



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:01 AM UTC

PDB ID : 3AM9 / pdb_00003am9
Title : Complex of bovine xanthine dehydrogenase and trihydroxy FYX-051
Authors : Matsumoto, K.; Okamoto, K.; Ashizawa, N.; Matsumura, T.; Kusano, T.;
Nishino, T.
Deposited on : 2010-08-18
Resolution : 2.17 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

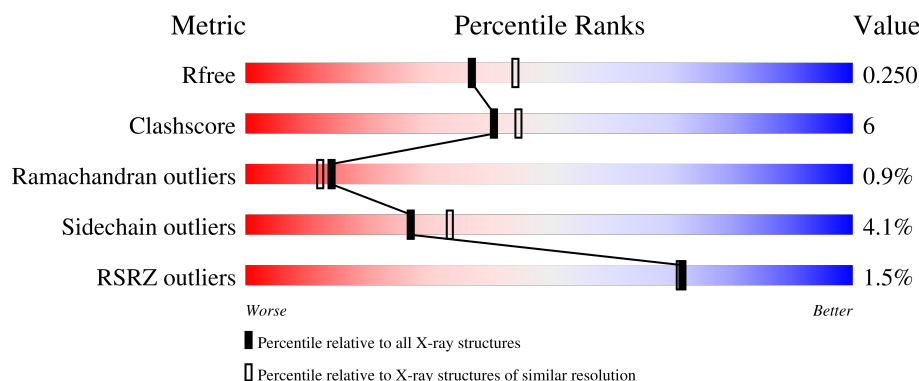
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	1332	2% 82% 13% ..
1	B	1332	% 80% 15% ..

2 Entry composition [i](#)

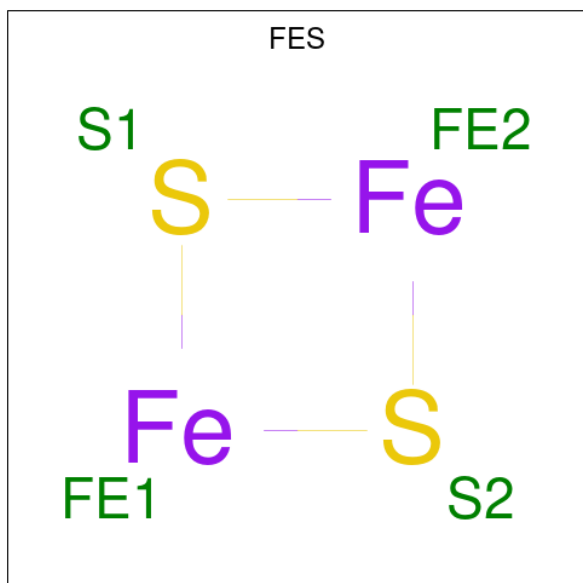
There are 10 unique types of molecules in this entry. The entry contains 22226 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1293	Total	C	N	O	S	0	0	0
			10041	6384	1721	1876	60			
1	B	1291	Total	C	N	O	S	0	0	0
			10027	6375	1719	1872	61			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



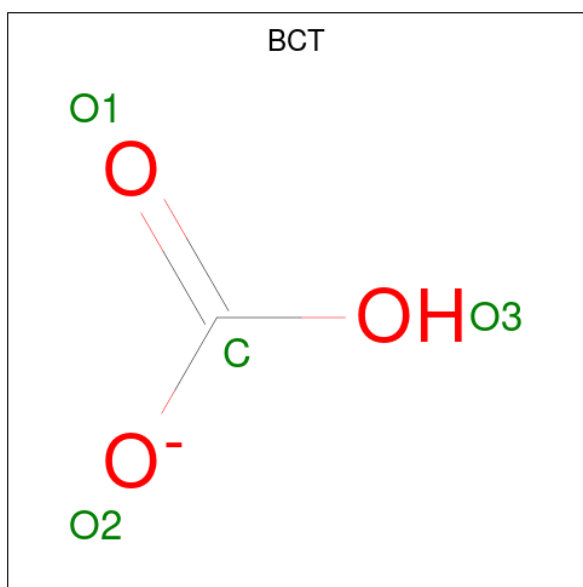
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | A | 2 | Total Ca
2 2 | 0 | 0 |
| 3 | B | 2 | Total Ca
2 2 | 0 | 0 |

- # FAD

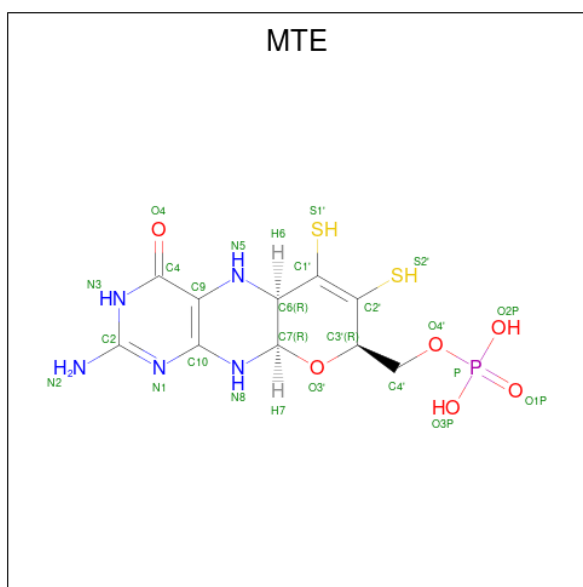
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- 



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

- Molecule 6 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (CCD ID: MTE) (formula: C₁₀H₁₄N₅O₆PS₂).



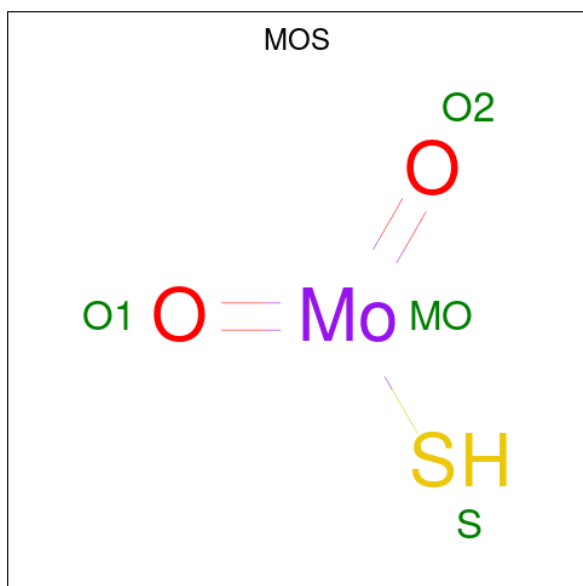
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

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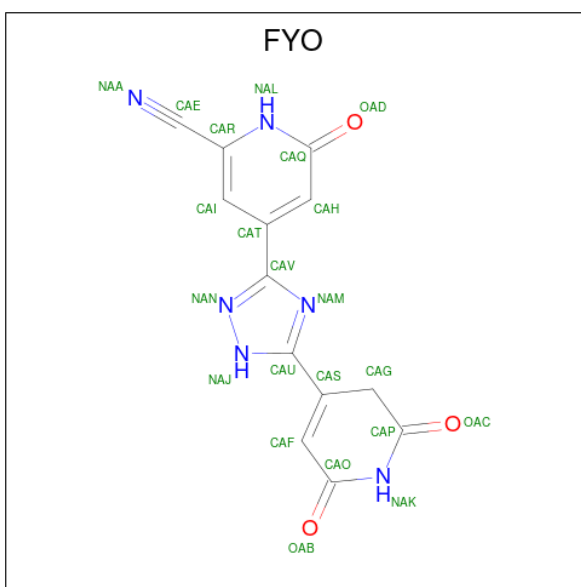
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (CCD ID: MOS) (formula: HMoO_2S).



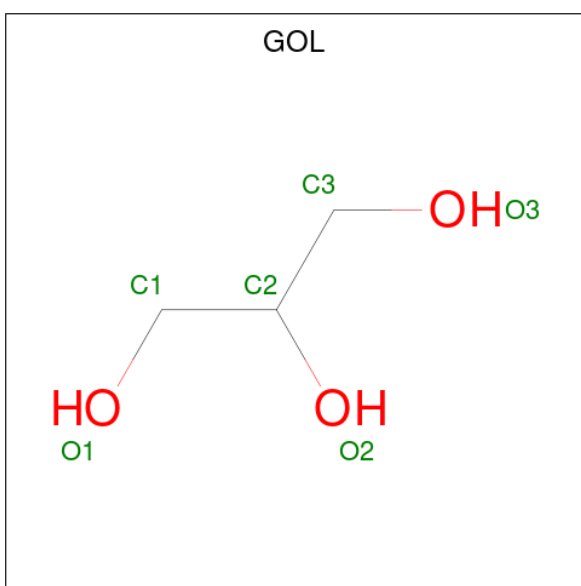
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	Mo	O	S	0	0
			3	1	1	1		
7	B	1	Total	Mo	O	S	0	0
			3	1	1	1		

- Molecule 8 is 4-[5-(2,6-dioxo-1,2,3,6-tetrahydropyridin-4-yl)-1H-1,2,4-triazol-3-yl]-6-oxo-1,6-dihydropyridine-2-carbonitrile (CCD ID: FYO) (formula: $\text{C}_{13}\text{H}_8\text{N}_6\text{O}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			22	13	6	3		
8	B	1	Total	C	N	O	0	0
			22	13	6	3		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		

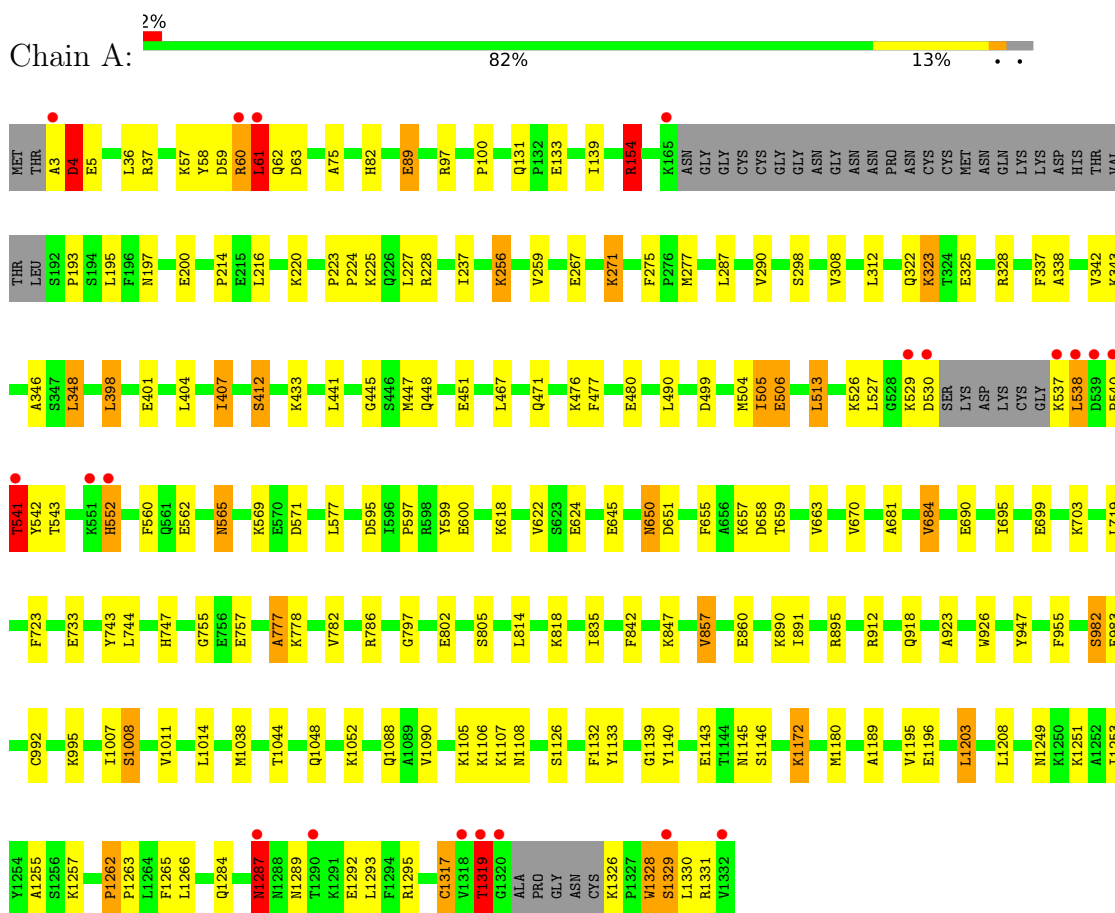
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	973	Total 973	O 973	0	0
10	B	941	Total 941	O 941	0	0

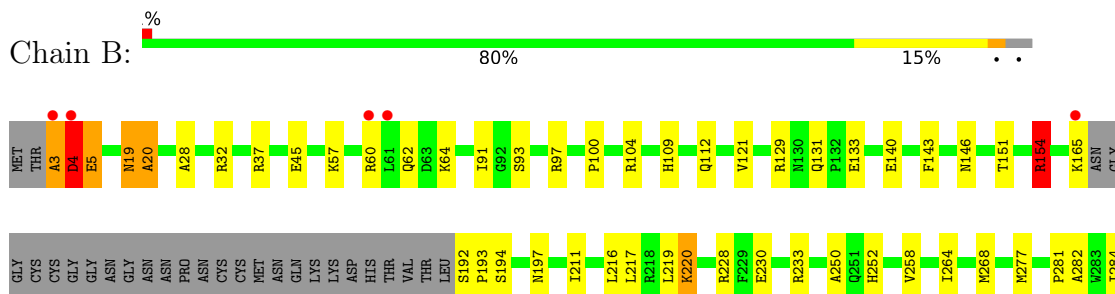
3 Residue-property plots

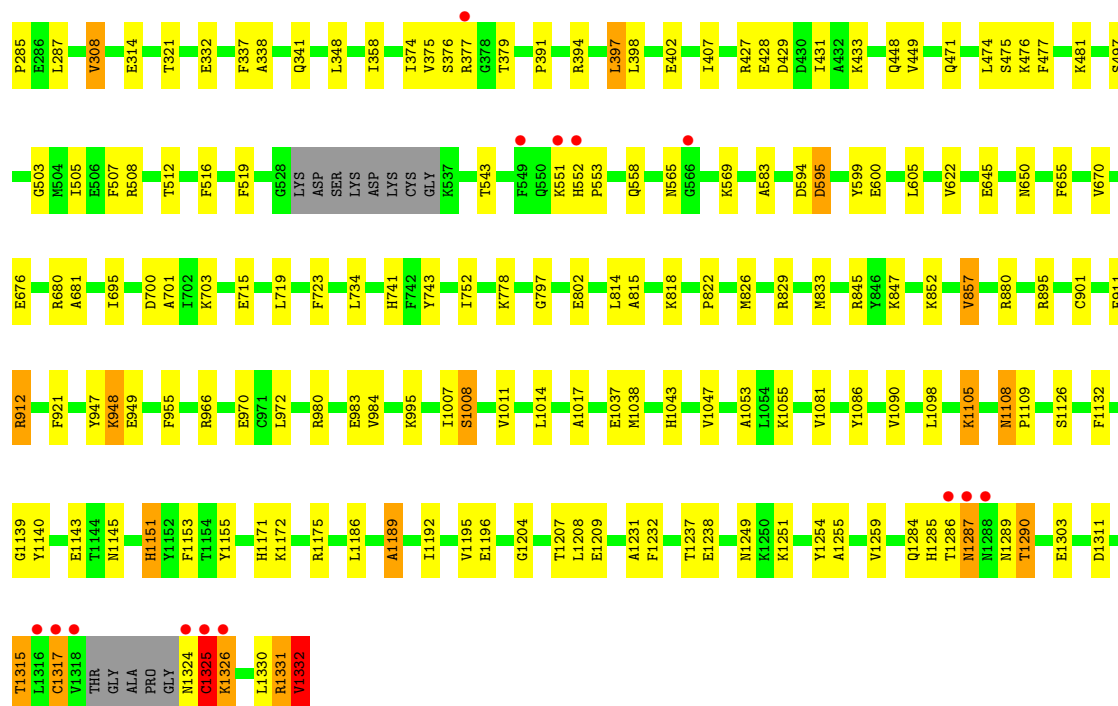
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Xanthine dehydrogenase/oxidase



• Molecule 1: Xanthine dehydrogenase/oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.92Å 124.72Å 146.19Å 90.00° 91.04° 90.00°	Depositor
Resolution (Å)	33.44 – 2.17 33.44 – 2.17	Depositor EDS
% Data completeness (in resolution range)	95.5 (33.44-2.17) 95.4 (33.44-2.17)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.174 , 0.243 (Not available) , 0.250	Depositor DCC
R_{free} test set	7582 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22226	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MTE, MOS, FAD, FES, BCT, GOL, FYO, CA

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	1.29	14/10260 (0.1%)	1.20	35/13885 (0.3%)
1	B	1.26	13/10246 (0.1%)	1.19	34/13867 (0.2%)
All	All	1.27	27/20506 (0.1%)	1.19	69/27752 (0.2%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4	ASP	CA-C	10.16	1.66	1.52
1	B	4	ASP	N-CA	8.95	1.57	1.46
1	A	4	ASP	CA-C	8.19	1.63	1.52
1	A	505	ILE	CA-CB	7.58	1.62	1.54
1	A	777	ALA	N-CA	7.54	1.55	1.46
1	A	663	VAL	CA-CB	7.25	1.62	1.53
1	A	538	LEU	CA-C	6.67	1.59	1.52
1	B	1090	VAL	CA-CB	6.48	1.61	1.54
1	B	28	ALA	CA-CB	5.96	1.62	1.53
1	B	1231	ALA	CA-CB	5.90	1.63	1.53
1	B	1317	CYS	N-CA	5.82	1.52	1.46
1	A	1319	THR	CA-CB	5.66	1.63	1.53
1	A	597	PRO	CA-C	5.58	1.59	1.52
1	B	1195	VAL	CA-CB	5.55	1.60	1.54
1	B	282	ALA	CA-CB	5.54	1.62	1.53
1	B	449	VAL	CA-CB	5.41	1.60	1.53
1	B	1189	ALA	CA-CB	5.30	1.61	1.53
1	A	552	HIS	CA-C	5.30	1.58	1.53
1	A	1330	LEU	N-CA	5.22	1.52	1.46
1	B	516	PHE	C-O	-5.21	1.18	1.24
1	A	259	VAL	CA-CB	5.20	1.61	1.54
1	A	1090	VAL	CA-C	5.14	1.59	1.52
1	A	1317	CYS	N-CA	5.13	1.51	1.46
1	B	583	ALA	CA-CB	5.10	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	LEU	CA-C	5.08	1.58	1.52
1	B	3	ALA	CA-C	5.07	1.63	1.52
1	A	622	VAL	CA-CB	5.02	1.61	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ASP	N-CA-C	11.16	134.58	110.80
1	B	5	GLU	N-CA-C	9.11	124.02	107.99
1	A	857	VAL	CB-CA-C	8.97	119.70	110.91
1	B	857	VAL	CB-CA-C	8.82	119.29	110.65
1	A	857	VAL	N-CA-C	-8.76	104.76	112.12
1	A	1330	LEU	N-CA-C	7.89	121.27	108.34
1	A	1328	TRP	CA-C-N	7.63	135.44	121.70
1	A	1328	TRP	C-N-CA	7.63	135.44	121.70
1	A	1328	TRP	N-CA-C	7.44	123.65	111.37
1	B	519	PHE	N-CA-C	-7.31	103.39	111.36
1	A	1108	ASN	CA-C-N	7.11	127.11	119.28
1	A	1108	ASN	C-N-CA	7.11	127.11	119.28
1	A	154	ARG	NE-CZ-NH2	-7.06	112.85	119.20
1	B	1207	THR	CB-CA-C	-6.96	100.19	109.16
1	A	1287	ASN	N-CA-C	6.89	119.91	109.23
1	B	197	ASN	CA-C-N	6.89	126.86	119.28
1	B	197	ASN	C-N-CA	6.89	126.86	119.28
1	A	154	ARG	CA-C-N	-6.83	111.95	119.19
1	A	154	ARG	C-N-CA	-6.83	111.95	119.19
1	B	1285	HIS	N-CA-C	6.79	122.41	113.30
1	A	891	ILE	N-CA-C	6.67	114.75	108.15
1	B	1287	ASN	N-CA-C	6.64	119.36	111.33
1	B	553	PRO	CA-C-N	6.39	126.15	119.76
1	B	553	PRO	C-N-CA	6.39	126.15	119.76
1	A	1317	CYS	N-CA-C	6.28	120.84	112.30
1	A	835	ILE	N-CA-C	6.17	117.18	111.45
1	B	1325	CYS	CA-C-N	5.98	132.47	121.70
1	B	1325	CYS	C-N-CA	5.98	132.47	121.70
1	A	651	ASP	N-CA-CB	-5.97	101.08	110.46
1	B	1108	ASN	CA-C-N	5.97	126.39	119.47
1	B	1108	ASN	C-N-CA	5.97	126.39	119.47
1	A	650	ASN	CA-C-N	5.92	133.07	122.06
1	A	650	ASN	C-N-CA	5.92	133.07	122.06
1	B	1105	LYS	N-CA-C	-5.89	104.78	111.14
1	A	480	GLU	N-CA-C	5.88	118.44	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	GLU	N-CA-CB	-5.86	102.51	110.95
1	A	412	SER	N-CA-CB	-5.80	101.30	110.06
1	A	1262	PRO	N-CA-C	5.80	117.77	110.70
1	A	62	GLN	N-CA-C	-5.73	106.33	113.38
1	B	19	ASN	CB-CA-C	5.72	121.80	110.42
1	B	1331	ARG	CA-C-N	5.69	131.94	121.70
1	B	1331	ARG	C-N-CA	5.69	131.94	121.70
1	B	857	VAL	N-CA-CB	-5.67	104.46	112.12
1	B	1047	VAL	N-CA-C	-5.67	104.82	111.00
1	A	684	VAL	N-CA-CB	-5.67	104.74	112.28
1	A	398	LEU	N-CA-C	-5.60	100.57	109.76
1	B	308	VAL	N-CA-C	-5.58	105.07	110.42
1	B	622	VAL	N-CA-C	5.43	117.39	112.29
1	A	1328	TRP	O-C-N	-5.24	116.09	122.11
1	A	1203	LEU	CA-CB-CG	5.20	134.49	116.30
1	B	595	ASP	N-CA-C	-5.20	106.45	112.89
1	A	982	SER	N-CA-C	-5.17	105.72	111.36
1	B	1151	HIS	N-CA-C	-5.17	105.34	111.69
1	A	220	LYS	N-CA-C	-5.16	106.08	112.38
1	B	154	ARG	CB-CG-CD	-5.15	99.45	111.30
1	B	1317	CYS	N-CA-C	5.15	118.59	112.72
1	B	3	ALA	CA-C-N	5.12	131.31	121.54
1	B	3	ALA	C-N-CA	5.12	131.31	121.54
1	A	755	GLY	N-CA-C	-5.09	107.67	115.00
1	B	1332	VAL	N-CA-CB	5.08	120.14	111.50
1	B	703	LYS	N-CA-C	-5.08	105.82	111.36
1	A	4	ASP	CB-CA-C	5.06	120.50	110.42
1	A	526	LYS	N-CA-C	-5.06	105.85	112.23
1	A	139	ILE	N-CA-C	5.05	115.27	110.42
1	A	565	ASN	N-CA-C	5.04	121.54	110.80
1	A	75	ALA	CA-C-N	-5.03	114.62	119.90
1	A	75	ALA	C-N-CA	-5.03	114.62	119.90
1	B	1237	THR	CA-C-N	-5.03	116.01	123.05
1	B	1237	THR	C-N-CA	-5.03	116.01	123.05

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	10041	0	10044	130	0
1	B	10027	0	10027	131	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	53	0	31	1	0
4	B	53	0	31	2	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	24	0	10	1	0
6	B	24	0	10	1	0
7	A	3	0	0	1	0
7	B	3	0	0	1	0
8	A	22	0	8	2	0
8	B	22	0	8	5	0
9	B	12	0	16	2	0
10	A	973	0	0	21	0
10	B	941	0	0	13	0
All	All	22226	0	20185	262	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 6.

All (262) 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:A:506:GLU:HG2	10:A:2141:HOH:O	1.40	1.17
1:A:504:MET:SD	10:A:1779:HOH:O	2.09	1.09
1:A:540:PRO:O	1:A:541:THR:HB	1.52	1.08
1:A:3:ALA:HB2	10:A:2268:HOH:O	1.52	1.07
1:A:60:ARG:HG2	1:A:60:ARG:HH11	1.22	1.03
1:B:358:ILE:HD13	1:B:431:ILE:HG23	1.50	0.94
1:A:1180:MET:CE	1:A:1263:PRO:HB3	1.97	0.94
1:B:4:ASP:HB3	1:B:228:ARG:O	1.68	0.92
1:A:3:ALA:HB1	1:A:228:ARG:H	1.32	0.91
1:A:131:GLN:HE21	1:A:133:GLU:H	1.16	0.91
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.72	0.90
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:NH1	10:B:1669:HOH:O	2.09	0.85
1:A:818:LYS:HE2	10:A:2283:HOH:O	1.77	0.83
1:A:1180:MET:HE1	1:A:1263:PRO:HB3	1.59	0.83
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.45	0.82
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.43	0.81
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.45	0.81
1:A:154:ARG:CD	1:A:1196:GLU:OE2	2.28	0.81
1:B:217:LEU:O	1:B:220:LYS:HE2	1.79	0.81
1:A:1180:MET:HE3	1:A:1263:PRO:HB3	1.63	0.81
1:A:467:LEU:O	1:A:471:GLN:HG2	1.81	0.79
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	1.80	0.79
1:B:966:ARG:O	1:B:970:GLU:HG3	1.83	0.78
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.47	0.78
1:A:562:GLU:HB2	10:A:1573:HOH:O	1.84	0.76
1:A:802:GLU:OE1	8:A:1335:FYO:NAN	2.19	0.76
1:A:3:ALA:O	1:A:4:ASP:C	2.28	0.75
1:A:3:ALA:HB1	1:A:228:ARG:N	2.02	0.73
1:B:3:ALA:HA	1:B:230:GLU:HB2	1.73	0.71
1:A:404:LEU:HD21	1:A:407:ILE:HD11	1.73	0.71
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.74	0.70
1:B:1331:ARG:O	1:B:1332:VAL:HG23	1.91	0.70
1:A:1257:LYS:HE3	10:A:1807:HOH:O	1.92	0.70
1:A:3:ALA:HA	1:A:227:LEU:HD22	1.74	0.69
1:A:541:THR:HG22	1:A:542:TYR:HD1	1.57	0.68
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.59	0.68
1:A:323:LYS:NZ	10:A:1707:HOH:O	2.25	0.68
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.59	0.68
1:A:237:ILE:CD1	1:A:277:MET:HE3	2.25	0.67
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.29	0.67
1:B:474:LEU:O	1:B:475:SER:HB2	1.95	0.66
1:B:594:ASP:OD1	9:B:1338:GOL:H32	1.96	0.66
1:B:1287:ASN:HB3	1:B:1289:ASN:HB3	1.77	0.66
1:A:1328:TRP:HB3	1:A:1329:SER:HB2	1.76	0.66
1:A:60:ARG:HG2	1:A:60:ARG:NH1	2.01	0.66
1:A:3:ALA:O	1:A:5:GLU:N	2.29	0.65
7:A:1334:MOS:O1	7:A:1334:MOS:MO	1.66	0.64
1:B:19:ASN:O	1:B:20:ALA:CB	2.46	0.63
7:B:1334:MOS:MO	7:B:1334:MOS:O1	1.69	0.63
1:B:264:ILE:HD11	4:B:4005:FAD:H3B	1.80	0.63
1:A:540:PRO:O	1:A:541:THR:CB	2.39	0.62
1:B:19:ASN:O	1:B:20:ALA:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:ILE:O	1:B:1008:SER:HB3	1.99	0.62
1:A:58:TYR:OH	1:A:63:ASP:OD1	2.16	0.62
1:B:802:GLU:OE1	8:B:1335:FYO:NAN	2.32	0.62
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.00	0.62
1:A:645:GLU:HG2	1:A:650:ASN:ND2	2.14	0.61
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.65	0.61
1:B:715:GLU:HG3	1:B:895:ARG:HB2	1.82	0.61
1:A:1289:ASN:ND2	1:A:1292:GLU:HB2	2.15	0.61
1:B:1175:ARG:HG3	1:B:1238:GLU:HB3	1.83	0.61
1:A:995:LYS:HZ3	1:A:1284:GLN:HE21	1.48	0.60
1:B:826:MET:H	9:B:1338:GOL:H12	1.67	0.60
1:B:4:ASP:CB	1:B:228:ARG:O	2.46	0.60
1:A:1287:ASN:HD22	1:A:1289:ASN:H	1.48	0.60
1:B:140:GLU:OE2	1:B:551:LYS:HE3	2.02	0.59
1:A:1287:ASN:ND2	1:A:1289:ASN:HB3	2.17	0.59
1:A:1146:SER:HB3	10:A:1909:HOH:O	2.03	0.58
1:B:1105:LYS:HD2	10:B:1837:HOH:O	2.03	0.58
1:A:154:ARG:HD2	1:A:1196:GLU:OE2	2.02	0.58
1:A:504:MET:HE3	10:A:2264:HOH:O	2.02	0.58
1:B:1008:SER:HA	1:B:1081:VAL:HG11	1.84	0.58
1:A:59:ASP:OD2	1:A:61:LEU:HB3	2.05	0.57
1:A:1038:MET:HG3	6:A:1333:MTE:C4	2.35	0.56
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.02	0.56
1:A:346:ALA:HB1	4:A:3005:FAD:H4'	1.87	0.56
1:A:1292:GLU:HG2	1:A:1293:LEU:N	2.20	0.56
1:A:719:LEU:HD11	1:A:895:ARG:HB3	1.88	0.56
8:A:1335:FYO:HAH	10:A:2289:HOH:O	2.04	0.56
1:A:237:ILE:CD1	1:A:277:MET:CE	2.83	0.56
1:A:995:LYS:NZ	1:A:1284:GLN:NE2	2.52	0.55
1:B:1324:ASN:O	1:B:1325:CYS:HB2	2.05	0.55
1:A:447:MET:HG2	1:A:527:LEU:HD13	1.87	0.55
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.06	0.55
1:B:818:LYS:HE2	10:B:1609:HOH:O	2.06	0.55
1:B:427:ARG:NH2	1:B:1171:HIS:O	2.40	0.55
1:A:1132:PHE:CD1	1:B:1126:SER:HB2	2.43	0.54
1:A:237:ILE:HD13	1:A:277:MET:CE	2.37	0.54
1:A:1105:LYS:HE2	10:A:1942:HOH:O	2.07	0.54
1:B:1289:ASN:OD1	1:B:1289:ASN:C	2.50	0.54
1:A:529:LYS:O	1:A:530:ASP:HB2	2.06	0.54
1:B:471:GLN:HG3	10:B:2245:HOH:O	2.07	0.54
1:A:995:LYS:HZ3	1:A:1284:GLN:NE2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASN:O	1:A:200:GLU:HG2	2.08	0.53
1:B:154:ARG:CD	1:B:1196:GLU:OE2	2.56	0.53
1:B:348:LEU:HD13	1:B:407:ILE:HD13	1.90	0.53
1:A:1180:MET:HE1	1:A:1266:LEU:HD12	1.90	0.53
1:B:3:ALA:HB3	1:B:19:ASN:OD1	2.09	0.52
1:A:131:GLN:HE21	1:A:133:GLU:N	1.97	0.52
1:A:338:ALA:HB1	1:A:342:VAL:HB	1.92	0.52
1:B:217:LEU:O	1:B:220:LYS:CE	2.53	0.52
1:A:60:ARG:HH11	1:A:60:ARG:CG	2.09	0.52
1:A:695:ILE:HD11	10:A:1836:HOH:O	2.10	0.52
1:B:284:ILE:HB	1:B:287:LEU:HD12	1.92	0.51
1:B:605:LEU:HD12	1:B:815:ALA:HB2	1.92	0.51
1:A:343:LYS:HE3	10:A:2055:HOH:O	2.09	0.51
1:A:703:LYS:HG3	1:A:703:LYS:O	2.09	0.51
1:B:1324:ASN:HA	1:B:1326:LYS:HB3	1.91	0.51
1:A:1140:TYR:OH	1:A:1145:ASN:ND2	2.36	0.51
1:A:1180:MET:HE3	1:A:1195:VAL:HG22	1.92	0.51
1:B:146:ASN:ND2	1:B:341:GLN:HE22	2.08	0.51
1:A:506:GLU:CD	1:A:506:GLU:H	2.18	0.51
1:A:154:ARG:HD2	10:A:1458:HOH:O	2.10	0.51
1:A:195:LEU:HD22	1:A:1189:ALA:HA	1.92	0.51
1:B:655:PHE:CE1	1:B:814:LEU:HD23	2.45	0.51
1:A:154:ARG:HD3	1:A:1196:GLU:CD	2.35	0.50
1:A:193:PRO:HG2	1:A:560:PHE:CE1	2.46	0.50
1:A:645:GLU:CG	1:A:650:ASN:HD22	2.19	0.50
1:B:1287:ASN:HB3	1:B:1289:ASN:CB	2.41	0.50
1:B:376:SER:HB3	1:B:402:GLU:HG2	1.93	0.50
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	2.11	0.50
1:A:57:LYS:NZ	10:A:1872:HOH:O	2.45	0.50
1:B:4:ASP:CG	1:B:5:GLU:H	2.20	0.50
1:B:1289:ASN:O	1:B:1290:THR:HB	2.12	0.50
1:B:37:ARG:CD	1:B:595:ASP:O	2.59	0.49
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.94	0.49
1:A:404:LEU:CD2	1:A:407:ILE:HD11	2.42	0.49
1:A:58:TYR:CE2	1:A:60:ARG:HB2	2.47	0.49
1:A:655:PHE:CE1	1:A:814:LEU:HD23	2.47	0.49
1:A:657:LYS:O	1:A:658:ASP:HB2	2.12	0.49
1:B:131:GLN:HE21	1:B:133:GLU:H	1.61	0.49
1:B:250:ALA:HB2	1:B:377:ARG:HB2	1.94	0.49
1:A:1126:SER:HB2	1:B:1132:PHE:CD1	2.48	0.49
1:B:1311:ASP:O	1:B:1315:THR:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:HG21	1:A:348:LEU:HG	1.93	0.49
1:B:308:VAL:HG21	1:B:348:LEU:HG	1.95	0.49
1:B:217:LEU:O	1:B:220:LYS:HG3	2.13	0.48
1:B:995:LYS:HZ1	1:B:1284:GLN:NE2	2.12	0.48
1:B:655:PHE:HE1	1:B:814:LEU:CD2	2.24	0.48
1:B:995:LYS:NZ	1:B:1284:GLN:NE2	2.60	0.48
1:A:540:PRO:HA	1:A:543:THR:HG23	1.95	0.48
1:B:1315:THR:O	1:B:1315:THR:CG2	2.59	0.48
1:B:252:HIS:CD2	1:B:277:MET:HE1	2.48	0.48
1:A:1007:ILE:O	1:A:1008:SER:HB3	2.13	0.48
1:B:143:PHE:HB3	1:B:1232:PHE:CE1	2.49	0.48
1:A:82:HIS:HA	1:A:216:LEU:HD21	1.96	0.47
1:B:507:PHE:HB2	1:B:1303:GLU:HG3	1.96	0.47
1:A:624:GLU:HG3	10:A:2285:HOH:O	2.13	0.47
1:B:980:ARG:HD2	10:B:1687:HOH:O	2.13	0.47
1:A:1044:THR:O	1:A:1048:GLN:HG3	2.13	0.47
1:B:165:LYS:O	1:B:165:LYS:HG3	2.14	0.47
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.49	0.47
1:B:358:ILE:CD1	1:B:431:ILE:HG23	2.32	0.47
1:B:391:PRO:HG3	1:B:397:LEU:HD23	1.97	0.47
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.96	0.47
1:B:192:SER:N	1:B:193:PRO:CD	2.78	0.47
1:B:695:ILE:HG23	1:B:700:ASP:HB3	1.96	0.47
1:A:267:GLU:HA	1:A:271:LYS:HG2	1.97	0.47
1:B:645:GLU:HG2	1:B:650:ASN:ND2	2.25	0.47
1:B:1140:TYR:OH	1:B:1145:ASN:ND2	2.48	0.47
1:A:322:GLN:O	1:A:412:SER:HB3	2.15	0.47
1:B:680:ARG:HD2	10:B:1560:HOH:O	2.14	0.47
1:A:61:LEU:H	1:A:63:ASP:H	1.63	0.47
1:B:569:LYS:HE3	10:B:1473:HOH:O	2.15	0.46
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.97	0.46
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.23	0.46
1:B:154:ARG:HD2	1:B:1196:GLU:OE2	2.14	0.46
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.16	0.46
1:B:216:LEU:HA	1:B:219:LEU:HD12	1.97	0.46
1:A:1172:LYS:HE2	1:A:1172:LYS:HB2	1.57	0.46
1:B:802:GLU:OE1	8:B:1335:FYO:HAI	2.15	0.46
1:B:258:VAL:HG22	1:B:264:ILE:HG13	1.97	0.45
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.82	0.45
1:A:58:TYR:HE2	1:A:60:ARG:HB2	1.82	0.45
1:B:192:SER:HB2	10:B:1938:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:SER:HA	10:B:1712:HOH:O	2.16	0.45
1:A:3:ALA:HA	1:A:227:LEU:CD2	2.44	0.45
1:B:1153:PHE:HB2	1:B:1155:TYR:CZ	2.52	0.45
1:B:394:ARG:HD3	10:B:1527:HOH:O	2.16	0.45
1:B:948:LYS:O	1:B:949:GLU:C	2.60	0.45
1:B:146:ASN:HD21	1:B:341:GLN:HE22	1.65	0.45
1:A:723:PHE:CZ	1:A:847:LYS:HE2	2.52	0.44
1:A:1287:ASN:ND2	1:A:1289:ASN:CB	2.80	0.44
1:A:599:TYR:HA	1:B:599:TYR:HA	2.00	0.44
1:B:428:GLU:HG2	10:B:1742:HOH:O	2.17	0.44
1:A:995:LYS:HZ1	1:A:1284:GLN:HE21	1.59	0.44
1:B:552:HIS:HE1	1:B:1172:LYS:HD2	1.82	0.44
1:B:1325:CYS:N	1:B:1326:LYS:CB	2.80	0.44
1:B:376:SER:O	1:B:377:ARG:C	2.59	0.44
8:B:1335:FYO:HAH	10:B:2247:HOH:O	2.18	0.43
1:A:337:PHE:O	1:A:338:ALA:C	2.58	0.43
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.34	0.43
1:A:1014:LEU:HD23	1:A:1014:LEU:HA	1.86	0.43
1:B:701:ALA:CB	1:B:901:CYS:HB3	2.48	0.43
1:A:777:ALA:HB1	1:A:782:VAL:O	2.19	0.43
1:A:37:ARG:HD3	1:A:595:ASP:O	2.19	0.43
1:A:256:LYS:HE2	10:A:2057:HOH:O	2.19	0.43
1:A:490:LEU:HB2	1:A:513:LEU:HD22	2.00	0.43
1:B:1108:ASN:N	1:B:1109:PRO:HD3	2.33	0.43
1:A:1251:LYS:HE2	10:A:1924:HOH:O	2.19	0.43
1:B:281:PRO:HB2	1:B:287:LEU:HD13	2.00	0.43
1:A:256:LYS:HG3	1:A:275:PHE:CD2	2.54	0.43
1:A:571:ASP:OD2	1:A:1052:LYS:NZ	2.41	0.43
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.83	0.43
1:A:325:GLU:HB2	1:A:412:SER:OG	2.19	0.43
1:B:508:ARG:O	1:B:512:THR:HG23	2.19	0.43
1:B:880:ARG:NH2	8:B:1335:FYO:OAD	2.50	0.43
1:B:1315:THR:O	1:B:1315:THR:HG23	2.17	0.43
1:A:97:ARG:NH1	10:A:2131:HOH:O	2.51	0.42
1:A:441:LEU:HB3	1:A:451:GLU:HB2	2.01	0.42
1:B:1011:VAL:CG2	1:B:1014:LEU:HD12	2.48	0.42
1:B:3:ALA:N	10:B:2169:HOH:O	2.52	0.42
1:B:911:PHE:O	1:B:912:ARG:C	2.61	0.42
1:B:1038:MET:HG3	6:B:1333:MTE:C4	2.49	0.42
1:A:1328:TRP:CA	1:A:1329:SER:HB2	2.49	0.42
1:B:37:ARG:HD3	1:B:595:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLN:HG3	1:B:151:THR:HG22	2.01	0.42
1:A:541:THR:HG22	1:A:542:TYR:CD1	2.46	0.42
1:A:36:LEU:HD22	1:A:89:GLU:CG	2.47	0.42
1:A:1180:MET:HE3	1:A:1263:PRO:CB	2.42	0.42
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.55	0.42
1:B:32:ARG:HH12	1:B:676:GLU:CD	2.27	0.42
1:B:605:LEU:C	1:B:605:LEU:HD23	2.45	0.42
1:B:972:LEU:HD23	1:B:972:LEU:HA	1.81	0.42
1:B:129:ARG:HH11	1:B:129:ARG:HD2	1.67	0.42
1:A:1328:TRP:CB	1:A:1329:SER:HB2	2.46	0.41
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.55	0.41
1:B:337:PHE:CE1	4:B:4005:FAD:C2	3.04	0.41
1:B:503:GLY:C	1:B:505:ILE:HD12	2.46	0.41
1:A:747:HIS:HD1	1:A:805:SER:HA	1.86	0.41
1:B:448:GLN:HB2	1:B:477:PHE:CE2	2.54	0.41
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	2.01	0.41
1:B:1151:HIS:CE1	1:B:1251:LYS:HD2	2.55	0.41
1:A:733:GLU:O	1:A:1295:ARG:HD2	2.20	0.41
1:A:448:GLN:HB2	1:A:477:PHE:CE2	2.55	0.41
1:A:1265:PHE:O	1:A:1265:PHE:CG	2.74	0.41
1:B:1186:LEU:HD21	1:B:1254:TYR:HB2	2.02	0.41
1:A:842:PHE:CD2	1:A:918:GLN:HG2	2.54	0.41
1:A:719:LEU:CD1	1:A:860:GLU:HG2	2.51	0.41
1:B:1331:ARG:C	1:B:1332:VAL:HG23	2.45	0.41
1:A:97:ARG:NH1	1:A:97:ARG:HB2	2.36	0.41
1:B:91:ILE:HD11	1:B:121:VAL:CG1	2.51	0.41
1:B:109:HIS:CE1	1:B:1189:ALA:HB1	2.56	0.41
1:B:338:ALA:HA	1:B:429:ASP:OD1	2.21	0.41
1:B:752:ILE:HD13	1:B:822:PRO:HB3	2.03	0.41
1:A:290:VAL:HA	1:A:298:SER:O	2.21	0.41
1:A:723:PHE:CE2	1:A:847:LYS:HE2	2.56	0.41
1:B:233:ARG:NH1	1:B:680:ARG:HD3	2.36	0.41
1:B:723:PHE:CZ	1:B:847:LYS:HE3	2.56	0.41
1:B:1204:GLY:HA3	1:B:1209:GLU:OE2	2.21	0.41
1:A:328:ARG:HD2	10:A:1713:HOH:O	2.22	0.40
1:B:100:PRO:O	1:B:104:ARG:HG3	2.21	0.40
1:B:829:ARG:O	1:B:833:MET:HG3	2.21	0.40
1:A:618:LYS:HD3	1:A:690:GLU:HB2	2.03	0.40
1:B:284:ILE:HA	1:B:285:PRO:HD3	1.99	0.40
1:B:1014:LEU:HD11	8:B:1335:FYO:HAGA	2.03	0.40
1:B:374:ILE:HG21	1:B:398:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:HIS:HA	1:B:911:PHE:CE1	2.57	0.40
1:B:1259:VAL:O	1:B:1259:VAL:HG22	2.22	0.40
1:A:214:PRO:HD2	10:A:2013:HOH:O	2.21	0.40
1:B:734:LEU:HD21	1:B:921:PHE:CE2	2.57	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	1285/1332 (96%)	1220 (95%)	53 (4%)	12 (1%)	14	12
1	B	1283/1332 (96%)	1227 (96%)	45 (4%)	11 (1%)	14	12
All	All	2568/2664 (96%)	2447 (95%)	98 (4%)	23 (1%)	14	12

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	565	ASN
1	A	1319	THR
1	A	1329	SER
1	B	4	ASP
1	B	20	ALA
1	A	4	ASP
1	A	61	LEU
1	A	541	THR
1	B	62	GLN
1	B	1008	SER
1	B	1290	THR
1	B	1325	CYS
1	A	445	GLY
1	A	912	ARG

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Mol	Chain	Res	Type
1	A	1008	SER
1	B	912	ARG
1	B	397	LEU
1	B	797	GLY
1	A	797	GLY
1	A	947	TYR
1	A	1139	GLY
1	B	947	TYR
1	B	1139	GLY

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	1097/1128 (97%)	1046 (95%)	51 (5%)	24	29
1	B	1096/1128 (97%)	1057 (96%)	39 (4%)	31	39
All	All	2193/2256 (97%)	2103 (96%)	90 (4%)	27	33

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	61	LEU
1	A	89	GLU
1	A	100	PRO
1	A	154	ARG
1	A	225	LYS
1	A	256	LYS
1	A	271	LYS
1	A	287	LEU
1	A	312	LEU
1	A	323	LYS
1	A	348	LEU
1	A	398	LEU
1	A	401	GLU

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Mol	Chain	Res	Type
1	A	407	ILE
1	A	433	LYS
1	A	476	LYS
1	A	499	ASP
1	A	505	ILE
1	A	506	GLU
1	A	513	LEU
1	A	537	LYS
1	A	538	LEU
1	A	541	THR
1	A	552	HIS
1	A	569	LYS
1	A	600	GLU
1	A	659	THR
1	A	684	VAL
1	A	699	GLU
1	A	743	TYR
1	A	744	LEU
1	A	857	VAL
1	A	890	LYS
1	A	982	SER
1	A	983	GLU
1	A	992	CYS
1	A	1011	VAL
1	A	1106	LYS
1	A	1107	LYS
1	A	1143	GLU
1	A	1172	LYS
1	A	1203	LEU
1	A	1208	LEU
1	A	1253	ILE
1	A	1262	PRO
1	A	1287	ASN
1	A	1317	CYS
1	A	1319	THR
1	A	1326	LYS
1	A	1331	ARG
1	B	4	ASP
1	B	57	LYS
1	B	60	ARG
1	B	64	LYS
1	B	93	SER

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Mol	Chain	Res	Type
1	B	97	ARG
1	B	154	ARG
1	B	194	SER
1	B	211	ILE
1	B	220	LYS
1	B	268	MET
1	B	314	GLU
1	B	321	THR
1	B	332	GLU
1	B	375	VAL
1	B	379	THR
1	B	433	LYS
1	B	476	LYS
1	B	481	LYS
1	B	497	SER
1	B	543	THR
1	B	565	ASN
1	B	600	GLU
1	B	743	TYR
1	B	845	ARG
1	B	852	LYS
1	B	857	VAL
1	B	948	LYS
1	B	983	GLU
1	B	984	VAL
1	B	1055	LYS
1	B	1143	GLU
1	B	1208	LEU
1	B	1286	THR
1	B	1315	THR
1	B	1317	CYS
1	B	1326	LYS
1	B	1330	LEU
1	B	1332	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	131	GLN
1	A	226	GLN
1	A	448	GLN

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Mol	Chain	Res	Type
1	A	473	GLN
1	A	650	ASN
1	A	728	ASN
1	A	1095	GLN
1	A	1145	ASN
1	A	1212	HIS
1	A	1284	GLN
1	A	1285	HIS
1	A	1287	ASN
1	A	1289	ASN
1	B	62	GLN
1	B	131	GLN
1	B	146	ASN
1	B	252	HIS
1	B	552	HIS
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	1137	ASN
1	B	1145	ASN
1	B	1212	HIS
1	B	1220	HIS
1	B	1284	GLN
1	B	1287	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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
8	FYO	B	1335	7	21,24,24	4.64	11 (52%)	23,34,34	8.70	15 (65%)
2	FES	B	4002	1	0,4,4	-	-	-		
7	MOS	A	1334	8,6	0,2,3	-	-	-		
2	FES	A	3002	1	0,4,4	-	-	-		
2	FES	B	4001	1	0,4,4	-	-	-		
9	GOL	B	1338	-	5,5,5	0.63	0	5,5,5	1.95	2 (40%)
2	FES	A	3001	1	0,4,4	-	-	-		
6	MTE	A	1333	7	21,26,26	1.20	2 (9%)	19,40,40	1.58	5 (26%)
4	FAD	B	4005	-	58,58,58	1.28	6 (10%)	85,89,89	1.86	20 (23%)
6	MTE	B	1333	7	21,26,26	1.45	2 (9%)	19,40,40	2.53	6 (31%)
5	BCT	B	1904	-	3,3,3	0.56	0	2,3,3	0.30	0
7	MOS	B	1334	8,6	0,2,3	-	-	-		
8	FYO	A	1335	7	21,24,24	4.77	10 (47%)	23,34,34	8.42	14 (60%)
5	BCT	A	1904	-	3,3,3	0.89	0	2,3,3	1.07	0
4	FAD	A	3005	-	58,58,58	1.30	7 (12%)	85,89,89	1.83	20 (23%)
9	GOL	B	1336	-	5,5,5	0.62	0	5,5,5	2.03	1 (20%)

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
8	FYO	B	1335	7	-	0/2/22/22	0/3/3/3
2	FES	B	4002	1	-	-	0/1/1/1
9	GOL	B	1338	-	-	2/4/4/4	-
2	FES	A	3002	1	-	-	0/1/1/1
2	FES	B	4001	1	-	-	0/1/1/1
2	FES	A	3001	1	-	-	0/1/1/1
6	MTE	A	1333	7	-	3/6/34/34	0/3/3/3
4	FAD	B	4005	-	-	6/34/50/50	0/6/6/6
6	MTE	B	1333	7	-	2/6/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FYO	A	1335	7	-	0/2/22/22	0/3/3/3
9	GOL	B	1336	-	-	2/4/4/4	-
4	FAD	A	3005	-	-	6/34/50/50	0/6/6/6

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1335	FYO	CAE-CAR	11.26	1.61	1.43
8	B	1335	FYO	CAE-CAR	10.95	1.60	1.43
8	B	1335	FYO	CAI-CAR	10.61	1.46	1.35
8	A	1335	FYO	CAI-CAR	8.92	1.44	1.35
8	A	1335	FYO	OAC-CAP	8.25	1.39	1.23
8	B	1335	FYO	OAD-CAQ	7.48	1.39	1.24
8	B	1335	FYO	OAC-CAP	7.38	1.37	1.23
8	A	1335	FYO	OAD-CAQ	7.19	1.38	1.24
8	A	1335	FYO	OAB-CAO	7.07	1.38	1.24
8	A	1335	FYO	CAG-CAS	-6.43	1.39	1.50
8	B	1335	FYO	OAB-CAO	6.12	1.36	1.24
8	B	1335	FYO	CAG-CAS	-5.69	1.41	1.50
8	A	1335	FYO	CAE-NAA	-4.71	1.06	1.14
4	A	3005	FAD	C4X-N5	4.03	1.39	1.30
6	B	1333	MTE	O4-C4	3.92	1.31	1.23
4	B	4005	FAD	C4X-N5	3.66	1.38	1.30
4	A	3005	FAD	P-O3P	3.35	1.63	1.59
4	A	3005	FAD	C8A-N7A	3.34	1.38	1.31
8	B	1335	FYO	CAU-NAM	3.29	1.38	1.33
8	A	1335	FYO	NAJ-NAN	3.24	1.43	1.36
4	B	4005	FAD	C2A-N1A	3.24	1.39	1.33
4	B	4005	FAD	C2A-N3A	3.01	1.39	1.33
4	B	4005	FAD	C10-N1	2.89	1.39	1.33
6	B	1333	MTE	C6-N5	2.78	1.49	1.46
4	B	4005	FAD	O4'-C4'	-2.74	1.37	1.43
8	A	1335	FYO	CAU-NAM	2.73	1.37	1.33
6	A	1333	MTE	O4-C4	2.67	1.28	1.23
4	B	4005	FAD	C9-C9A	2.55	1.43	1.39
8	A	1335	FYO	CAI-CAT	-2.43	1.38	1.43
4	A	3005	FAD	C1'-N10	2.34	1.53	1.47
8	B	1335	FYO	NAJ-NAN	2.32	1.41	1.36
4	A	3005	FAD	O3B-C3B	-2.31	1.37	1.43
4	A	3005	FAD	C2A-N1A	2.22	1.37	1.33
6	A	1333	MTE	C9-C10	2.19	1.42	1.38
8	B	1335	FYO	CAF-CAS	2.16	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1335	FYO	CAG-CAP	-2.14	1.41	1.48
4	A	3005	FAD	C5A-N7A	-2.08	1.35	1.39
8	B	1335	FYO	CAU-NAJ	2.00	1.36	1.34

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1335	FYO	CAR-CAE-NAA	-38.55	124.36	177.77
8	A	1335	FYO	CAR-CAE-NAA	-36.41	127.32	177.77
8	A	1335	FYO	OAD-CAQ-CAH	-8.24	114.09	125.46
8	B	1335	FYO	CAO-CAF-CAS	-7.40	117.55	122.41
8	A	1335	FYO	CAU-NAJ-NAN	-6.53	104.46	110.23
6	B	1333	MTE	O3'-C7-C6	6.49	113.29	108.96
8	A	1335	FYO	OAB-CAO-CAF	-6.30	116.77	125.46
8	A	1335	FYO	CAH-CAQ-NAL	5.95	122.64	115.24
8	B	1335	FYO	CAH-CAQ-NAL	5.87	122.54	115.24
6	B	1333	MTE	O3'-C7-N8	5.64	113.73	108.61
4	B	4005	FAD	N9A-C8A-N7A	-5.43	106.24	113.94
8	B	1335	FYO	CAF-CAO-NAK	5.28	121.81	115.24
4	B	4005	FAD	N3A-C2A-N1A	-5.20	120.71	128.58
4	A	3005	FAD	N3A-C2A-N1A	-5.15	120.79	128.58
8	B	1335	FYO	CAU-NAJ-NAN	-4.74	106.04	110.23
4	B	4005	FAD	C4-N3-C2	-4.60	117.47	125.64
4	B	4005	FAD	C5A-N7A-C8A	4.47	110.47	103.45
8	B	1335	FYO	CAP-NAK-CAO	-4.45	121.36	127.06
8	B	1335	FYO	CAS-CAU-NAJ	-4.41	119.22	125.67
8	A	1335	FYO	CAP-NAK-CAO	-4.31	121.53	127.06
8	A	1335	FYO	CAI-CAR-CAE	-4.31	113.83	121.70
9	B	1336	GOL	O3-C3-C2	-4.26	91.19	110.38
4	A	3005	FAD	C5A-C4A-N3A	-4.23	120.89	126.72
4	A	3005	FAD	C5X-C9A-N10	4.12	121.70	117.97
4	A	3005	FAD	C4X-C10-N10	4.01	122.22	116.48
8	A	1335	FYO	CAO-CAF-CAS	-3.99	119.79	122.41
4	A	3005	FAD	C9A-C5X-N5	-3.97	118.24	122.45
8	B	1335	FYO	OAD-CAQ-CAH	-3.97	119.98	125.46
8	A	1335	FYO	CAF-CAO-NAK	3.80	119.97	115.24
4	B	4005	FAD	C5A-C4A-N3A	-3.72	121.59	126.72
4	B	4005	FAD	N3A-C4A-N9A	3.63	133.34	127.17
4	B	4005	FAD	C4A-N9A-C8A	3.60	109.52	105.74
8	B	1335	FYO	CAT-CAH-CAQ	-3.60	118.05	120.79
6	A	1333	MTE	O3'-C7-N8	3.54	111.81	108.61
4	A	3005	FAD	C4A-C5A-N7A	-3.51	106.57	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3005	FAD	N9A-C8A-N7A	-3.49	108.99	113.94
4	B	4005	FAD	C4'-C3'-C2'	-3.38	107.94	113.57
4	A	3005	FAD	C5A-N7A-C8A	3.36	108.74	103.45
4	A	3005	FAD	C2A-N3A-C4A	3.31	119.91	111.83
8	A	1335	FYO	NAN-CAV-NAM	-3.30	108.24	114.66
6	B	1333	MTE	C2-N1-C10	3.27	119.14	113.36
4	B	4005	FAD	O2P-P-O3P	3.19	115.88	107.27
4	B	4005	FAD	C10-C4X-N5	-3.11	118.47	124.81
6	B	1333	MTE	O3P-P-O4'	-2.98	98.90	106.67
4	A	3005	FAD	C5A-C4A-N9A	2.96	109.03	105.81
4	B	4005	FAD	C4X-C4-N3	2.86	120.52	113.25
4	A	3005	FAD	C4-N3-C2	-2.84	120.60	125.64
4	A	3005	FAD	O3B-C3B-C4B	-2.82	102.98	111.08
4	A	3005	FAD	C10-C4X-N5	-2.81	119.07	124.81
8	B	1335	FYO	NAN-CAV-NAM	-2.76	109.29	114.66
8	A	1335	FYO	OAB-CAO-NAK	2.75	123.27	119.27
8	A	1335	FYO	OAD-CAQ-NAL	2.75	123.27	119.27
4	B	4005	FAD	C5X-N5-C4X	2.73	122.50	118.09
8	B	1335	FYO	OAB-CAO-CAF	-2.70	121.73	125.46
4	B	4005	FAD	C9A-C5X-N5	-2.69	119.60	122.45
4	A	3005	FAD	O2-C2-N1	-2.64	117.42	121.80
6	A	1333	MTE	O2P-P-O4'	-2.63	99.80	106.67
4	B	4005	FAD	C2A-N3A-C4A	2.60	118.18	111.83
4	B	4005	FAD	C4X-C10-N10	2.59	120.18	116.48
4	A	3005	FAD	C6-C5X-C9A	2.56	122.57	119.05
6	B	1333	MTE	N3-C2-N1	-2.55	118.66	123.32
8	B	1335	FYO	CAG-CAP-NAK	2.54	119.19	116.81
4	B	4005	FAD	O3'-C3'-C4'	2.49	114.58	108.93
4	B	4005	FAD	C4-C4X-C10	2.47	121.16	116.93
4	B	4005	FAD	C6A-C5A-C4A	2.44	120.51	117.18
8	A	1335	FYO	CAT-CAH-CAQ	-2.40	118.96	120.79
8	A	1335	FYO	CAG-CAP-NAK	2.32	118.98	116.81
9	B	1338	GOL	C3-C2-C1	-2.27	103.47	111.80
4	A	3005	FAD	O4B-C1B-N9A	-2.24	103.78	108.09
4	B	4005	FAD	C5'-C4'-C3'	2.24	116.45	112.22
8	B	1335	FYO	CAI-CAT-CAV	-2.24	112.17	120.45
4	A	3005	FAD	C2'-C1'-N10	2.24	120.77	110.20
6	A	1333	MTE	C2-N1-C10	2.23	117.29	113.36
6	A	1333	MTE	O4-C4-C9	-2.21	121.94	127.26
4	A	3005	FAD	C8M-C8-C9	-2.20	115.69	119.57
4	A	3005	FAD	C9A-N10-C10	-2.19	117.42	120.75
4	B	4005	FAD	C4X-C10-N1	-2.12	119.38	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1333	MTE	O4-C4-C9	-2.12	122.15	127.26
8	B	1335	FYO	CAH-CAT-CAV	2.10	124.64	120.94
8	B	1335	FYO	CAI-CAT-CAH	2.09	123.19	120.77
9	B	1338	GOL	O1-C1-C2	2.08	119.74	110.38
6	A	1333	MTE	O2P-P-O1P	2.03	118.75	110.83
4	A	3005	FAD	C5X-N5-C4X	2.00	121.32	118.09

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3005	FAD	N10-C1'-C2'-O2'
4	A	3005	FAD	N10-C1'-C2'-C3'
4	B	4005	FAD	N10-C1'-C2'-O2'
4	B	4005	FAD	N10-C1'-C2'-C3'
6	A	1333	MTE	C4'-O4'-P-O2P
6	A	1333	MTE	C4'-O4'-P-O3P
9	B	1336	GOL	C1-C2-C3-O3
9	B	1336	GOL	O2-C2-C3-O3
4	B	4005	FAD	C2'-C3'-C4'-C5'
4	B	4005	FAD	C2'-C3'-C4'-O4'
6	B	1333	MTE	C3'-C4'-O4'-P
9	B	1338	GOL	O1-C1-C2-O2
9	B	1338	GOL	O2-C2-C3-O3
4	A	3005	FAD	C2'-C3'-C4'-C5'
4	B	4005	FAD	O3'-C3'-C4'-O4'
6	A	1333	MTE	C3'-C4'-O4'-P
6	B	1333	MTE	C4'-O4'-P-O3P
4	A	3005	FAD	C2'-C3'-C4'-O4'
4	B	4005	FAD	O3'-C3'-C4'-C5'
4	A	3005	FAD	O3'-C3'-C4'-O4'
4	A	3005	FAD	O3'-C3'-C4'-C5'

There are no ring outliers.

9 monomers are involved in 16 short contacts:

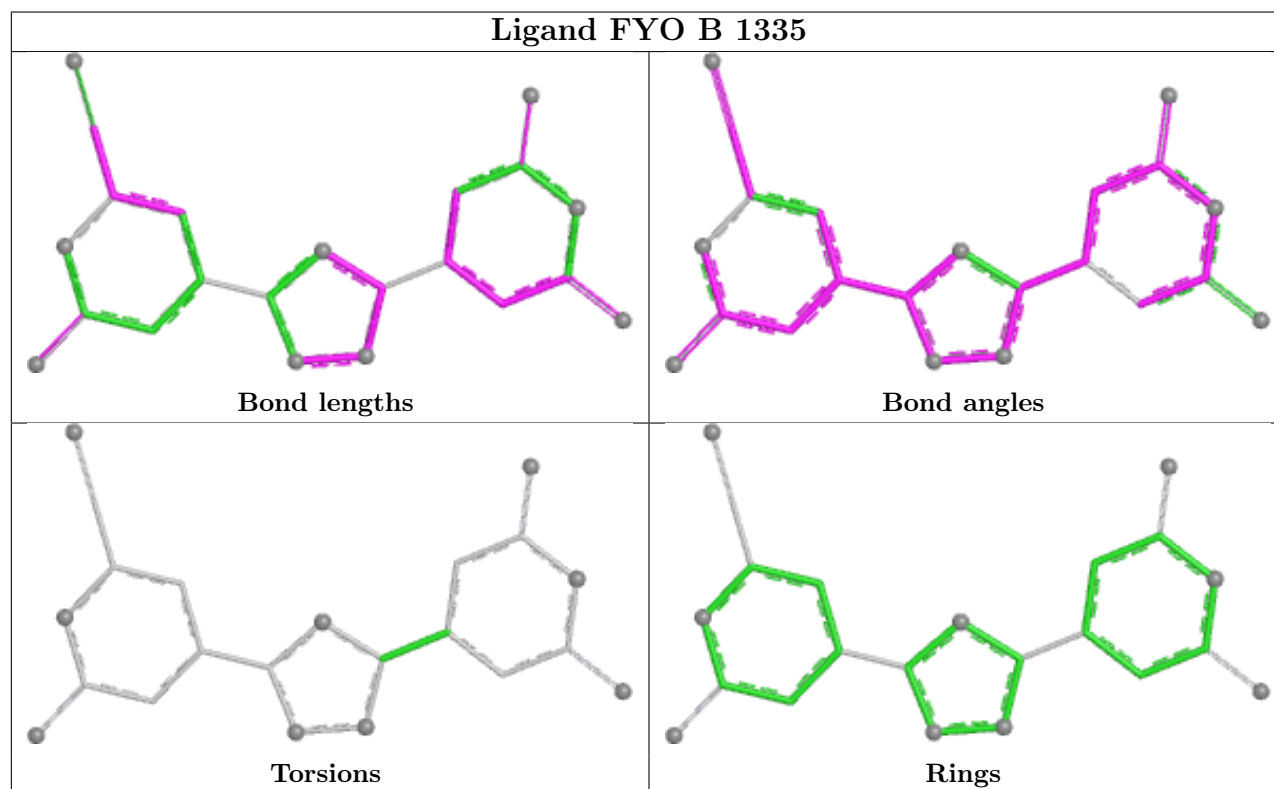
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1335	FYO	5	0
7	A	1334	MOS	1	0
9	B	1338	GOL	2	0
6	A	1333	MTE	1	0

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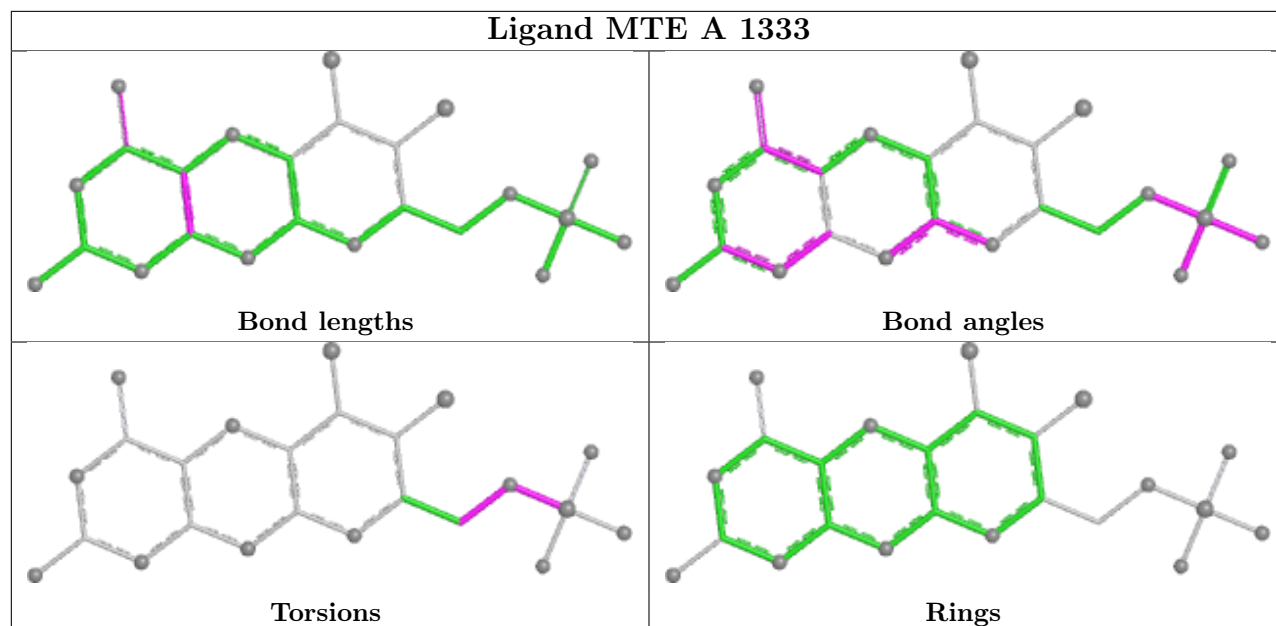
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4005	FAD	2	0
6	B	1333	MTE	1	0
7	B	1334	MOS	1	0
8	A	1335	FYO	2	0
4	A	3005	FAD	1	0

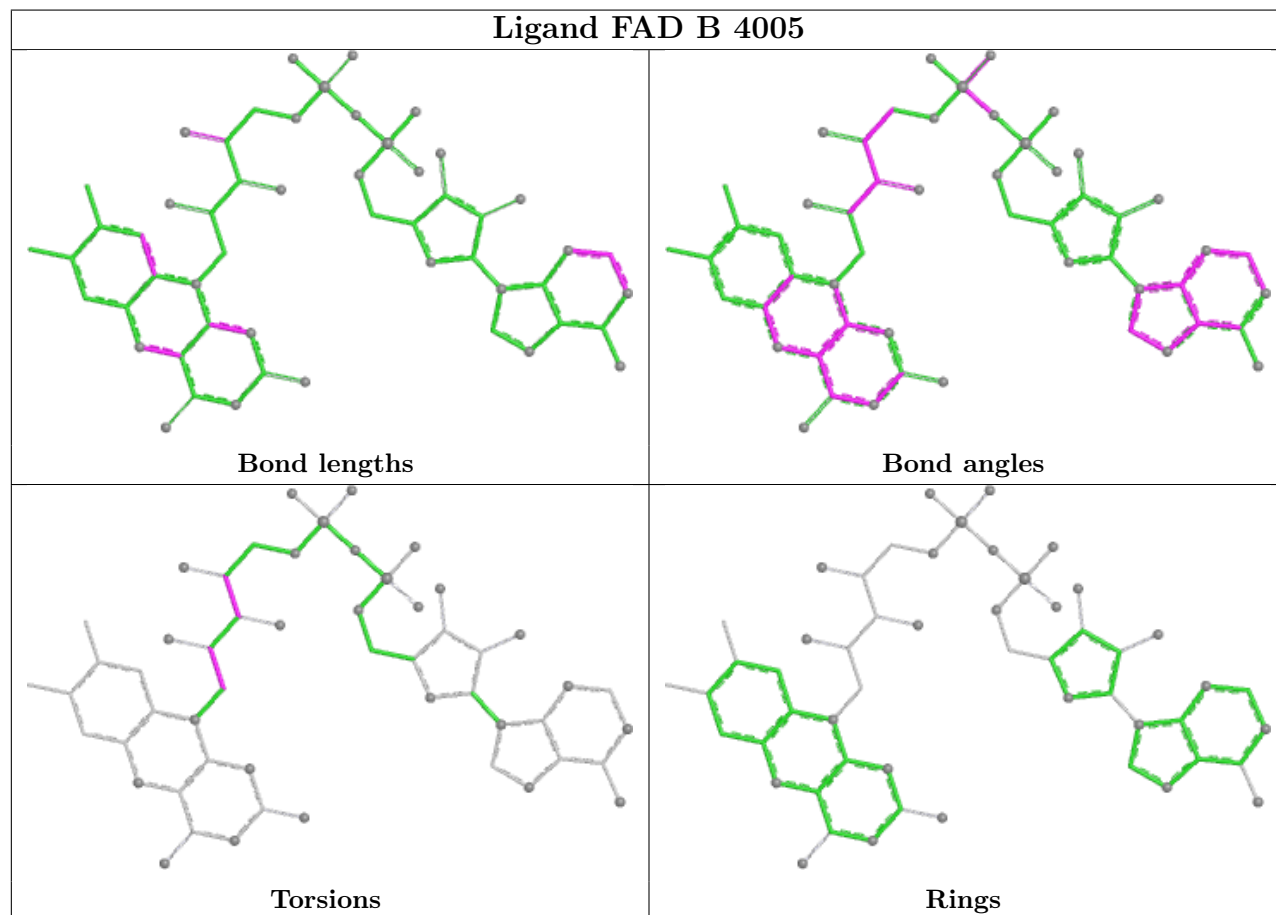
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



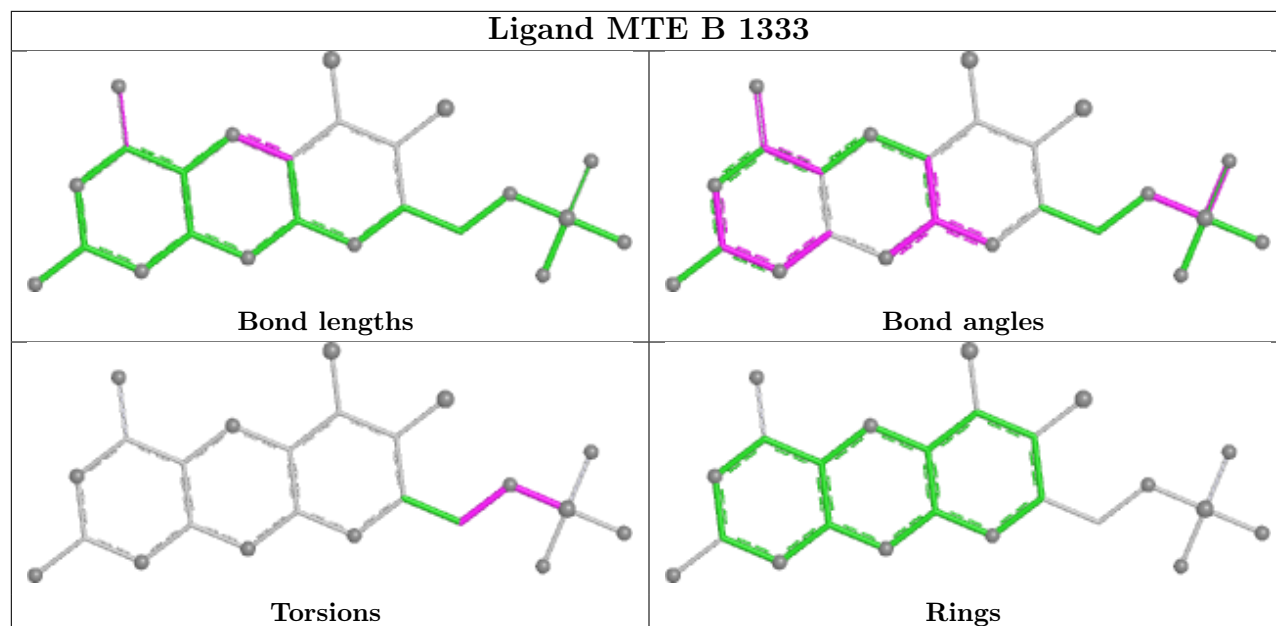
Ligand MTE A 1333



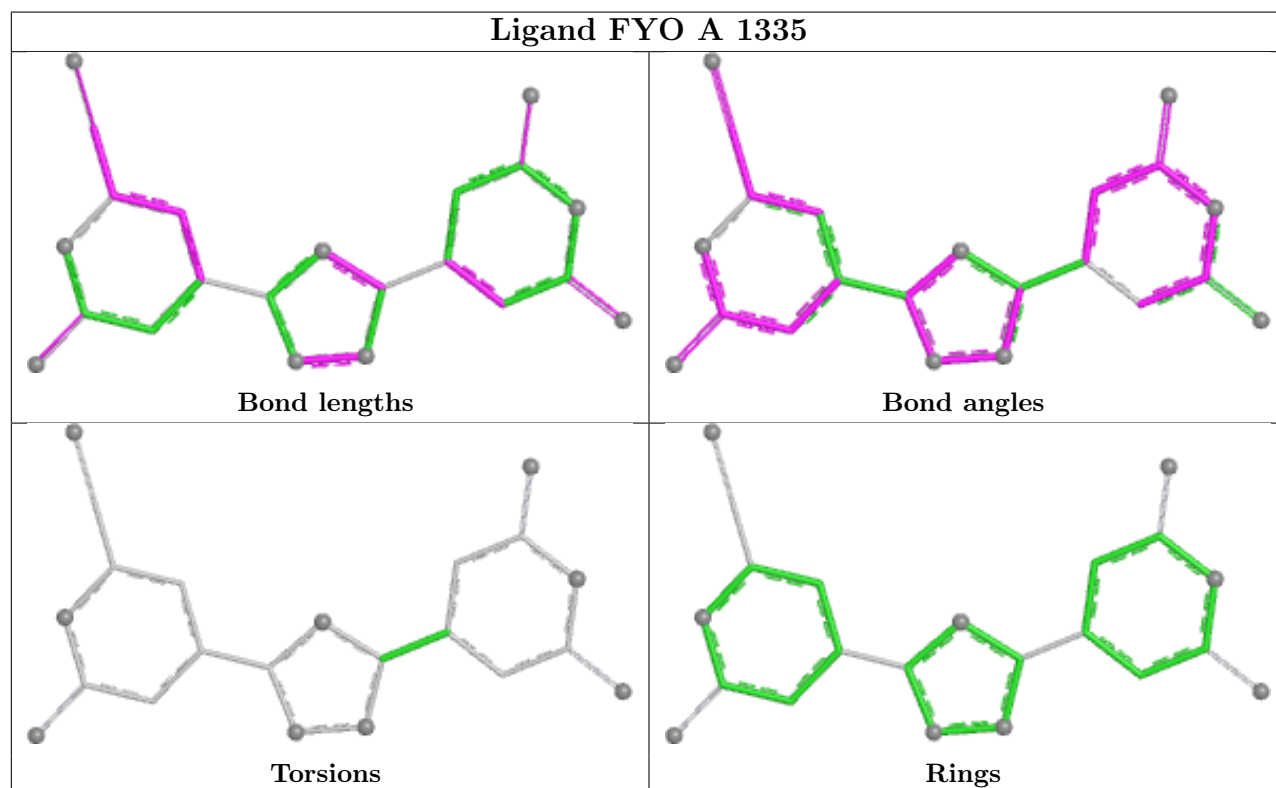
Ligand FAD B 4005

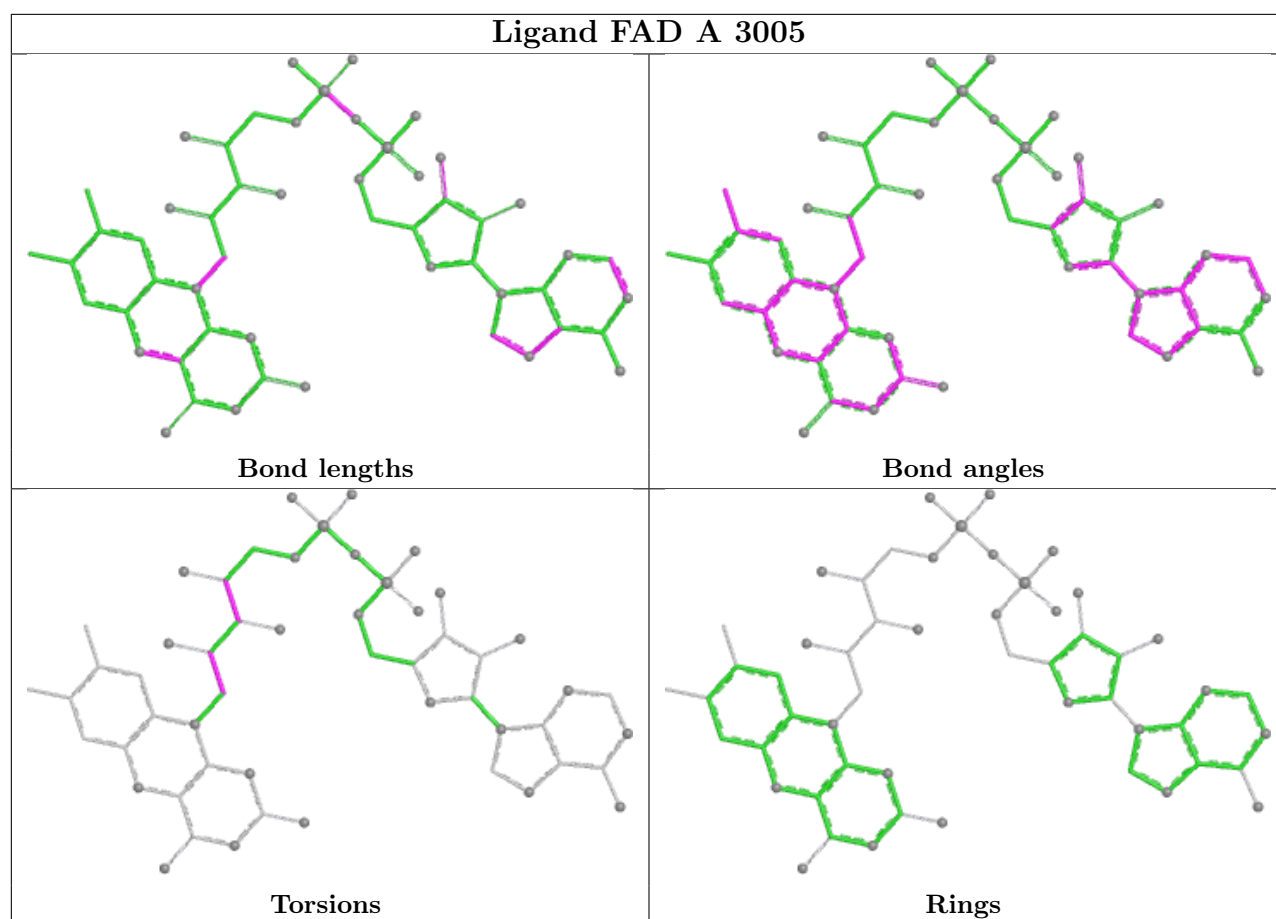


Ligand MTE B 1333



Ligand FYO A 1335





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	1293/1332 (97%)	-0.32	20 (1%) 72 71	12, 25, 44, 85	0
1	B	1291/1332 (96%)	-0.41	19 (1%) 72 71	13, 25, 45, 72	0
All	All	2584/2664 (96%)	-0.37	39 (1%) 72 71	12, 25, 45, 85	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ALA	7.4
1	A	538	LEU	7.0
1	B	4	ASP	4.9
1	A	540	PRO	4.5
1	B	1286	THR	4.0
1	B	552	HIS	3.9
1	B	1316	LEU	3.6
1	A	1320	GLY	3.6
1	B	1318	VAL	3.6
1	A	1319	THR	3.6
1	A	530	ASP	3.5
1	A	1318	VAL	3.5
1	A	539	ASP	3.4
1	A	537	LYS	3.2
1	B	1324	ASN	3.1
1	A	529	LYS	3.0
1	A	552	HIS	3.0
1	A	1329	SER	3.0
1	A	1287	ASN	2.9
1	B	1325	CYS	2.9
1	A	61	LEU	2.8
1	B	61	LEU	2.8
1	B	1287	ASN	2.7
1	A	1290	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1326	LYS	2.6
1	B	566	GLY	2.5
1	A	541	THR	2.5
1	A	551	LYS	2.5
1	A	60	ARG	2.4
1	B	549	PHE	2.3
1	A	165	LYS	2.3
1	B	377	ARG	2.3
1	B	1317	CYS	2.2
1	B	60	ARG	2.2
1	B	1288	ASN	2.2
1	B	551	LYS	2.2
1	A	1332	VAL	2.1
1	A	3	ALA	2.1
1	B	165	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

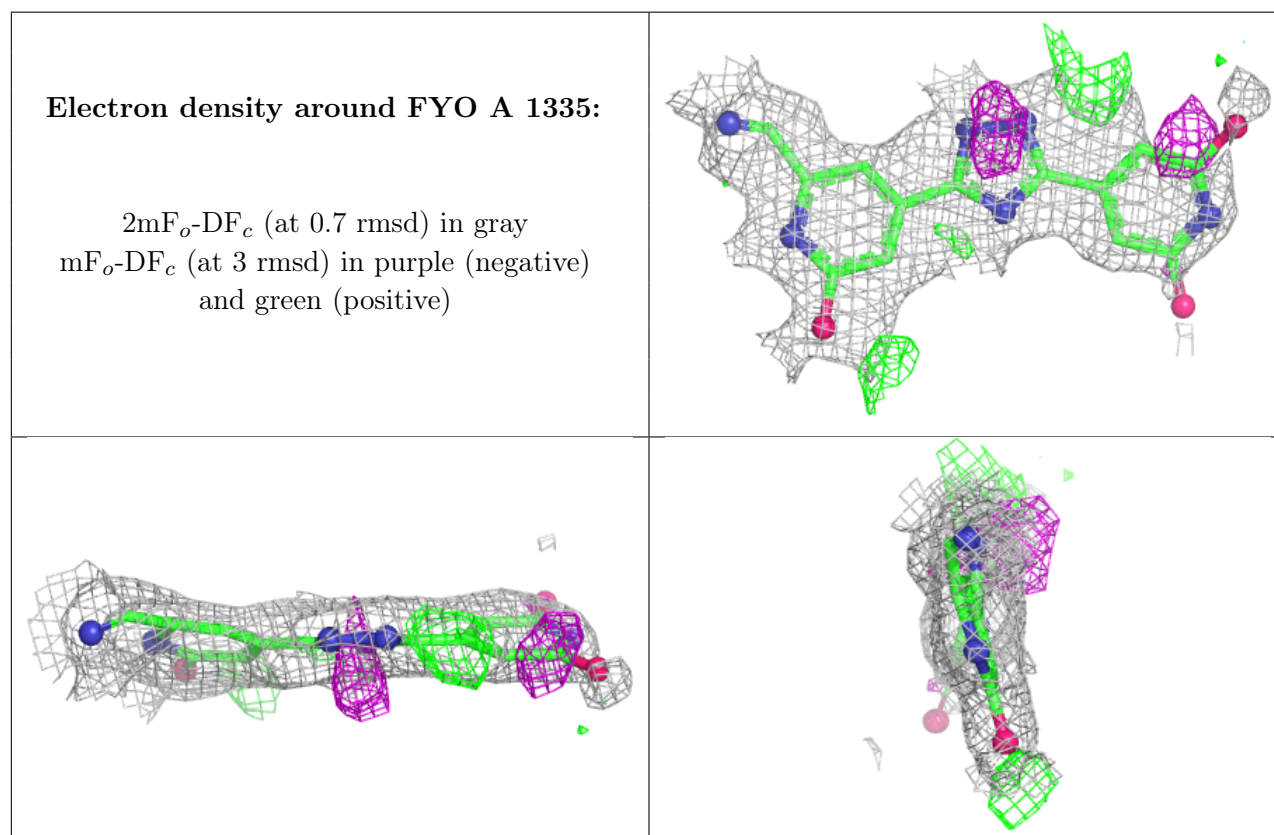
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FYO	A	1335	22/22	0.83	0.14	25,41,59,61	0
8	FYO	B	1335	22/22	0.88	0.12	20,37,60,65	0
9	GOL	B	1336	6/6	0.89	0.09	22,24,29,36	0
9	GOL	B	1338	6/6	0.89	0.13	38,38,41,44	0
3	CA	A	1336	1/1	0.96	0.08	38,38,38,38	0
3	CA	B	1337	1/1	0.96	0.09	34,34,34,34	0
4	FAD	A	3005	53/53	0.97	0.06	15,23,26,29	0
4	FAD	B	4005	53/53	0.97	0.05	16,22,26,31	0

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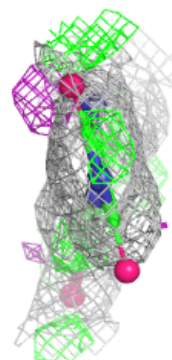
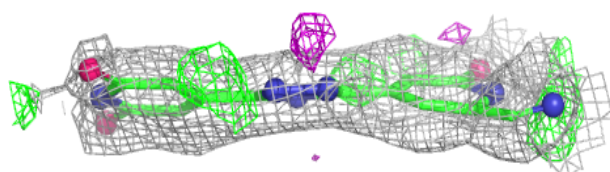
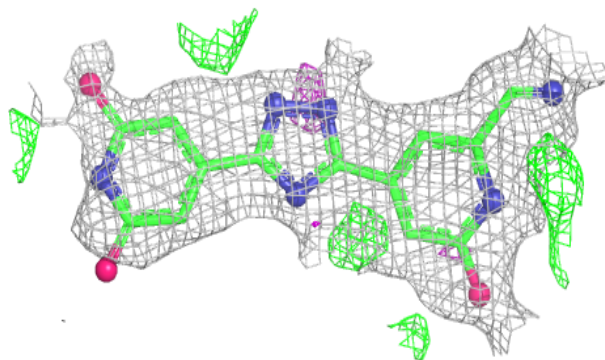
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BCT	A	1904	4/4	0.97	0.07	24,24,24,25	0
5	BCT	B	1904	4/4	0.97	0.09	18,19,20,20	0
3	CA	A	3008	1/1	0.98	0.03	25,25,25,25	0
6	MTE	A	1333	24/24	0.98	0.04	12,18,20,23	0
3	CA	B	4008	1/1	0.99	0.03	21,21,21,21	0
6	MTE	B	1333	24/24	0.99	0.03	14,16,18,21	0
2	FES	B	4002	4/4	0.99	0.02	14,15,16,17	0
7	MOS	B	1334	3/4	1.00	0.01	18,18,20,20	0
2	FES	B	4001	4/4	1.00	0.02	15,17,18,18	0
2	FES	A	3001	4/4	1.00	0.02	16,17,18,19	0
2	FES	A	3002	4/4	1.00	0.03	16,17,17,18	0
7	MOS	A	1334	3/4	1.00	0.02	22,22,22,24	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.

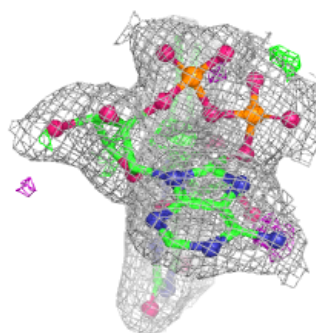
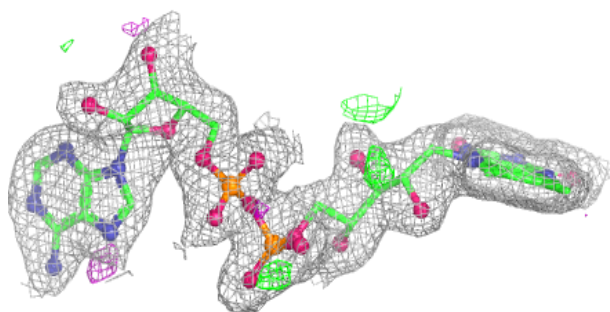
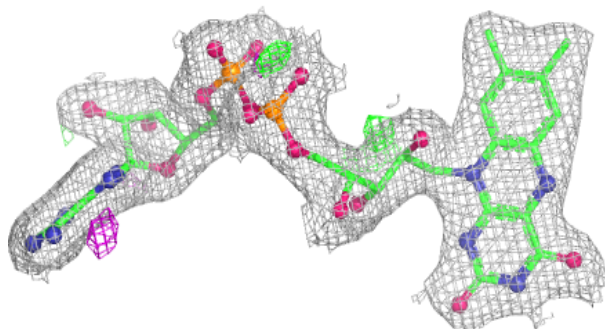


Electron density around FYO B 1335:

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

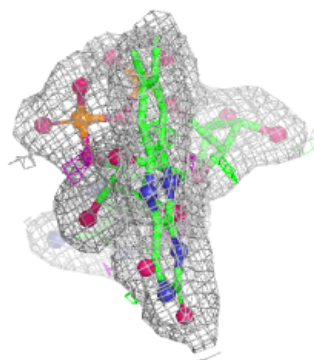
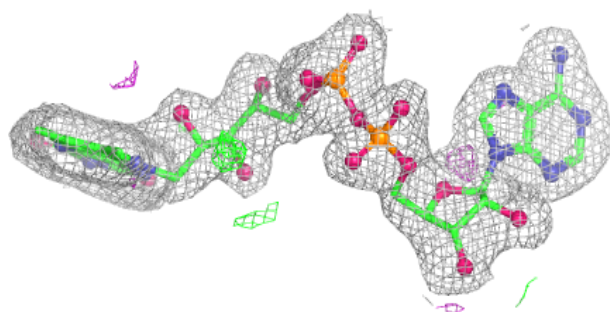
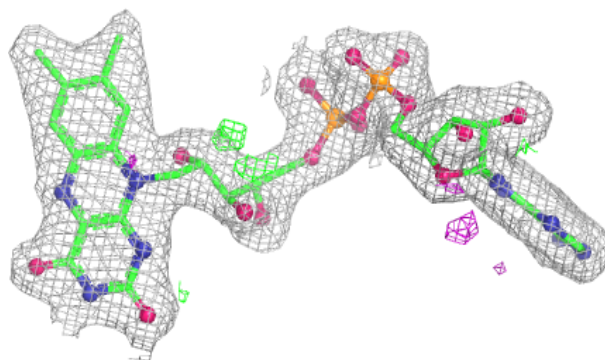
**Electron density around FAD A 3005:**

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



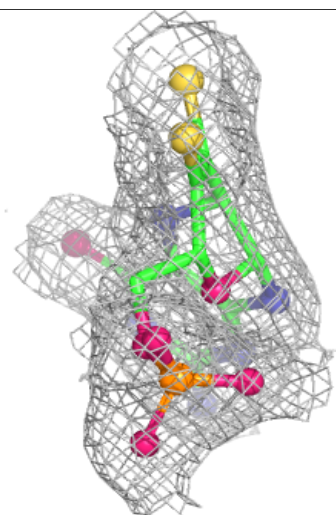
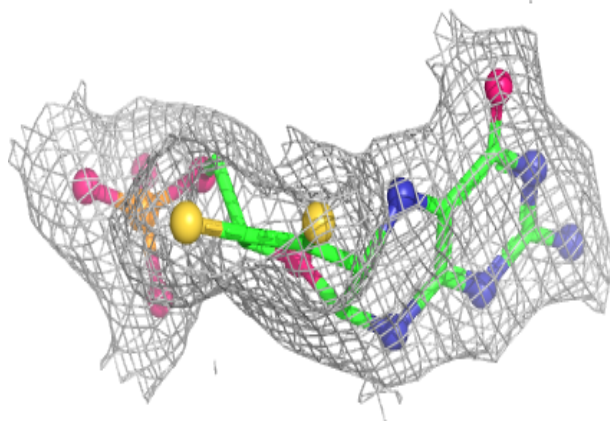
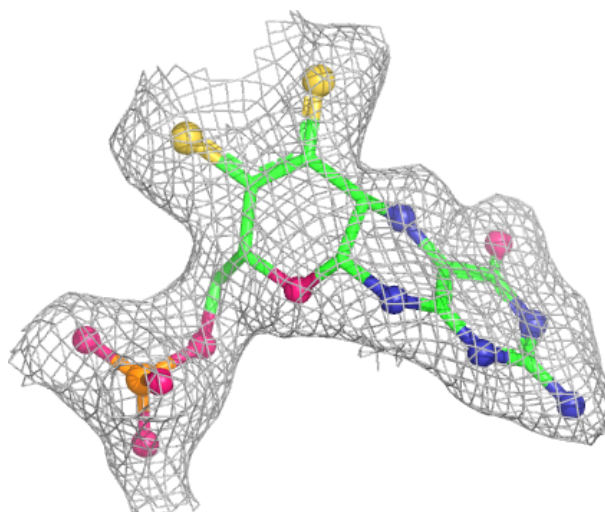
Electron density around FAD B 4005:

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



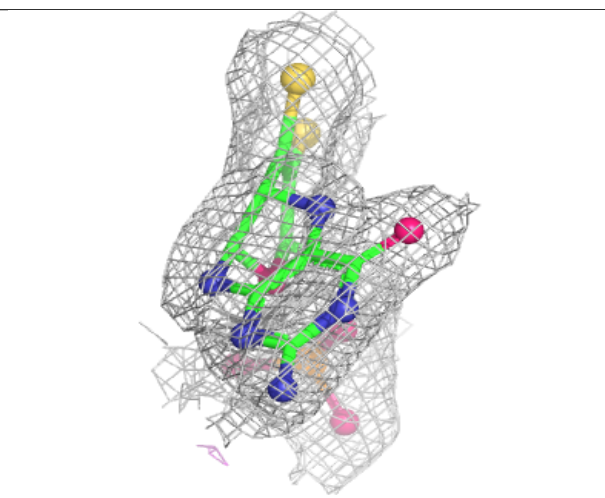
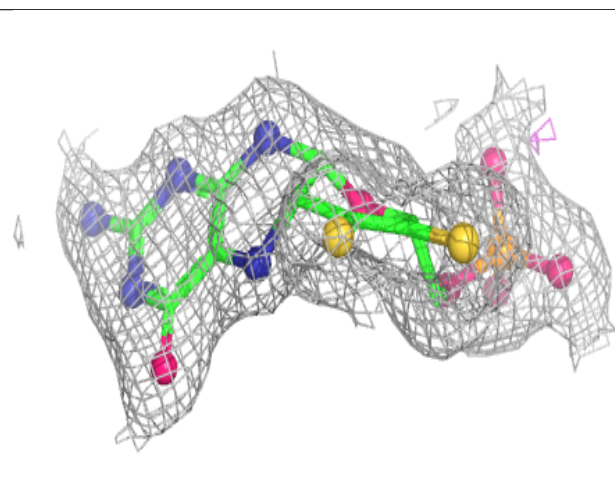
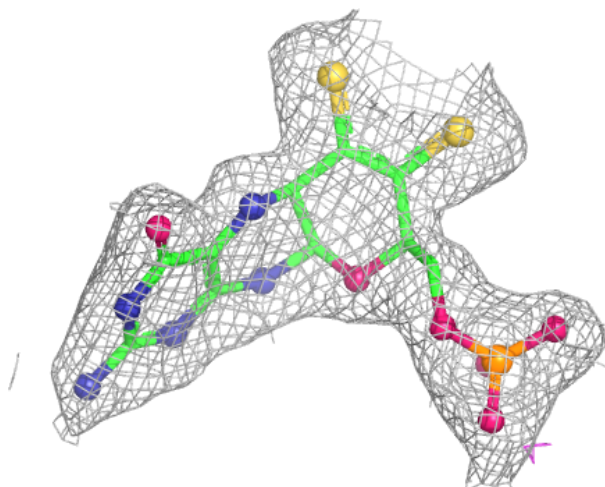
Electron density around MTE A 1333:

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



Electron density around MTE B 1333:

$2mF_o-DF_c$ (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.