GLN	2.7
1	A	73	MET	2.7
1	A	86	PHE	2.6
2	C	403	VAL	2.5
2	C	30	TYR	2.5
2	C	174	ILE	2.4
2	C	380	THR	2.4
2	C	244	VAL	2.4
2	C	99	ASN	2.4
2	C	53	THR	2.4
2	C	196	LEU	2.4
2	C	56	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	399	LEU	2.3
1	A	12	SER	2.3
1	B	580	THR	2.3
1	B	56	VAL	2.3
2	C	363	MET	2.3
1	A	11	GLY	2.3
1	A	75	LEU	2.1
1	B	13	LEU	2.1
2	C	253	LEU	2.1
2	C	274	SER	2.1
2	C	304	LEU	2.1
2	C	153	CYS	2.1
2	C	180	PHE	2.1
2	C	67	ILE	2.1
1	B	35	PRO	2.1
1	A	34	ASN	2.1
1	A	543	ASN	2.1
2	C	28	LEU	2.1
2	C	101	TRP	2.1
2	C	419	GLU	2.0
2	C	94	GLU	2.0
2	C	335	MET	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	2CO	A	345	8/9	0.86	0.11	91,100,130,132	0
1	2CO	B	345	8/9	0.90	0.11	92,102,133,135	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

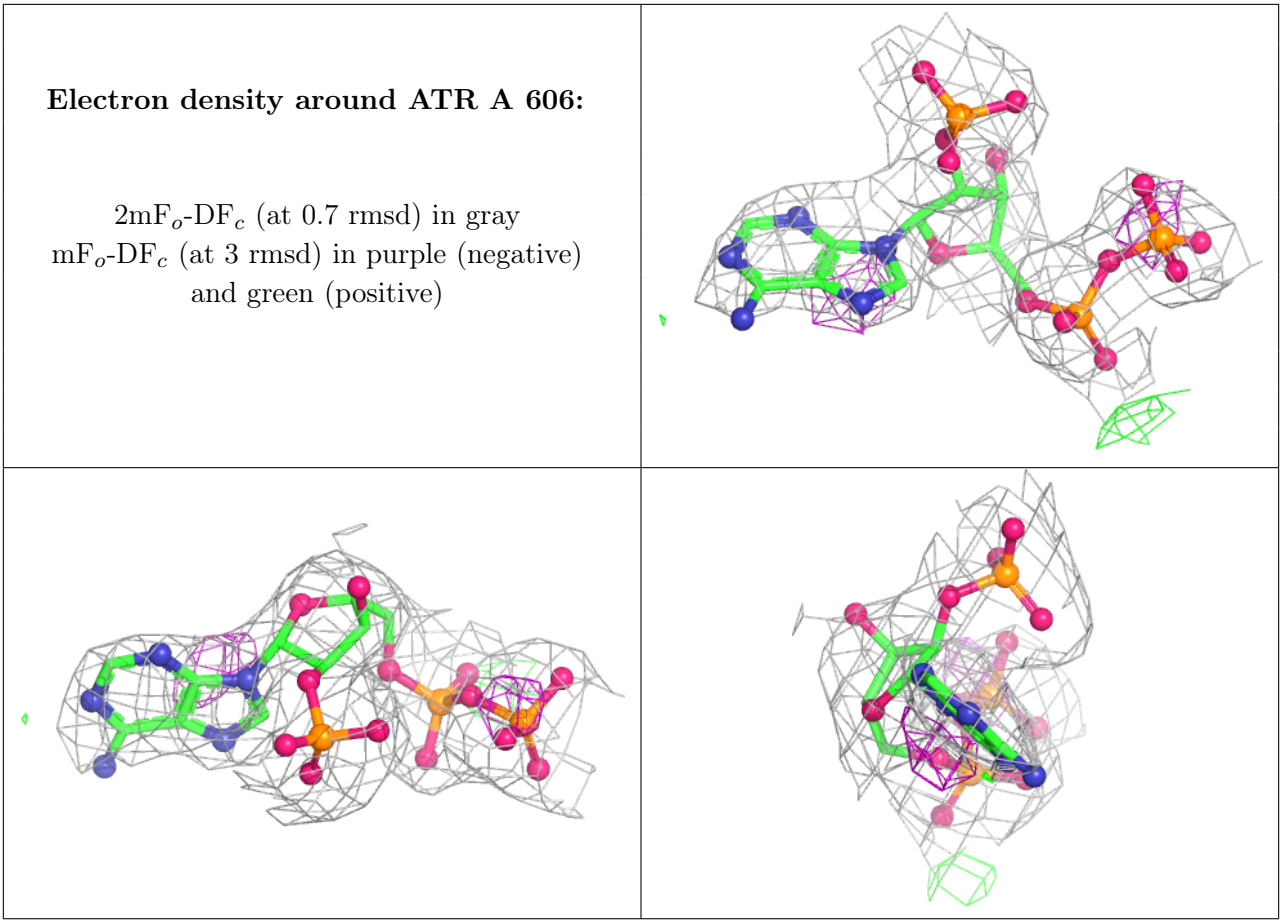
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MPD	A	604	8/8	0.82	0.54	121,131,138,138	0
4	MPD	A	605	8/8	0.85	0.26	131,147,151,151	0
4	MPD	B	604	8/8	0.85	0.31	76,88,101,108	8
4	MPD	A	603	8/8	0.86	0.29	98,101,117,118	0
5	ATR	A	606	31/31	0.87	0.20	76,86,99,103	31
3	FAD	C	601	53/53	0.89	0.20	98,126,141,148	0
4	MPD	A	602	8/8	0.91	0.24	102,118,125,131	0
4	MPD	B	603	8/8	0.91	0.33	103,113,117,118	0
4	MPD	B	602	8/8	0.92	0.25	90,109,121,127	0
3	FAD	B	601	53/53	0.96	0.17	54,68,88,90	0
3	FAD	A	601	53/53	0.96	0.18	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.

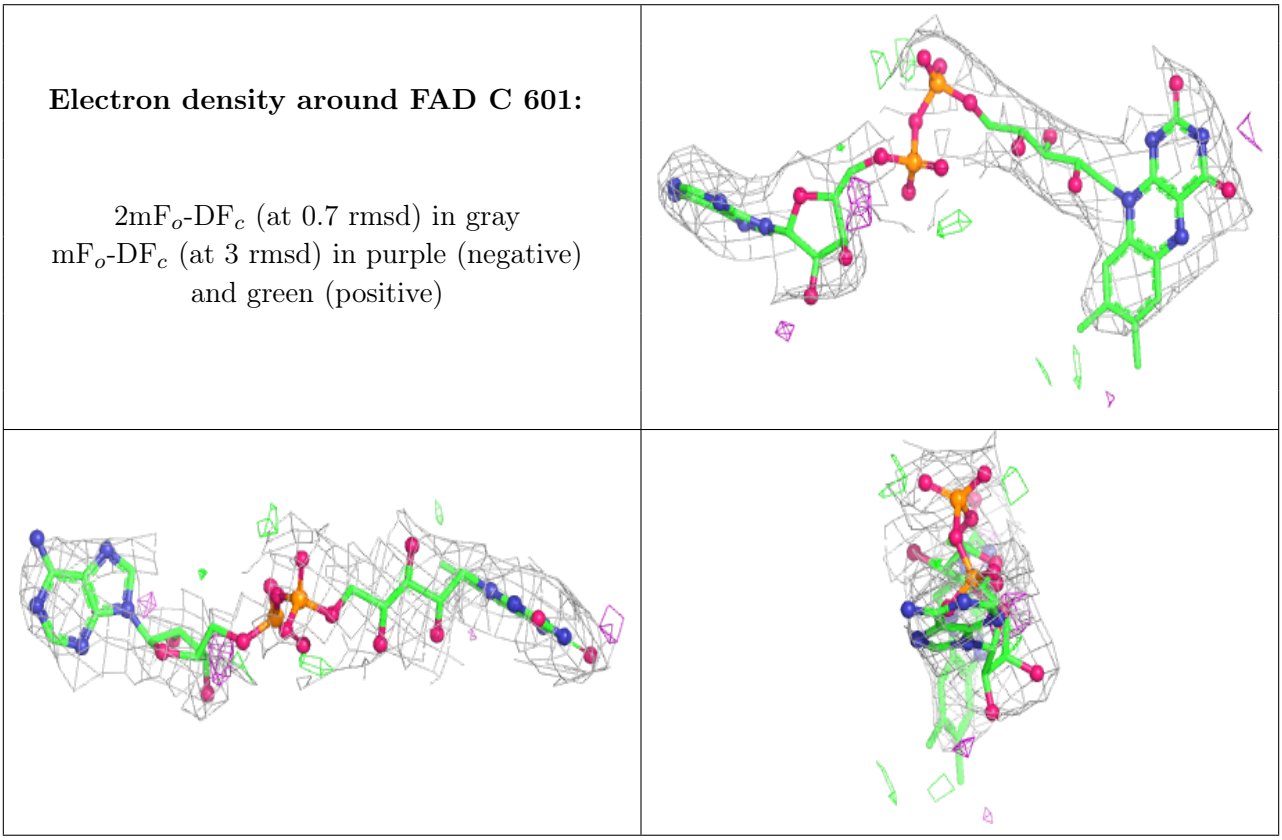
Electron density around ATR A 606:

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



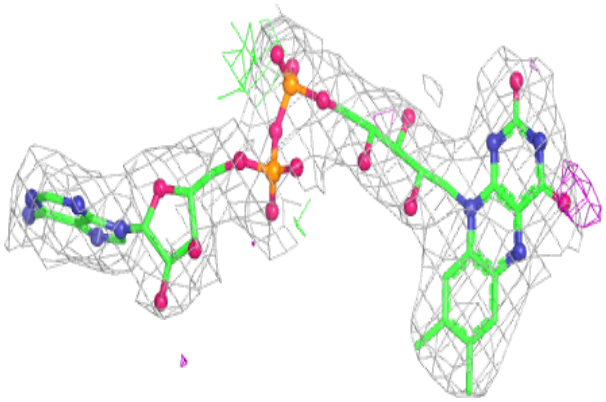
Electron density around FAD C 601:

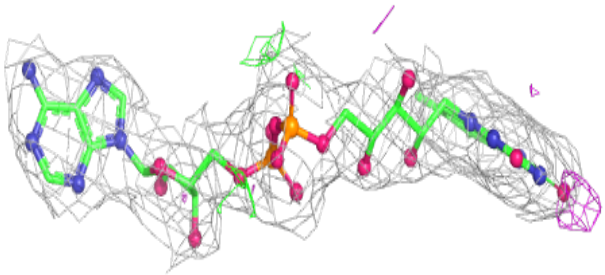
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

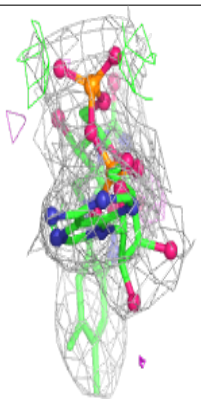


Electron density around FAD B 601:

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

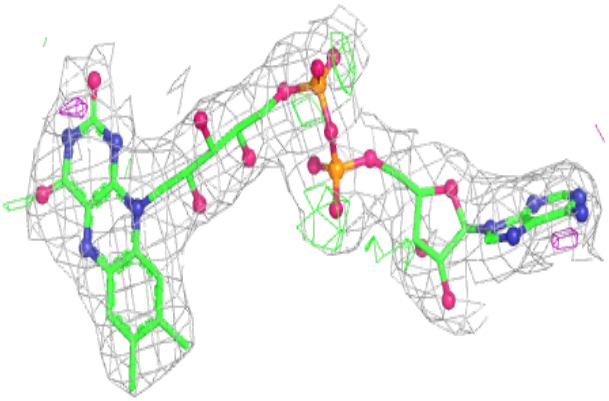


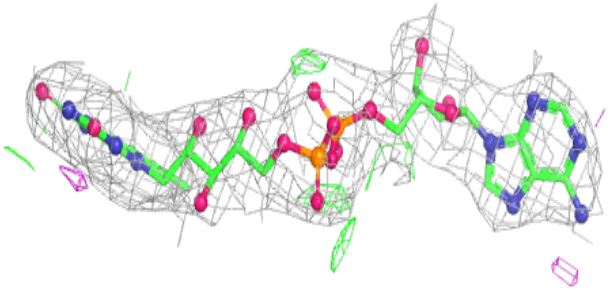


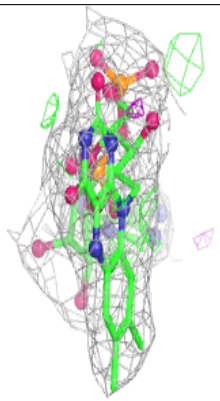


Electron density around FAD A 601:

$2mF_o$-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.