



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:28 AM UTC

PDB ID : 7P0X / pdb_00007p0x
Title : Crystal structure of Thioredoxin reductase from Brugia Malayi
Authors : Fata, F.; Ardini, M.; Silvestri, I.; Gabriele, F.; Cheng, Q.; Arner, E.S.J.; Williams, D.L.
Deposited on : 2021-06-30
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

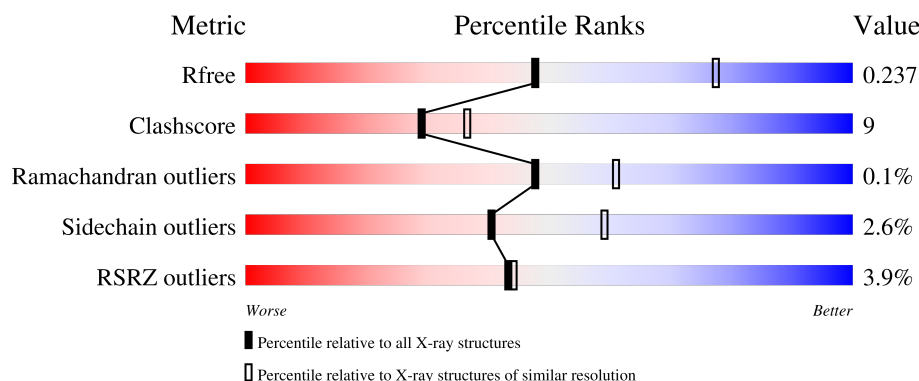
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	598	
1	B	598	
2	C	598	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13517 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	576	Total	C	N	O	S	0	1	0
			4486	2862	752	843	29			
1	B	581	Total	C	N	O	S	0	1	0
			4511	2875	757	848	30			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	550	Total	C	N	O	S	0	0	0
			4270	2732	718	792	28			

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



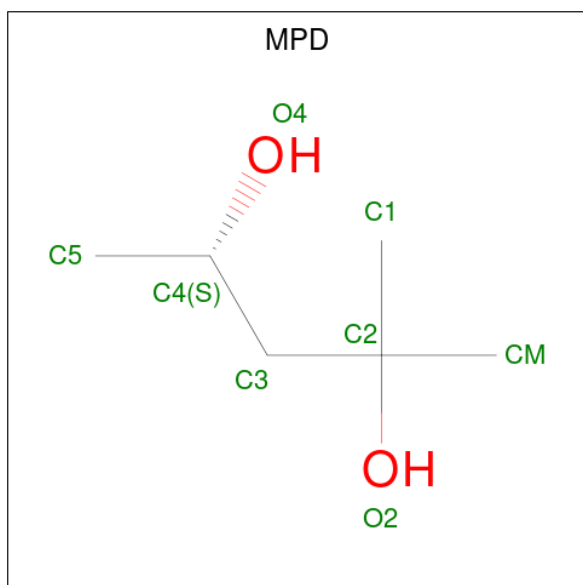
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Cl	0	0
			3	3		

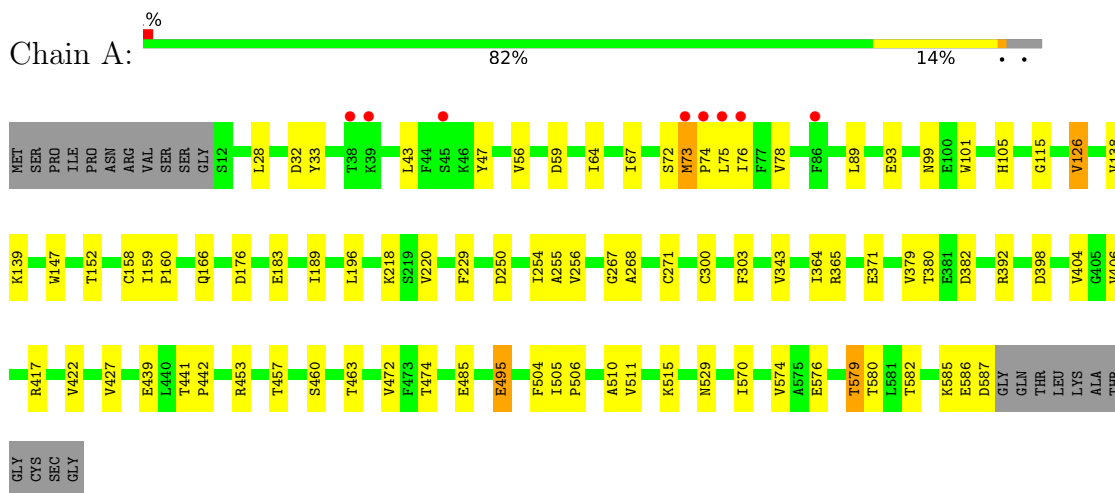
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	34	Total 34	O 34	0	0
7	B	26	Total 26	O 26	0	0
7	C	2	Total 2	O 2	0	0

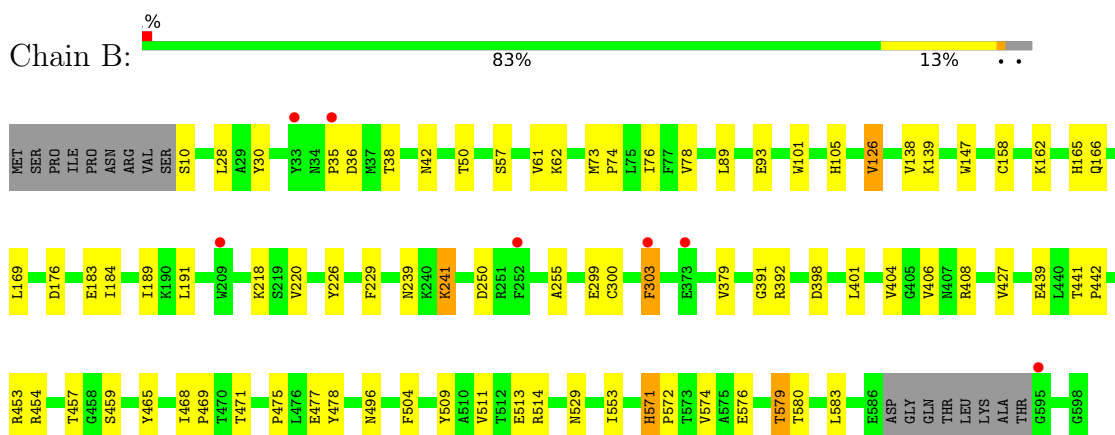
3 Residue-property plots [i](#)

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.

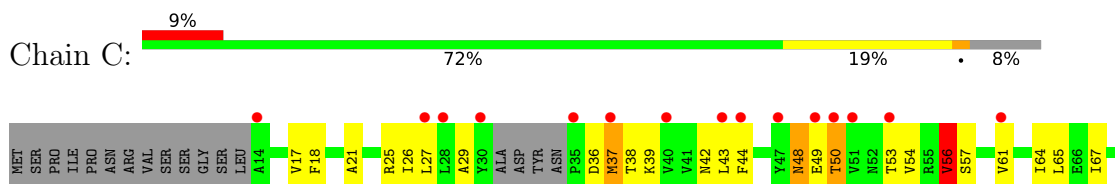
- Molecule 1: Glutaredoxin domain-containing protein

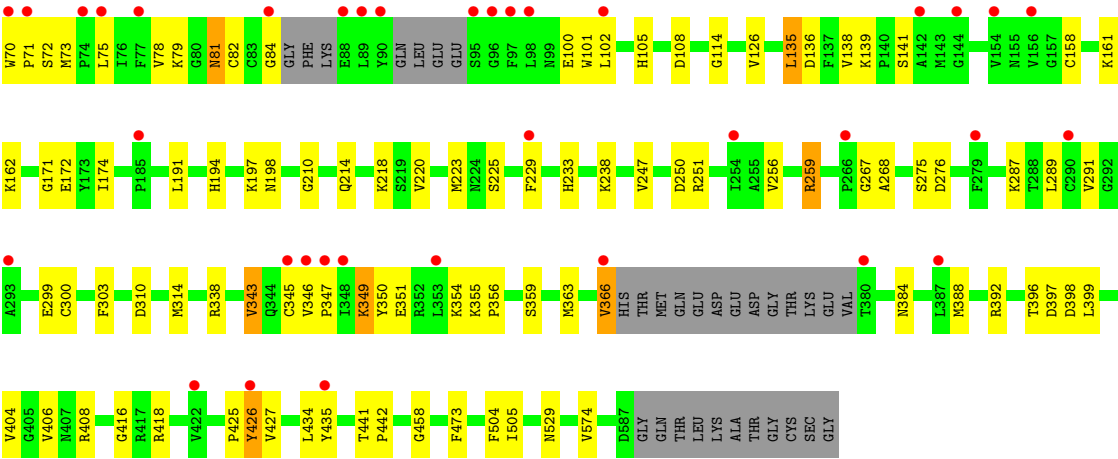


- Molecule 1: Glutaredoxin domain-containing protein



- Molecule 2: Glutaredoxin domain-containing protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	146.92Å 258.99Å 129.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 2.55 48.90 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.90-2.55) 99.9 (48.90-2.55)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.197 , 0.237 0.200 , 0.237	Depositor DCC
R_{free} test set	3847 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 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	13517	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEC, CSO, FAD, MPD, CL, NA

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	5/4570 (0.1%)	1.41	13/6177 (0.2%)
1	B	1.11	3/4584 (0.1%)	1.36	4/6190 (0.1%)
2	C	1.10	0/4352	1.43	12/5878 (0.2%)
All	All	1.12	8/13506 (0.1%)	1.40	29/18245 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	582	THR	C-N	-7.58	1.22	1.33
1	B	583	LEU	C-O	7.13	1.32	1.23
1	A	115	GLY	C-O	6.21	1.29	1.24
1	A	176	ASP	C-O	5.59	1.30	1.24
1	B	571	HIS	CE1-NE2	5.54	1.38	1.32
1	B	475	PRO	C-O	-5.24	1.17	1.24
1	A	463	THR	C-O	-5.21	1.17	1.23
1	A	196	LEU	C-O	5.01	1.29	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	81	ASN	N-CA-C	14.98	129.74	111.02
2	C	349	LYS	N-CA-C	14.38	141.42	110.80
2	C	349	LYS	CB-CA-C	-8.87	92.76	110.42
2	C	426	TYR	CB-CA-C	8.42	122.19	110.06
1	A	73	MET	N-CA-C	7.28	122.66	112.75
2	C	359	SER	CB-CA-C	-6.84	100.08	111.23
1	A	255	ALA	CA-C-N	6.59	130.97	121.02
1	A	255	ALA	C-N-CA	6.59	130.97	121.02
1	B	50	THR	CB-CA-C	5.98	119.61	109.75
2	C	346	VAL	N-CA-C	-5.85	103.60	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ASP	CA-CB-CG	5.62	118.22	112.60
2	C	50	THR	N-CA-C	5.56	122.64	110.80
2	C	81	ASN	CB-CA-C	-5.50	102.17	112.30
1	A	72	SER	CA-C-N	5.47	127.59	120.26
1	A	72	SER	C-N-CA	5.47	127.59	120.26
2	C	37	MET	CA-C-N	-5.46	114.37	122.56
2	C	37	MET	C-N-CA	-5.46	114.37	122.56
1	A	152	THR	CA-CB-OG1	-5.41	101.48	109.60
1	A	510	ALA	CA-C-N	5.37	129.50	121.77
1	A	510	ALA	C-N-CA	5.37	129.50	121.77
2	C	416	GLY	CA-C-N	5.25	130.54	122.77
2	C	416	GLY	C-N-CA	5.25	130.54	122.77
1	B	303	PHE	CB-CA-C	5.21	119.72	110.85
1	A	32	ASP	CA-C-N	5.20	131.47	121.54
1	A	32	ASP	C-N-CA	5.20	131.47	121.54
1	B	509	TYR	CA-C-N	5.10	127.36	120.38
1	B	509	TYR	C-N-CA	5.10	127.36	120.38
1	A	371	GLU	CB-CA-C	5.04	117.95	109.48
1	A	463	THR	CA-CB-OG1	-5.00	102.09	109.60

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	4486	0	4510	52	0
1	B	4511	0	4530	63	0
2	C	4270	0	4320	118	0
3	A	53	0	31	1	0
3	B	53	0	31	3	0
3	C	53	0	31	9	0
4	A	16	0	28	4	0
4	B	8	0	14	5	0
5	A	2	0	0	0	0
6	B	3	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	34	0	0	0	0
7	B	26	0	0	1	0
7	C	2	0	0	0	0
All	All	13517	0	13495	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)
1:B:300:CYS:HA	1:B:303:PHE:CE2	1.67	1.29
1:B:38:THR:HG22	1:B:42:ASN:OD1	1.54	1.08
1:A:105:HIS:HD2	1:A:250:ASP:OD1	1.39	1.05
2:C:50:THR:O	2:C:50:THR:HG22	1.64	0.95
2:C:81:ASN:HD21	2:C:426:TYR:CA	1.82	0.90
2:C:81:ASN:HD21	2:C:426:TYR:N	1.70	0.90
1:A:105:HIS:CD2	1:A:250:ASP:OD1	2.29	0.84
2:C:75:LEU:HD13	2:C:82:CYS:SG	2.18	0.82
2:C:81:ASN:ND2	2:C:426:TYR:HA	1.95	0.81
2:C:36:ASP:C	2:C:38:THR:H	1.87	0.81
2:C:233:HIS:NE2	2:C:426:TYR:CE1	2.50	0.80
1:A:56:VAL:HG21	1:A:73:MET:HE1	1.63	0.78
2:C:65:LEU:HD13	2:C:72:SER:HA	1.65	0.78
2:C:48:ASN:OD1	2:C:49:GLU:N	2.17	0.78
2:C:81:ASN:ND2	2:C:426:TYR:CA	2.48	0.76
2:C:161:LYS:HE2	2:C:299:GLU:OE2	1.84	0.76
2:C:36:ASP:C	2:C:38:THR:N	2.44	0.75
2:C:81:ASN:HD21	2:C:426:TYR:HA	1.52	0.74
1:B:300:CYS:CA	1:B:303:PHE:CE2	2.61	0.74
1:A:579:THR:HG22	1:A:580:THR:HG23	1.68	0.73
1:A:365:ARG:HD3	1:A:382:ASP:OD1	1.89	0.73
2:C:75:LEU:CD1	2:C:82:CYS:SG	2.77	0.71
2:C:256:VAL:O	3:C:601:FAD:H8A	1.91	0.71
1:A:576:GLU:O	1:A:579:THR:HB	1.93	0.69
1:A:586:GLU:HA	1:A:586:GLU:OE2	1.92	0.69
1:A:139:LYS:NZ	1:A:398:ASP:OD2	2.26	0.68
1:B:139:LYS:NZ	1:B:398:ASP:OD2	2.27	0.68
2:C:434:LEU:HD23	2:C:435:TYR:N	2.09	0.67
1:B:165:HIS:HE1	1:B:477:GLU:OE2	1.76	0.67
1:B:579:THR:HG22	1:B:580:THR:HG23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:VAL:HG21	1:A:73:MET:CE	2.25	0.67
2:C:139:LYS:NZ	2:C:398:ASP:OD2	2.29	0.65
1:A:73:MET:O	1:A:74:PRO:C	2.35	0.65
1:B:576:GLU:O	1:B:579:THR:HB	1.96	0.64
1:B:76:ILE:HD13	1:B:89:LEU:HD22	1.79	0.64
1:A:166:GLN:NE2	6:B:603:CL:CL	2.67	0.64
1:B:35:PRO:O	1:B:36:ASP:HB2	1.98	0.63
2:C:65:LEU:CD1	2:C:72:SER:HA	2.28	0.63
2:C:349:LYS:HE2	2:C:351:GLU:OE2	1.99	0.63
1:A:392:ARG:H	4:A:603:MPD:H4	1.64	0.62
2:C:50:THR:O	2:C:50:THR:CG2	2.37	0.62
2:C:256:VAL:HB	3:C:601:FAD:N7A	2.15	0.62
2:C:81:ASN:HD21	2:C:426:TYR:H	1.46	0.61
2:C:397:ASP:HA	2:C:408:ARG:HH22	1.66	0.61
2:C:21:ALA:HB2	2:C:27:LEU:HD23	1.81	0.61
2:C:355:LYS:N	2:C:356:PRO:CD	2.63	0.60
1:B:453:ARG:O	1:B:457:THR:HB	2.01	0.60
2:C:36:ASP:O	2:C:38:THR:N	2.34	0.60
1:A:453:ARG:O	1:A:457:THR:HB	2.02	0.60
2:C:349:LYS:CE	2:C:351:GLU:OE2	2.50	0.60
2:C:194:HIS:HD2	2:C:197:LYS:HE2	1.65	0.60
2:C:161:LYS:NZ	3:C:601:FAD:O4	2.33	0.59
2:C:287:LYS:HG2	2:C:310:ASP:HB3	1.84	0.59
1:B:166:GLN:NE2	6:B:604:CL:CL	2.72	0.59
1:B:165:HIS:CE1	1:B:169:LEU:HD11	2.38	0.59
1:B:300:CYS:HA	1:B:303:PHE:HE2	1.56	0.59
2:C:102:LEU:O	2:C:102:LEU:HD23	2.03	0.59
1:B:38:THR:HG22	1:B:42:ASN:CG	2.28	0.58
2:C:81:ASN:OD1	2:C:81:ASN:C	2.44	0.58
2:C:229:PHE:CD2	2:C:404:VAL:HG21	2.38	0.58
2:C:396:THR:HG23	2:C:399:LEU:HD12	1.86	0.58
1:A:365:ARG:HD2	1:A:380:THR:HB	1.86	0.58
2:C:171:GLY:O	2:C:174:ILE:HG12	2.04	0.58
1:A:76:ILE:HD13	1:A:89:LEU:HD22	1.84	0.57
2:C:194:HIS:HA	2:C:197:LYS:HG2	1.87	0.57
1:A:229:PHE:CD1	1:A:404:VAL:HG21	2.40	0.57
1:B:299:GLU:O	1:B:303:PHE:CD2	2.57	0.57
1:A:43:LEU:HD11	1:A:93:GLU:HG3	1.87	0.56
2:C:108:ASP:O	2:C:251:ARG:HG3	2.06	0.56
2:C:355:LYS:N	2:C:356:PRO:HD2	2.20	0.56
2:C:81:ASN:ND2	2:C:426:TYR:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:48:ASN:OD1	2:C:49:GLU:O	2.23	0.56
2:C:314:MET:HG2	2:C:345:CYS:HB3	1.87	0.56
1:A:73:MET:O	1:A:75:LEU:N	2.39	0.56
2:C:197:LYS:HG3	2:C:198:ASN:N	2.21	0.56
1:B:38:THR:O	1:B:42:ASN:N	2.23	0.56
1:B:454:ARG:HG3	1:B:459:SER:O	2.05	0.55
1:B:300:CYS:HA	1:B:303:PHE:CZ	2.36	0.55
2:C:48:ASN:CG	2:C:49:GLU:N	2.63	0.55
2:C:71:PRO:O	2:C:72:SER:C	2.50	0.55
1:B:299:GLU:O	1:B:303:PHE:HD2	1.91	0.54
2:C:425:PRO:O	2:C:426:TYR:CD2	2.61	0.54
2:C:172:GLU:HG3	2:C:338:ARG:HH12	1.72	0.54
1:B:229:PHE:CD1	1:B:404[A]:VAL:HG21	2.43	0.54
2:C:291:VAL:HG12	2:C:388:MET:HA	1.90	0.54
1:B:391:GLY:HA3	4:B:602:MPD:HM2	1.90	0.53
2:C:57:SER:O	2:C:61:VAL:HG23	2.08	0.53
2:C:67:ILE:O	2:C:418:ARG:NH2	2.42	0.53
1:B:496:ASN:HB3	1:B:529:ASN:ND2	2.23	0.53
4:A:603:MPD:H52	4:A:603:MPD:O2	2.09	0.53
2:C:347:PRO:HB3	2:C:350:TYR:CZ	2.44	0.53
1:A:189:ILE:HG23	1:B:183:GLU:O	2.09	0.52
1:B:126:VAL:HG11	1:B:218:LYS:HB3	1.90	0.52
2:C:259:ARG:NH2	2:C:276:ASP:OD2	2.42	0.52
2:C:349:LYS:O	2:C:349:LYS:HG2	2.09	0.52
1:B:38:THR:CG2	1:B:42:ASN:OD1	2.42	0.52
1:B:105:HIS:HD2	1:B:250:ASP:OD1	1.92	0.52
2:C:434:LEU:HD23	2:C:434:LEU:C	2.33	0.52
1:A:439:GLU:OE2	4:A:603:MPD:H12	2.10	0.52
2:C:126:VAL:HG11	2:C:218:LYS:HB3	1.92	0.51
1:B:105:HIS:CD2	1:B:250:ASP:OD1	2.63	0.51
2:C:44:PHE:HB3	2:C:48:ASN:HD22	1.76	0.51
2:C:70:TRP:CE2	2:C:84:GLY:O	2.64	0.51
1:B:176:ASP:OD2	1:B:514:ARG:NH1	2.44	0.50
2:C:105:HIS:CD2	2:C:250:ASP:OD1	2.63	0.50
2:C:287:LYS:HB2	2:C:384:ASN:OD1	2.10	0.50
2:C:172:GLU:HG3	2:C:338:ARG:NH1	2.27	0.50
1:B:300:CYS:HA	1:B:303:PHE:CD2	2.39	0.50
1:A:404:VAL:HG12	1:A:404:VAL:O	2.11	0.50
1:A:495:GLU:CD	1:A:495:GLU:H	2.20	0.49
2:C:233:HIS:CE1	2:C:426:TYR:CE1	3.00	0.49
2:C:349:LYS:O	2:C:349:LYS:CG	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:404:VAL:HG12	2:C:404:VAL:O	2.12	0.49
2:C:225:SER:OG	2:C:238:LYS:N	2.46	0.49
2:C:17:VAL:HG22	2:C:54:VAL:HG11	1.94	0.49
2:C:29:ALA:HA	2:C:54:VAL:O	2.12	0.49
2:C:105:HIS:HD2	2:C:250:ASP:OD1	1.95	0.49
2:C:404:VAL:HG11	2:C:427:VAL:HG21	1.95	0.48
2:C:81:ASN:ND2	2:C:426:TYR:CB	2.77	0.48
2:C:233:HIS:NE2	2:C:426:TYR:CD1	2.81	0.48
2:C:78:VAL:HB	2:C:101:TRP:CH2	2.48	0.48
2:C:289:LEU:HD22	2:C:366:VAL:HG21	1.94	0.48
1:B:165:HIS:CE1	1:B:477:GLU:OE2	2.63	0.48
1:A:56:VAL:CG2	1:A:73:MET:CE	2.92	0.48
1:B:78:VAL:HB	1:B:101:TRP:CH2	2.49	0.48
2:C:17:VAL:HG21	2:C:56:VAL:HG13	1.95	0.48
2:C:75:LEU:HD11	2:C:82:CYS:SG	2.53	0.47
2:C:314:MET:HG2	2:C:343:VAL:HG22	1.96	0.47
2:C:21:ALA:CB	2:C:27:LEU:HD23	2.44	0.47
1:A:138:VAL:HG11	1:A:147:TRP:CE2	2.49	0.47
2:C:135:LEU:HD13	2:C:223:MET:HB2	1.96	0.47
1:B:10:SER:O	1:B:57:SER:HA	2.14	0.47
1:B:404[A]:VAL:HG12	1:B:404[A]:VAL:O	2.13	0.47
1:B:579:THR:CG2	7:B:726:HOH:O	2.63	0.47
1:B:439:GLU:OE2	4:B:602:MPD:O4	2.32	0.47
1:B:30:TYR:CD1	1:B:30:TYR:C	2.93	0.46
1:B:404[A]:VAL:HG11	1:B:427:VAL:HG21	1.96	0.46
2:C:79:LYS:O	2:C:251:ARG:NH1	2.48	0.46
2:C:291:VAL:CG1	2:C:388:MET:HA	2.46	0.46
1:B:93:GLU:C	1:B:93:GLU:OE1	2.58	0.46
1:B:126:VAL:HG21	1:B:220:VAL:HG22	1.96	0.46
1:A:78:VAL:HB	1:A:101:TRP:CH2	2.50	0.46
1:A:441:THR:HB	1:A:442:PRO:HD3	1.97	0.46
1:A:417:ARG:NH1	1:A:422:VAL:O	2.46	0.46
2:C:399:LEU:HD21	3:C:601:FAD:H61A	1.81	0.46
1:A:406:VAL:HG21	1:A:427:VAL:HG11	1.97	0.46
2:C:256:VAL:HB	3:C:601:FAD:C8A	2.46	0.46
1:A:126:VAL:HG11	1:A:218:LYS:HB3	1.98	0.46
2:C:363:MET:HG2	2:C:384:ASN:HA	1.97	0.46
1:A:93:GLU:C	1:A:93:GLU:OE1	2.60	0.45
2:C:256:VAL:HG12	3:C:601:FAD:N7A	2.31	0.45
1:A:56:VAL:HG11	1:A:64:ILE:HD12	1.99	0.45
1:B:504:PHE:CE1	1:B:574:VAL:HG13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:73:MET:HE2	2:C:75:LEU:HB3	1.99	0.45
1:A:47:TYR:HE1	1:A:99:ASN:HD22	1.64	0.45
1:A:365:ARG:HH11	1:A:382:ASP:CG	2.25	0.44
1:B:401:LEU:HD12	1:B:408:ARG:HD3	1.98	0.44
2:C:194:HIS:CD2	2:C:197:LYS:HE2	2.50	0.44
2:C:406:VAL:HG21	2:C:427:VAL:HG11	1.99	0.44
1:A:183:GLU:O	1:B:189:ILE:HG23	2.18	0.44
2:C:26:ILE:HD12	2:C:78:VAL:HG22	1.99	0.44
1:B:126:VAL:HG21	1:B:220:VAL:CG2	2.48	0.44
2:C:135:LEU:HD11	2:C:223:MET:HE3	1.98	0.44
2:C:171:GLY:O	2:C:174:ILE:CG1	2.65	0.44
2:C:504:PHE:CE1	2:C:574:VAL:HG13	2.53	0.44
1:A:404:VAL:O	1:A:404:VAL:CG1	2.66	0.44
3:B:601:FAD:H9	3:B:601:FAD:H1'1	1.84	0.44
2:C:418:ARG:HH21	2:C:418:ARG:HG3	1.83	0.44
1:B:61:VAL:HG13	1:B:62:LYS:N	2.32	0.44
1:B:239:ASN:HD21	1:B:241:LYS:HG2	1.82	0.43
1:B:406:VAL:HG21	1:B:427:VAL:HG11	2.01	0.43
1:B:138:VAL:HG11	1:B:147:TRP:CE2	2.53	0.43
2:C:256:VAL:CB	3:C:601:FAD:N7A	2.81	0.43
2:C:396:THR:HG22	2:C:396:THR:O	2.18	0.43
1:B:226:TYR:CZ	3:B:601:FAD:N6A	2.86	0.43
2:C:434:LEU:C	2:C:434:LEU:CD2	2.91	0.43
1:A:485:GLU:OE2	1:A:585:LYS:HE2	2.19	0.43
1:B:496:ASN:HB3	1:B:529:ASN:HD22	1.83	0.43
1:B:255:ALA:O	3:B:601:FAD:H52A	2.18	0.43
1:B:439:GLU:OE2	4:B:602:MPD:C4	2.66	0.43
2:C:18:PHE:HB3	2:C:458:GLY:O	2.18	0.43
2:C:300:CYS:HA	2:C:303:PHE:CE2	2.53	0.43
1:A:73:MET:O	1:A:73:MET:SD	2.77	0.43
2:C:191:LEU:HD13	2:C:191:LEU:C	2.44	0.43
1:A:33:TYR:HD1	1:A:33:TYR:O	2.02	0.43
3:A:601:FAD:H9	3:A:601:FAD:H1'1	1.88	0.43
1:B:571:HIS:HA	1:B:572:PRO:HA	1.81	0.42
2:C:425:PRO:O	2:C:426:TYR:CG	2.72	0.42
1:A:67:ILE:HD13	1:A:460:SER:HB3	2.01	0.42
1:A:504:PHE:CE1	1:A:574:VAL:HG13	2.54	0.42
2:C:250:ASP:C	2:C:251:ARG:HG2	2.44	0.42
1:B:441:THR:HB	1:B:442:PRO:HD3	2.00	0.42
2:C:135:LEU:CD1	2:C:223:MET:HB2	2.49	0.42
2:C:126:VAL:HG21	2:C:220:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:HG21	1:A:220:VAL:HG22	2.02	0.42
2:C:25:ARG:O	2:C:26:ILE:HD13	2.20	0.42
2:C:256:VAL:CG1	3:C:601:FAD:N7A	2.83	0.42
1:A:404:VAL:HG11	1:A:427:VAL:HG21	2.01	0.42
2:C:291:VAL:CG1	2:C:388:MET:SD	3.08	0.42
1:B:73:MET:HB3	1:B:74:PRO:HA	2.01	0.42
2:C:354:LYS:C	2:C:356:PRO:HD2	2.45	0.42
1:B:465:TYR:HA	1:B:468:ILE:HD11	2.02	0.42
2:C:26:ILE:HD13	2:C:78:VAL:HA	2.01	0.42
1:B:239:ASN:HD21	1:B:241:LYS:CD	2.33	0.41
4:A:603:MPD:H53	4:A:603:MPD:HM1	2.02	0.41
1:B:191:LEU:C	1:B:191:LEU:HD13	2.45	0.41
2:C:126:VAL:HG21	2:C:220:VAL:HG22	2.02	0.41
2:C:223:MET:HE1	2:C:247:VAL:HG21	2.01	0.41
1:A:472:VAL:HG12	1:A:474:THR:HG23	2.02	0.41
2:C:162:LYS:HE3	2:C:473:PHE:CE2	2.55	0.41
2:C:267:GLY:O	2:C:268:ALA:C	2.63	0.41
1:A:267:GLY:O	1:A:268:ALA:C	2.63	0.41
1:B:404[A]:VAL:O	1:B:404[A]:VAL:CG1	2.68	0.41
2:C:349:LYS:HE3	2:C:351:GLU:OE2	2.20	0.41
1:A:159:ILE:HB	1:A:160:PRO:CD	2.51	0.41
1:A:505:ILE:O	1:A:506:PRO:C	2.64	0.41
1:A:570:ILE:HD11	1:B:469:PRO:HB2	2.03	0.41
1:A:254:ILE:HG22	1:A:256:VAL:HG13	2.03	0.41
1:A:300:CYS:HA	1:A:303:PHE:CE2	2.56	0.41
1:B:392:ARG:N	4:B:602:MPD:H11	2.36	0.41
1:B:392:ARG:O	4:B:602:MPD:H31	2.20	0.41
2:C:39:LYS:HA	2:C:42:ASN:HB2	2.02	0.41
2:C:229:PHE:CD2	2:C:404:VAL:CG2	3.03	0.41
2:C:314:MET:SD	2:C:345:CYS:HB3	2.61	0.41
1:A:271:CYS:HB3	1:A:364:ILE:HG12	2.03	0.40
1:B:471:THR:HA	1:B:478:TYR:O	2.22	0.40
1:A:159:ILE:HB	1:A:160:PRO:HD3	2.03	0.40
2:C:210:GLY:O	2:C:214:GLN:HB2	2.20	0.40
2:C:392:ARG:CD	3:C:601:FAD:HM81	2.51	0.40
1:A:254:ILE:CG2	1:A:256:VAL:HG13	2.51	0.40
2:C:114:GLY:HA3	2:C:136:ASP:HB2	2.02	0.40
1:B:239:ASN:ND2	1:B:241:LYS:HG2	2.36	0.40
2:C:404:VAL:O	2:C:404:VAL:CG1	2.70	0.40
2:C:441:THR:HB	2:C:442:PRO:HD3	2.03	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	574/598 (96%)	553 (96%)	21 (4%)	0	100	100
1	B	576/598 (96%)	553 (96%)	23 (4%)	0	100	100
2	C	540/598 (90%)	504 (93%)	34 (6%)	2 (0%)	30	39
All	All	1690/1794 (94%)	1610 (95%)	78 (5%)	2 (0%)	48	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	37	MET
2	C	56	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	488/503 (97%)	476 (98%)	12 (2%)	42	60
1	B	489/503 (97%)	478 (98%)	11 (2%)	45	64
2	C	465/504 (92%)	449 (97%)	16 (3%)	32	48
All	All	1442/1510 (96%)	1403 (97%)	39 (3%)	40	58

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU

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Mol	Chain	Res	Type
1	A	126	VAL
1	A	158	CYS
1	A	343	VAL
1	A	379	VAL
1	A	495	GLU
1	A	511	VAL
1	A	515	LYS
1	A	529[A]	ASN
1	A	529[B]	ASN
1	A	579	THR
1	A	587	ASP
1	B	28	LEU
1	B	126	VAL
1	B	158	CYS
1	B	162	LYS
1	B	184	ILE
1	B	241	LYS
1	B	379	VAL
1	B	511	VAL
1	B	513	GLU
1	B	553	ILE
1	B	579	THR
2	C	43	LEU
2	C	48	ASN
2	C	53	THR
2	C	56	VAL
2	C	64	ILE
2	C	100	GLU
2	C	135	LEU
2	C	138	VAL
2	C	141	SER
2	C	158	CYS
2	C	259	ARG
2	C	275	SER
2	C	343	VAL
2	C	366	VAL
2	C	505	ILE
2	C	529	ASN

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	34	ASN
1	A	99	ASN
1	A	105	HIS
1	A	155	ASN
1	A	208	ASN
1	A	224	ASN
1	B	99	ASN
1	B	155	ASN
1	B	165	HIS
1	B	166	GLN
1	B	203	HIS
1	B	208	ASN
1	B	224	ASN
1	B	529	ASN
2	C	81	ASN
2	C	155	ASN
2	C	208	ASN
2	C	519	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	CSO	B	345	1	3,6,7	0.66	0	1,6,8	0.30	0
1	CSO	A	345	1	3,6,7	0.62	0	1,6,8	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	CSO	B	345	1	-	1/1/5/7	-
1	CSO	A	345	1	-	1/1/5/7	-

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	CSO	N-CA-CB-SG
1	B	345	CSO	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](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	A	601	5	58,58,58	1.05	2 (3%)	85,89,89	0.74	2 (2%)
4	MPD	A	602	-	7,7,7	0.12	0	9,10,10	0.42	0
3	FAD	C	601	-	58,58,58	0.80	1 (1%)	85,89,89	0.70	1 (1%)
4	MPD	A	603	-	7,7,7	0.22	0	9,10,10	0.72	0
4	MPD	B	602	-	7,7,7	0.27	0	9,10,10	0.50	0
3	FAD	B	601	-	58,58,58	0.96	2 (3%)	85,89,89	0.71	1 (1%)

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	A	601	5	-	5/34/50/50	0/6/6/6
4	MPD	A	602	-	-	1/5/5/5	-
3	FAD	C	601	-	-	3/34/50/50	0/6/6/6
4	MPD	A	603	-	-	4/5/5/5	-
4	MPD	B	602	-	-	0/5/5/5	-
3	FAD	B	601	-	-	3/34/50/50	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	FAD	C2-N3	-2.68	1.33	1.39
3	A	601	FAD	C1'-C2'	-2.65	1.49	1.52
3	B	601	FAD	C1'-C2'	-2.61	1.49	1.52
3	B	601	FAD	C2-N3	-2.38	1.33	1.39
3	C	601	FAD	C1'-C2'	-2.28	1.49	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FAD	C4-N3-C2	-2.12	121.88	125.64
3	C	601	FAD	C4-N3-C2	-2.10	121.91	125.64
3	A	601	FAD	O4B-C1B-C2B	-2.08	102.17	106.62
3	A	601	FAD	O3B-C3B-C2B	-2.07	105.18	111.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	FAD	PA-O3P-P-O5'
3	C	601	FAD	PA-O3P-P-O5'
4	A	603	MPD	C2-C3-C4-O4
4	A	603	MPD	C2-C3-C4-C5
3	C	601	FAD	O4B-C4B-C5B-O5B
3	C	601	FAD	C3B-C4B-C5B-O5B
3	A	601	FAD	O4B-C4B-C5B-O5B
3	A	601	FAD	C3B-C4B-C5B-O5B
3	B	601	FAD	PA-O3P-P-O5'

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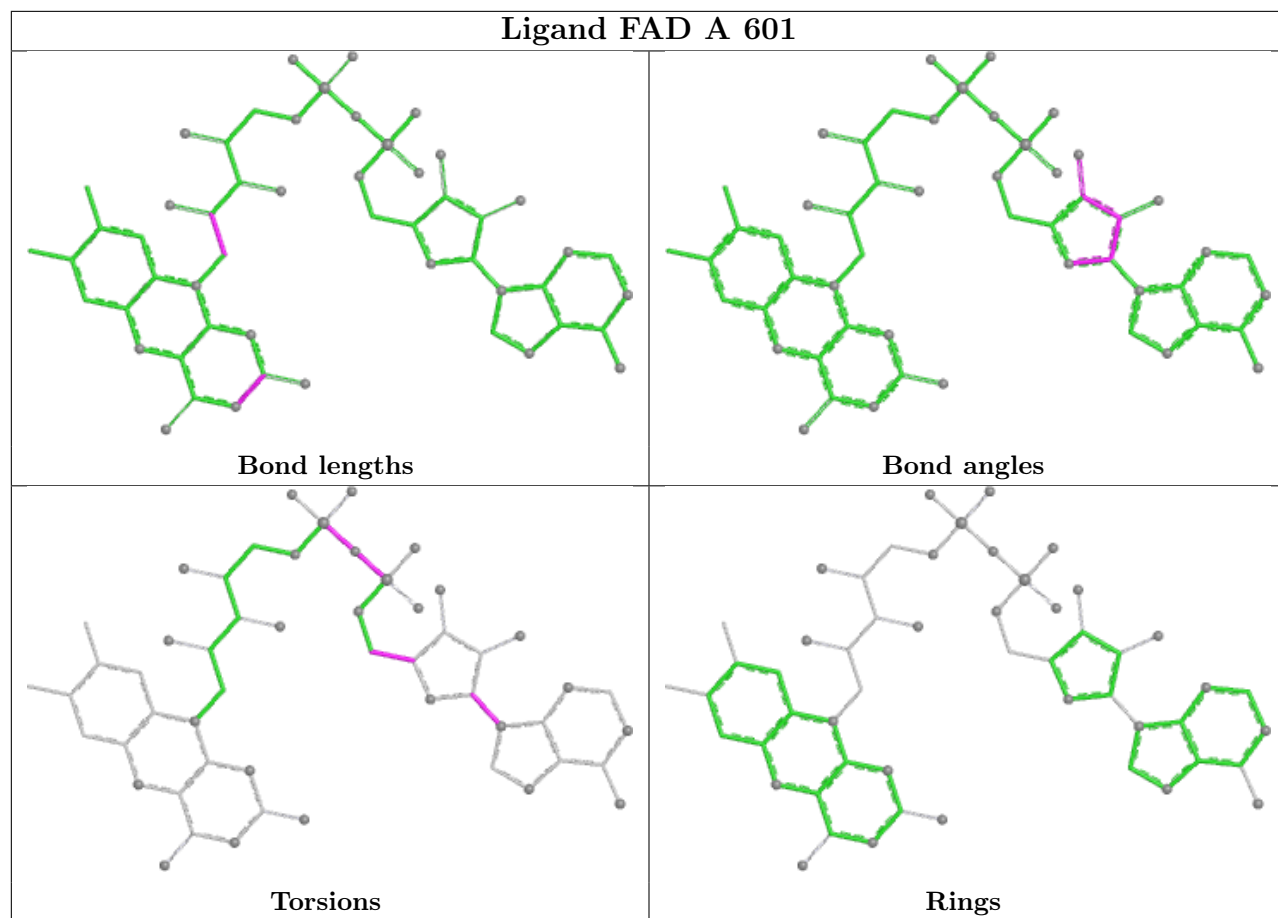
Mol	Chain	Res	Type	Atoms
3	A	601	FAD	C2B-C1B-N9A-C8A
3	B	601	FAD	C2B-C1B-N9A-C8A
3	B	601	FAD	O4B-C4B-C5B-O5B
4	A	603	MPD	O2-C2-C3-C4
4	A	602	MPD	C1-C2-C3-C4
4	A	603	MPD	CM-C2-C3-C4
3	A	601	FAD	P-O3P-PA-O2A

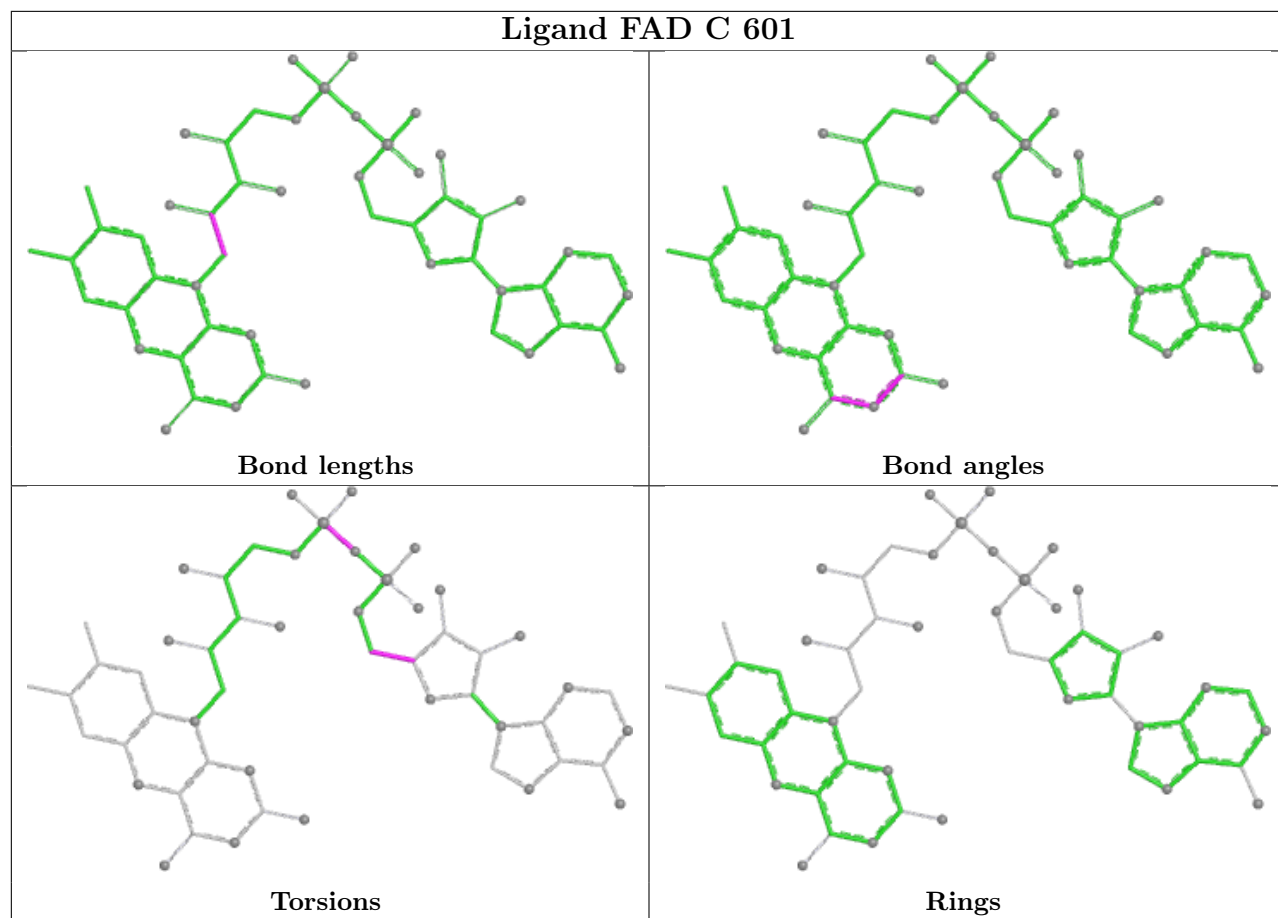
There are no ring outliers.

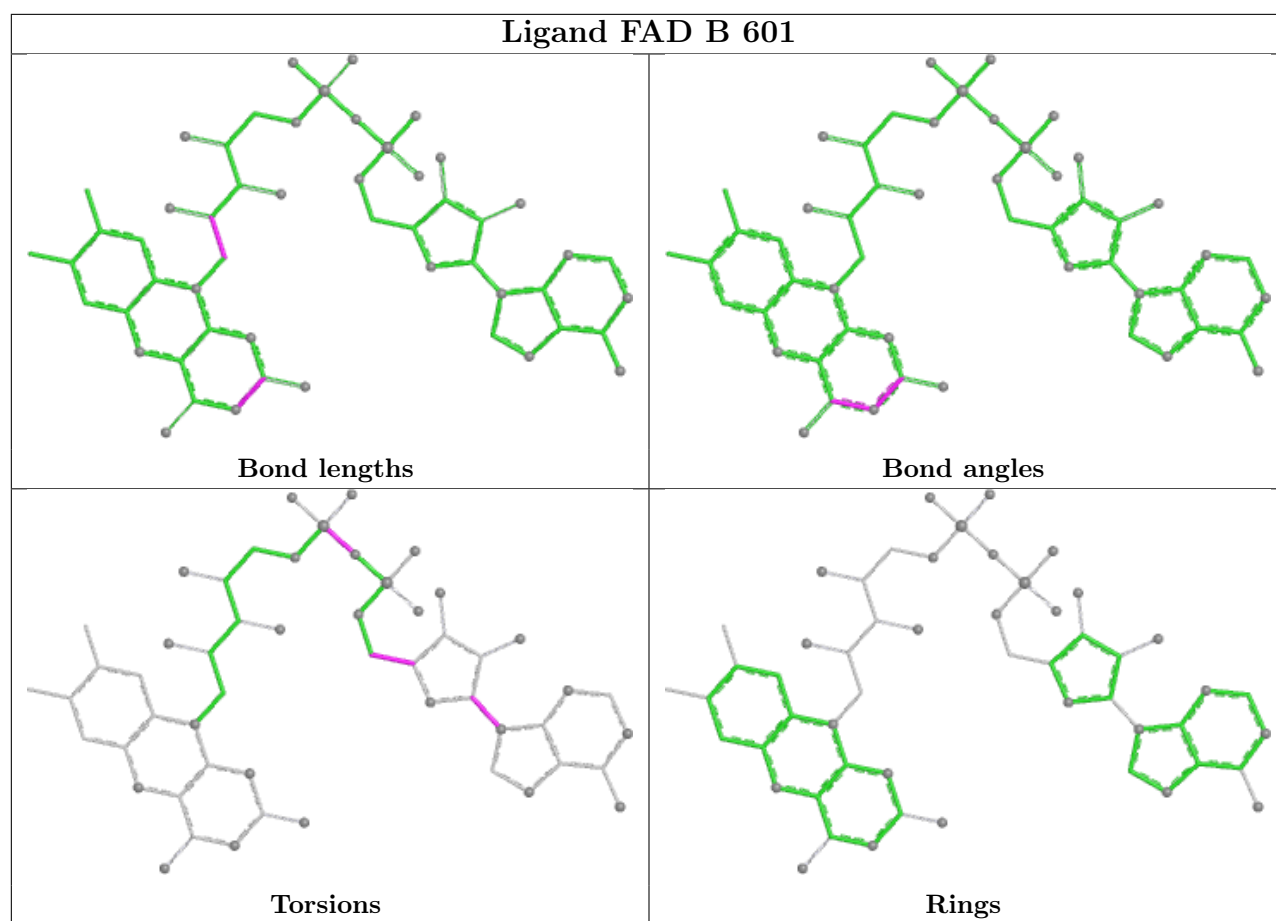
5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	FAD	1	0
3	C	601	FAD	9	0
4	A	603	MPD	4	0
4	B	602	MPD	5	0
3	B	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 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	575/598 (96%)	-0.19	8 (1%) 73 74	50, 78, 136, 206	2 (0%)
1	B	579/598 (96%)	-0.10	7 (1%) 76 77	45, 84, 144, 207	1 (0%)
2	C	550/598 (91%)	0.65	51 (9%) 14 13	59, 128, 205, 268	0
All	All	1704/1794 (94%)	0.11	66 (3%) 43 44	45, 92, 180, 268	3 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	348	ILE	5.4
2	C	290	CYS	5.3
2	C	95	SER	5.3
2	C	84	GLY	4.8
1	B	595	GLY	4.2
2	C	426	TYR	4.2
2	C	89	LEU	3.9
2	C	40	VAL	3.9
2	C	88	GLU	3.7
2	C	90	TYR	3.6
2	C	51	VAL	3.5
2	C	44	PHE	3.5
2	C	353	LEU	3.4
2	C	77	PHE	3.2
2	C	74	PRO	3.2
2	C	142	ALA	3.1
2	C	293	ALA	3.0
2	C	98	LEU	3.0
2	C	35	PRO	2.9
2	C	75	LEU	2.9
2	C	14	ALA	2.9
1	B	373	GLU	2.9
2	C	53	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	380	THR	2.8
2	C	279	PHE	2.8
2	C	43	LEU	2.8
2	C	102	LEU	2.8
2	C	345	CYS	2.8
2	C	70	TRP	2.7
2	C	346	VAL	2.7
2	C	50	THR	2.7
2	C	47	TYR	2.6
2	C	366	VAL	2.6
1	A	39	LYS	2.6
2	C	387	LEU	2.5
2	C	30	TYR	2.5
1	B	33	TYR	2.5
2	C	156	VAL	2.5
1	A	45	SER	2.5
2	C	37	MET	2.4
2	C	97	PHE	2.4
2	C	49	GLU	2.4
1	A	73	MET	2.3
1	B	303	PHE	2.3
1	A	75	LEU	2.3
2	C	422	VAL	2.3
2	C	347	PRO	2.3
2	C	229	PHE	2.3
2	C	61	VAL	2.3
2	C	27	LEU	2.2
2	C	185	PRO	2.2
2	C	266	PRO	2.2
1	A	76	ILE	2.2
1	A	86	PHE	2.2
2	C	96	GLY	2.2
2	C	435	TYR	2.1
1	A	38	THR	2.1
1	B	209	TRP	2.1
1	A	74	PRO	2.1
1	B	35	PRO	2.0
1	B	252	PHE	2.0
2	C	154	VAL	2.0
2	C	28	LEU	2.0
2	C	144	GLY	2.0
2	C	254	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	C	71	PRO	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSO	B	345	7/8	0.80	0.10	85,94,123,124	0
1	CSO	A	345	7/8	0.89	0.10	78,85,113,121	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

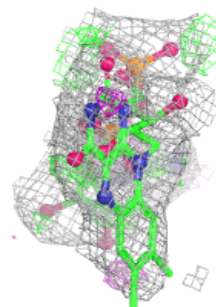
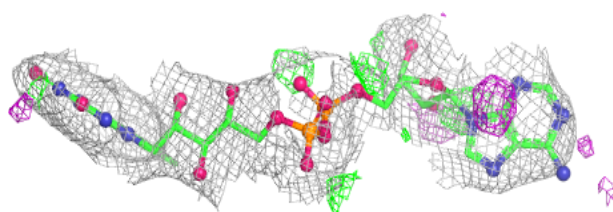
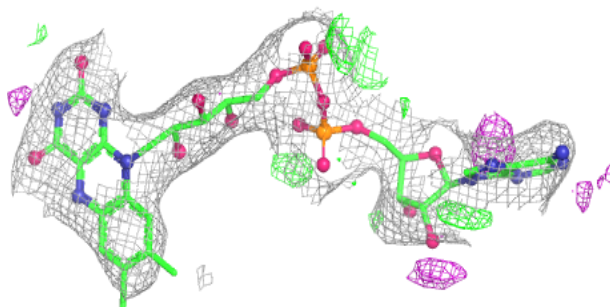
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MPD	B	602	8/8	0.71	0.21	91,104,107,110	0
4	MPD	A	603	8/8	0.78	0.22	88,103,105,111	0
4	MPD	A	602	8/8	0.85	0.26	90,112,118,119	0
5	NA	A	604	1/1	0.87	0.12	54,54,54,54	1
5	NA	A	605	1/1	0.90	0.23	66,66,66,66	1
6	CL	B	603	1/1	0.90	0.46	98,98,98,98	0
6	CL	B	604	1/1	0.90	0.38	98,98,98,98	0
3	FAD	C	601	53/53	0.92	0.10	86,109,132,137	0
6	CL	B	605	1/1	0.94	0.35	101,101,101,101	0
3	FAD	A	601	53/53	0.96	0.07	50,59,69,74	0
3	FAD	B	601	53/53	0.97	0.06	53,66,85,90	0

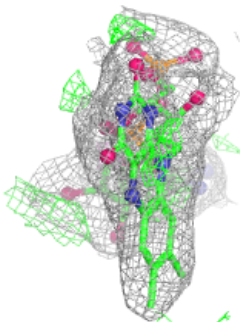
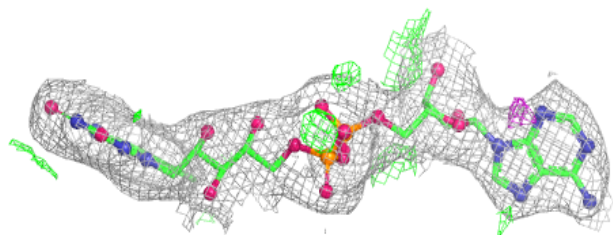
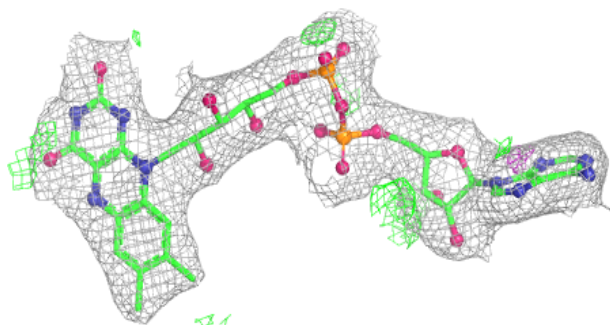
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

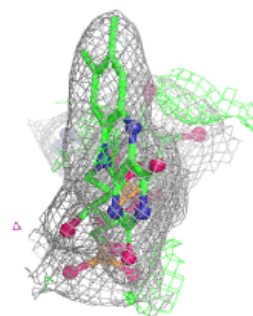
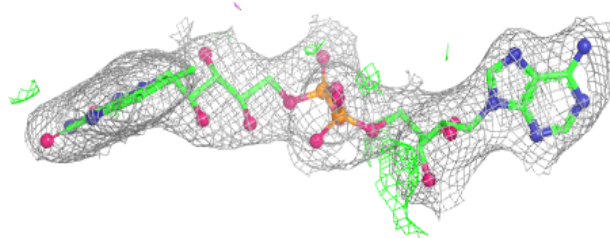
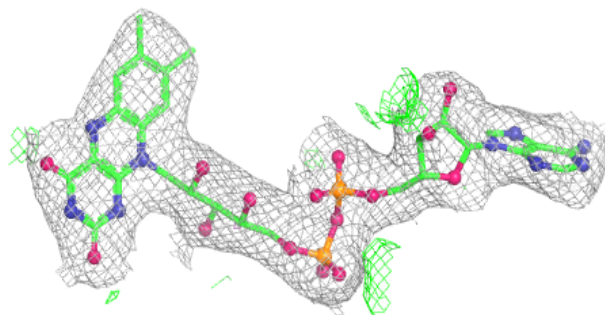
**Electron density around FAD A 601:**

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



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.