



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:15 PM UTC

PDB ID : 1V97 / pdb_00001v97
Title : Crystal Structure of Bovine Milk Xanthine Dehydrogenase FYX-051 bound form
Authors : Okamoto, K.; Matsumoto, K.; Hille, R.; Eger, B.T.; Pai, E.F.; Nishino, T.
Deposited on : 2004-01-21
Resolution : 1.94 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

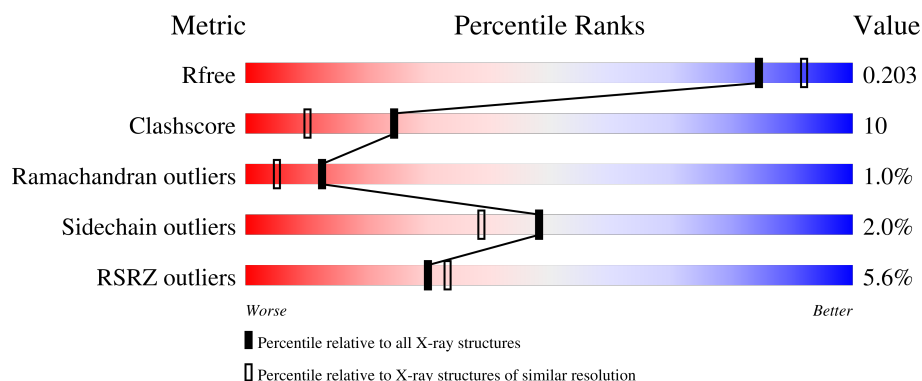
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	6% 77% 18% ..
1	B	1332	5% 77% 18% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MOS	A	3004	-	-	X	-
5	MOS	B	4004	-	-	X	-
8	ACY	A	3007	-	-	X	-
8	ACY	B	4007	-	-	X	-
9	GOL	A	5001	-	X	-	-
9	GOL	A	5003	-	X	-	-
9	GOL	A	5005	-	X	-	-
9	GOL	A	5007	-	X	-	-
9	GOL	B	5002	-	X	-	-
9	GOL	B	5004	-	X	-	-
9	GOL	B	5006	-	X	-	-
9	GOL	B	5008	-	X	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 22481 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.

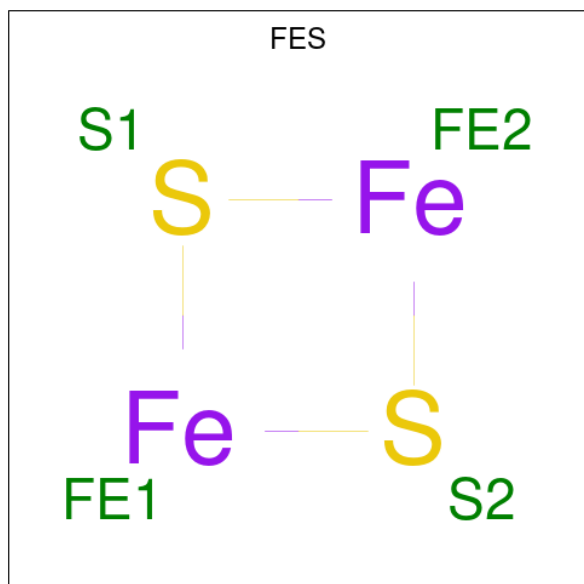
- Molecule 1 is a protein called Xanthine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1298	Total	C	N	O	S	0	0	0
			10071	6401	1727	1882	61			
1	B	1296	Total	C	N	O	S	0	0	0
			10054	6391	1724	1878	61			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

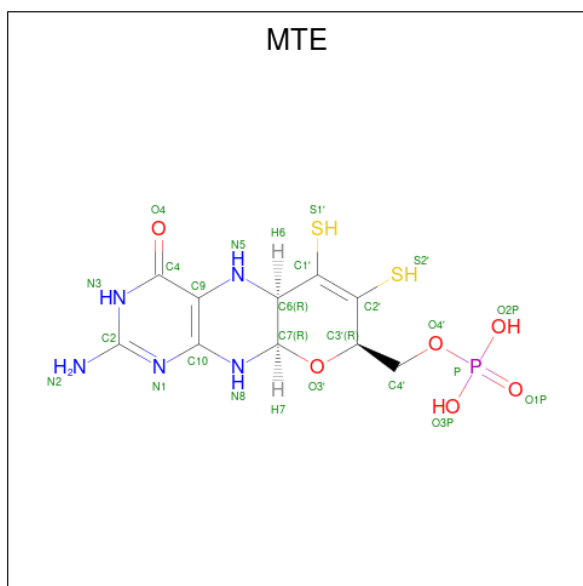
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

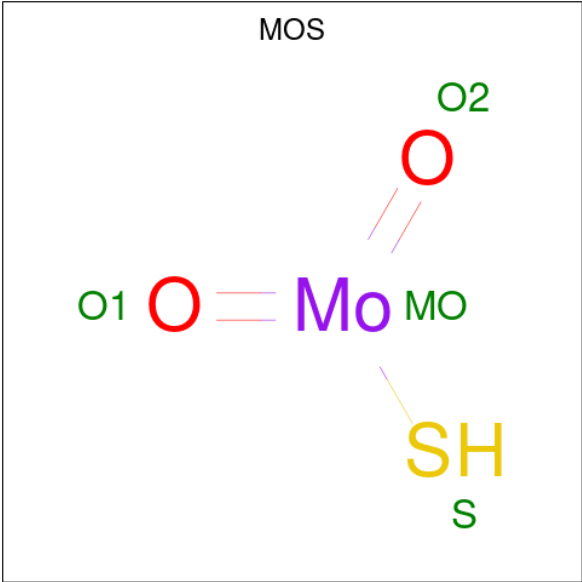
- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

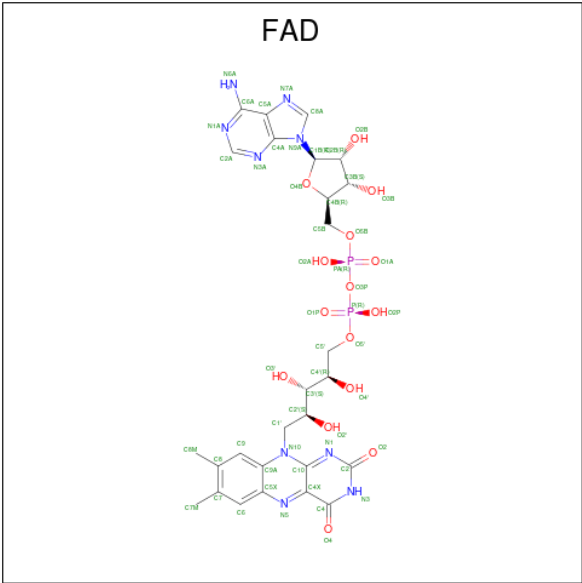
- Molecule 4 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (CCD ID: MTE) (formula: C₁₀H₁₄N₅O₆PS₂).





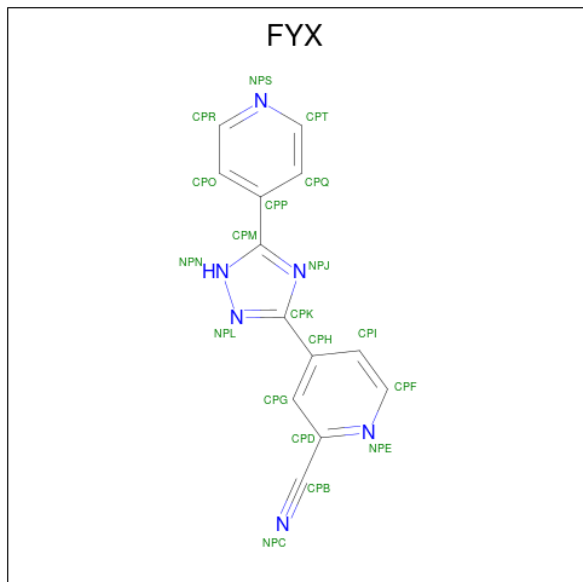
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
5	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



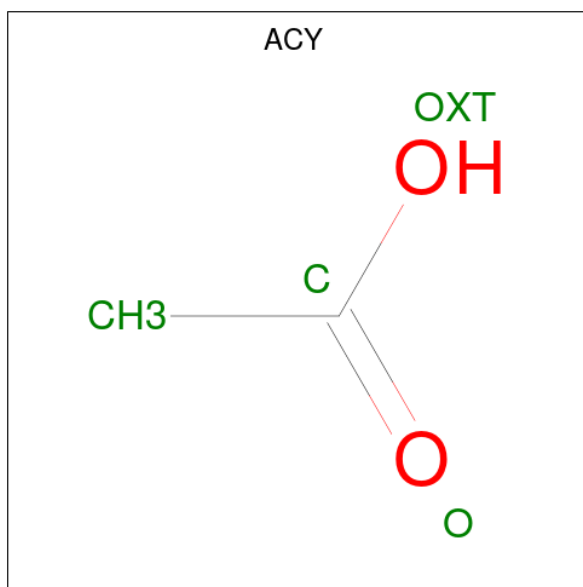
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
6	B	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 7 is 4-(5-PYRIDIN-4-YL-1H-1,2,4-TRIAZOL-3-YL)PYRIDINE-2-CARBONITRILE (CCD ID: FYX) (formula: $C_{13}H_8N_6$).



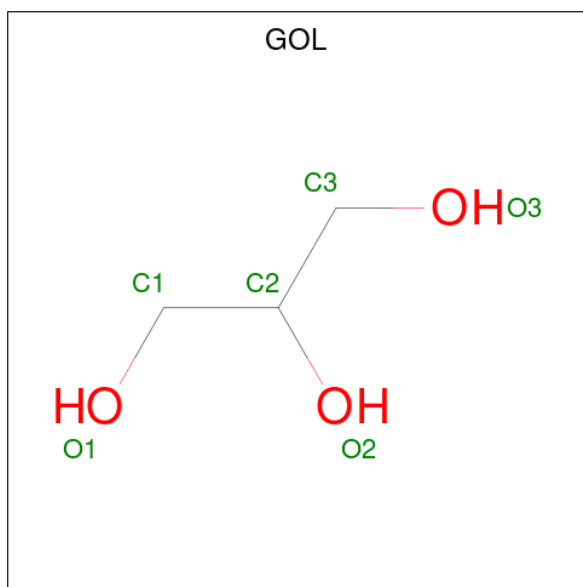
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			19	13	6		
7	B	1	Total	C	N	0	0
			19	13	6		

- Molecule 8 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



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

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



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

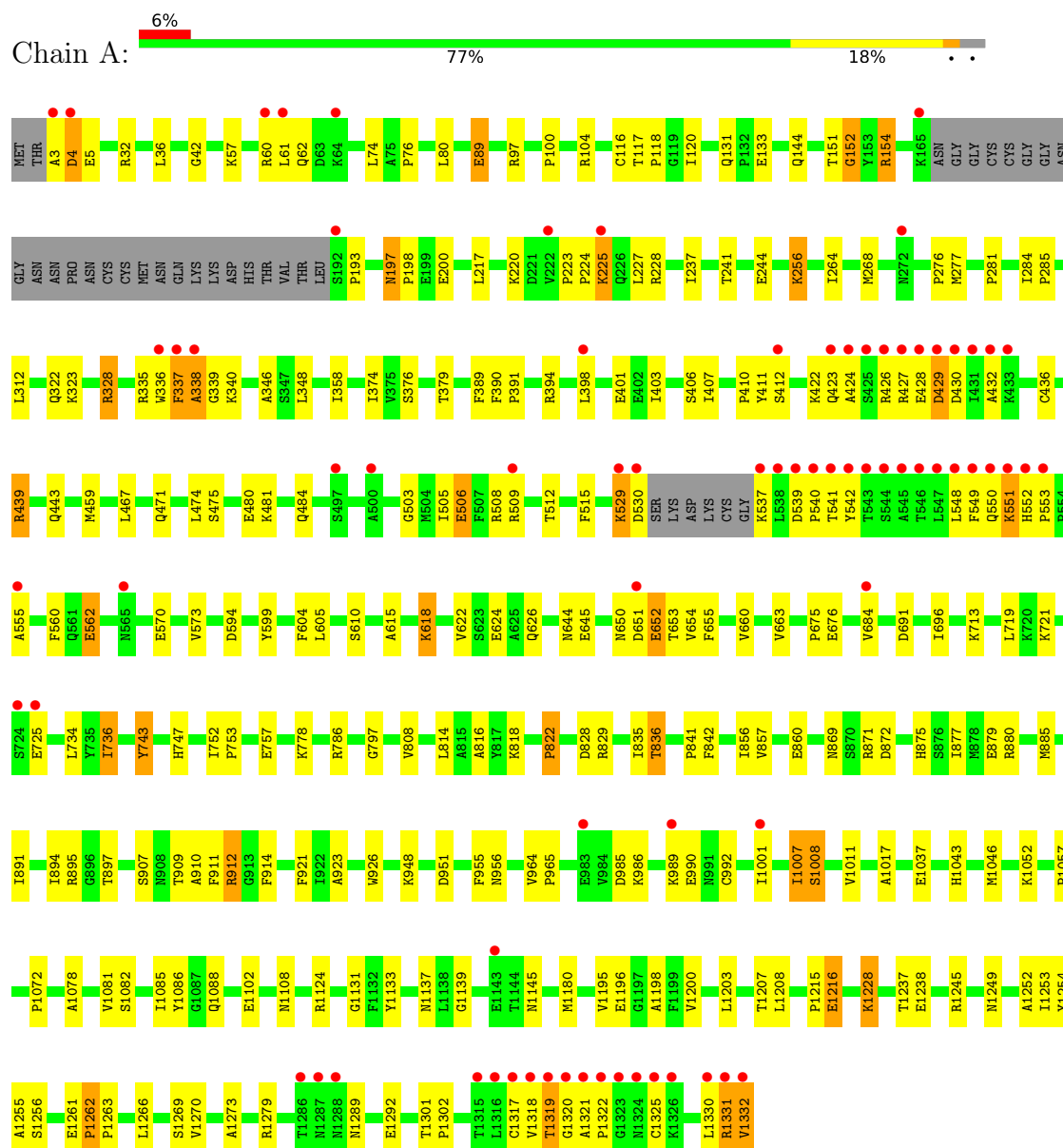
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1061	Total 1061	O 1061	0	0
10	B	1021	Total 1021	O 1021	0	0

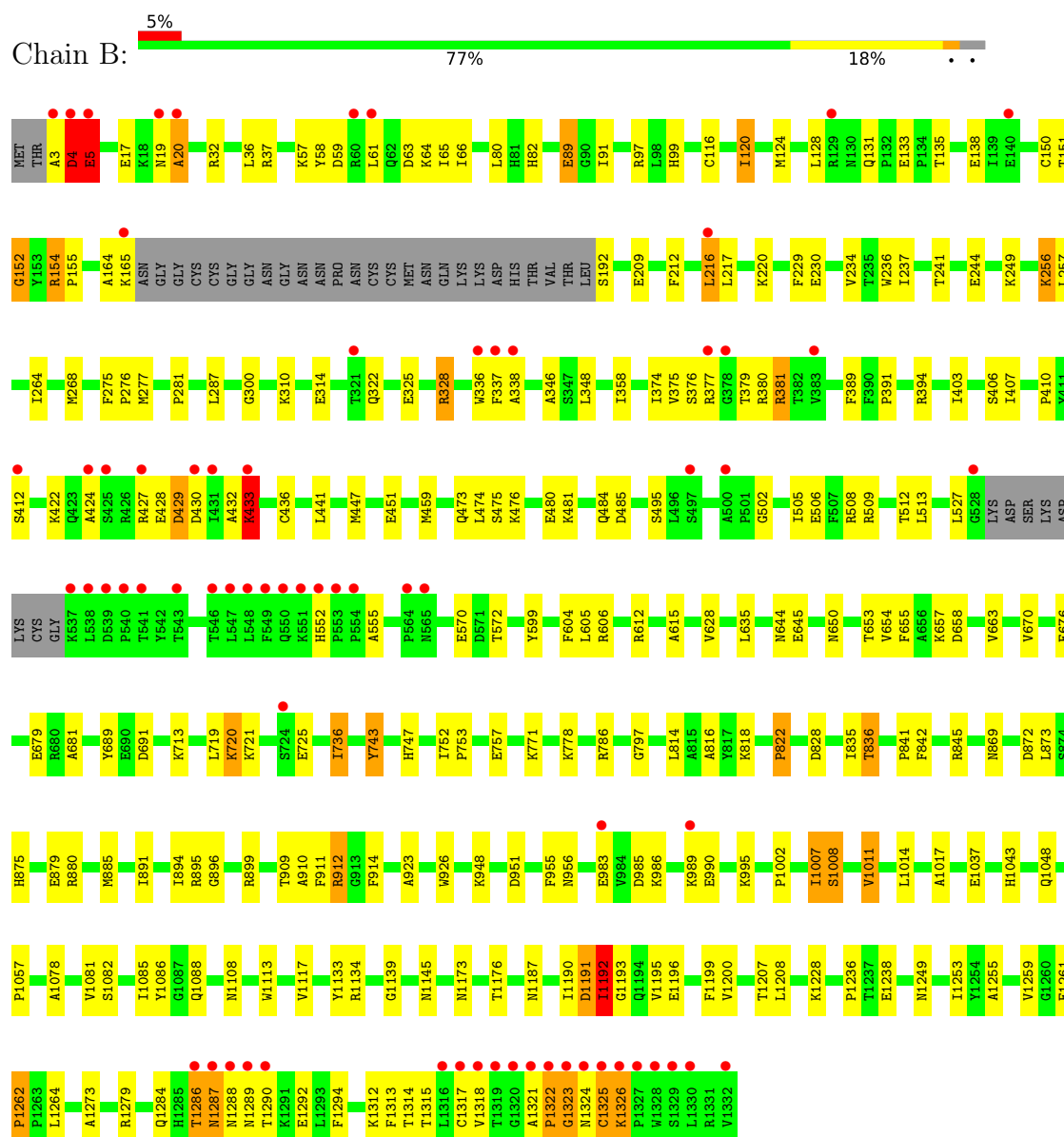
3 Residue-property plots [i](#)

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: Xanthine dehydrogenase



- Molecule 1: Xanthine dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.99Å 124.61Å 146.93Å 90.00° 90.99° 90.00°	Depositor
Resolution (Å)	40.00 – 1.94 40.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-1.94) 96.4 (40.00-1.94)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 1.94Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.178 , 0.208 0.173 , 0.203	Depositor DCC
R_{free} test set	6405 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22481	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: FES, ACY, CA, MOS, MTE, GOL, FAD, FYX

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	0.34	0/10292	0.91	38/13931 (0.3%)
1	B	0.35	0/10275	0.93	36/13909 (0.3%)
All	All	0.35	0/20567	0.92	74/27840 (0.3%)

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1191	ASP	N-CA-C	14.23	129.96	111.75
1	B	1192	ILE	N-CA-CB	-13.67	88.34	111.98
1	A	835	ILE	N-CA-C	12.07	122.67	111.45
1	A	151	THR	N-CA-C	12.05	124.49	111.36
1	B	835	ILE	N-CA-C	11.74	122.37	111.45
1	B	1192	ILE	N-CA-C	-11.36	96.70	113.39
1	A	836	THR	N-CA-C	8.73	123.49	113.01
1	B	5	GLU	N-CA-C	8.68	129.29	110.80
1	B	836	THR	N-CA-C	8.42	123.21	113.19
1	B	151	THR	N-CA-C	8.37	123.27	112.89
1	A	1262	PRO	N-CA-C	7.56	119.92	110.70
1	A	743	TYR	N-CA-C	-7.34	99.41	110.28
1	A	152	GLY	N-CA-C	-7.21	105.37	115.32
1	A	654	VAL	N-CA-C	-7.12	103.24	111.00
1	B	1262	PRO	N-CA-C	7.08	119.34	110.70
1	A	390	PHE	CA-C-N	6.96	126.21	118.97
1	A	390	PHE	C-N-CA	6.96	126.21	118.97
1	B	828	ASP	N-CA-C	-6.91	101.23	110.55
1	B	1011	VAL	N-CA-C	-6.86	101.32	107.56
1	B	654	VAL	N-CA-C	-6.81	103.58	111.00
1	B	743	TYR	N-CA-C	-6.77	100.26	110.28
1	B	956	ASN	N-CA-C	6.69	120.80	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	891	ILE	CA-C-N	6.61	126.11	119.24
1	A	891	ILE	C-N-CA	6.61	126.11	119.24
1	A	956	ASN	N-CA-C	6.42	120.46	112.24
1	A	80	LEU	N-CA-C	6.38	119.99	112.72
1	B	1273	ALA	N-CA-C	-6.34	104.44	111.36
1	A	1108	ASN	CA-C-N	6.32	126.53	119.32
1	A	1108	ASN	C-N-CA	6.32	126.53	119.32
1	B	869	ASN	N-CA-C	6.32	120.47	113.21
1	B	433	LYS	N-CA-C	-6.29	103.13	111.24
1	A	436	CYS	N-CA-C	6.27	118.30	108.96
1	B	150	CYS	N-CA-C	6.27	120.96	113.12
1	B	1085	ILE	N-CA-C	6.26	117.82	111.00
1	A	1273	ALA	N-CA-C	-6.25	104.55	111.36
1	B	1108	ASN	CA-C-N	6.22	126.41	119.32
1	B	1108	ASN	C-N-CA	6.22	126.41	119.32
1	A	696	ILE	N-CA-C	6.04	117.41	111.67
1	A	869	ASN	N-CA-C	6.00	120.29	113.15
1	A	1011	VAL	N-CA-C	-5.99	102.11	107.56
1	B	891	ILE	CA-C-N	5.99	126.15	119.32
1	B	891	ILE	C-N-CA	5.99	126.15	119.32
1	A	62	GLN	N-CA-C	-5.96	105.83	114.12
1	B	4	ASP	N-CA-C	5.90	123.38	110.80
1	B	234	VAL	N-CA-C	5.84	116.89	108.48
1	B	300	GLY	N-CA-C	-5.81	105.25	111.93
1	B	1193	GLY	N-CA-C	-5.80	105.77	112.73
1	B	80	LEU	N-CA-C	5.74	119.26	112.72
1	A	828	ASP	N-CA-C	-5.73	102.81	110.55
1	A	652	GLU	N-CA-C	5.72	117.30	109.18
1	A	1085	ILE	N-CA-C	5.68	117.19	111.00
1	B	1286	THR	N-CA-C	5.64	115.72	108.34
1	A	5	GLU	N-CA-C	5.63	118.49	110.10
1	B	152	GLY	N-CA-C	-5.57	107.56	115.30
1	A	1131	GLY	N-CA-C	-5.46	102.55	110.90
1	B	822	PRO	N-CA-C	-5.39	102.81	111.38
1	A	1007	ILE	N-CA-C	5.38	115.59	107.80
1	B	841	PRO	N-CA-C	-5.35	102.87	111.38
1	B	436	CYS	N-CA-C	5.34	116.92	108.96
1	A	822	PRO	N-CA-C	-5.33	102.90	111.38
1	A	663	VAL	N-CA-C	-5.33	102.64	109.30
1	B	663	VAL	N-CA-C	-5.32	102.65	109.30
1	A	410	PRO	N-CA-C	5.31	119.82	111.38
1	B	410	PRO	N-CA-C	5.29	119.79	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1228	LYS	N-CA-C	5.25	117.18	108.20
1	A	197	ASN	CA-C-N	5.24	125.04	119.28
1	A	197	ASN	C-N-CA	5.24	125.04	119.28
1	A	872	ASP	CB-CA-C	-5.13	110.64	116.54
1	A	443	GLN	N-CA-C	-5.10	103.04	110.08
1	B	1007	ILE	N-CA-C	5.09	115.18	107.80
1	B	1228	LYS	N-CA-C	5.08	116.89	108.20
1	A	1331	ARG	N-CA-C	5.03	117.19	110.35
1	A	1137	ASN	N-CA-C	5.03	118.33	111.39
1	A	841	PRO	N-CA-C	-5.02	103.40	111.38

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	10071	0	10071	193	0
1	B	10054	0	10053	211	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	24	0	10	1	0
4	B	24	0	10	1	0
5	A	4	0	0	2	0
5	B	4	0	0	2	0
6	A	53	0	31	3	0
6	B	53	0	31	3	0
7	A	19	0	7	0	0
7	B	19	0	7	0	0
8	A	4	0	3	3	0
8	B	4	0	3	4	0
9	A	24	0	16	5	0
9	B	24	0	15	3	0
10	A	1061	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	1021	0	0	14	0
All	All	22481	0	20257	404	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 10.

All (404) 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:340:LYS:NZ	10:A:6066:HOH:O	1.60	1.26
1:A:1088:GLN:NE2	9:A:5007:GOL:O3	1.86	1.08
1:A:3:ALA:HB1	1:A:228:ARG:H	1.17	1.06
1:B:1286:THR:HG22	1:B:1287:ASN:H	1.28	0.98
1:B:229:PHE:HA	10:B:5161:HOH:O	1.65	0.95
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.35	0.89
1:A:3:ALA:HB1	1:A:228:ARG:N	1.91	0.83
1:A:736:ILE:CG2	1:A:842:PHE:HB2	2.08	0.83
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.43	0.82
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.46	0.81
1:B:1289:ASN:HB3	1:B:1292:GLU:HB2	1.60	0.81
1:B:131:GLN:HE21	1:B:133:GLU:H	1.25	0.81
1:B:249:LYS:HD3	1:B:257:LEU:HD11	1.62	0.81
1:A:422:LYS:HE3	1:A:432:ALA:HB2	1.63	0.80
1:B:736:ILE:CG2	1:B:842:PHE:HB2	2.10	0.80
1:B:433:LYS:HE3	1:B:433:LYS:HA	1.64	0.80
1:A:719:LEU:HD11	1:A:895:ARG:HB2	1.65	0.79
1:A:1088:GLN:HE22	9:A:5007:GOL:C3	1.95	0.79
1:B:1253:ILE:HD12	9:B:5008:GOL:H12	1.63	0.78
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.17	0.78
1:B:17:GLU:HG3	1:B:20:ALA:HB2	1.66	0.78
1:B:1321:ALA:HB1	1:B:1322:PRO:HD2	1.64	0.78
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.49	0.77
1:B:509:ARG:O	1:B:513:LEU:HD13	1.84	0.77
1:A:594:ASP:OD1	9:A:5003:GOL:O3	2.01	0.76
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	1.84	0.76
1:B:57:LYS:HZ3	1:B:66:ILE:HD11	1.50	0.76
1:B:3:ALA:HB3	1:B:19:ASN:C	2.11	0.75
1:B:19:ASN:O	1:B:20:ALA:HB3	1.85	0.75
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.86	0.75
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.50	0.75
1:B:1088:GLN:HG2	1:B:1133:TYR:CD1	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:NZ	1:B:66:ILE:HD11	2.02	0.74
1:A:264:ILE:HG22	1:A:268:MET:HE2	1.69	0.74
1:A:509:ARG:NH1	1:A:1317:CYS:HB2	2.05	0.72
1:A:131:GLN:HE21	1:A:133:GLU:H	1.36	0.71
1:A:358:ILE:HD11	10:A:6068:HOH:O	1.89	0.71
1:B:3:ALA:N	1:B:19:ASN:HA	2.05	0.70
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	1.87	0.70
1:A:736:ILE:O	1:A:736:ILE:HG23	1.91	0.69
1:A:719:LEU:HD11	1:A:895:ARG:CB	2.23	0.69
1:B:1286:THR:HG22	1:B:1287:ASN:N	2.05	0.68
1:A:1180:MET:HE1	1:A:1266:LEU:HD12	1.76	0.67
1:A:736:ILE:HG21	1:A:842:PHE:HB2	1.76	0.66
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.77	0.66
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.59	0.66
1:B:36:LEU:HD22	1:B:89:GLU:HG3	1.75	0.66
1:A:914:PHE:HA	8:A:3007:ACY:H1	1.77	0.66
1:A:505:ILE:O	1:A:509:ARG:HG3	1.96	0.65
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.61	0.65
1:A:1289:ASN:HD22	1:A:1292:GLU:HB2	1.59	0.65
1:B:555:ALA:HB3	1:B:1238:GLU:HG3	1.79	0.65
1:A:573:VAL:HG21	1:A:1052:LYS:HD2	1.76	0.65
1:B:495:SER:HA	1:B:509:ARG:NH1	2.12	0.65
1:A:506:GLU:HG2	1:A:1319:THR:HB	1.77	0.64
5:B:4004:MOS:MO	5:B:4004:MOS:O2	1.68	0.64
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.79	0.64
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.79	0.64
1:B:17:GLU:CG	1:B:20:ALA:HB2	2.28	0.64
1:B:32:ARG:HH12	1:B:676:GLU:CD	2.06	0.64
5:A:3004:MOS:O2	5:A:3004:MOS:MO	1.70	0.63
1:B:19:ASN:O	1:B:20:ALA:CB	2.45	0.63
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.63	0.63
1:A:541:THR:CG2	1:A:992:CYS:HB2	2.29	0.63
1:B:911:PHE:H	8:B:4007:ACY:H3	1.64	0.63
1:A:336:TRP:HB3	1:A:427:ARG:O	1.99	0.63
1:A:335:ARG:NH2	1:A:549:PHE:HB3	2.14	0.62
1:A:684:VAL:HG12	1:A:684:VAL:O	2.00	0.62
1:B:375:VAL:HG22	1:B:380:ARG:HG3	1.81	0.62
1:B:986:LYS:HA	1:B:989:LYS:NZ	2.14	0.62
1:A:217:LEU:O	1:A:220:LYS:HG2	2.00	0.62
1:A:474:LEU:O	1:A:475:SER:HB2	2.00	0.62
1:B:995:LYS:HZ1	1:B:1284:GLN:HE21	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ARG:HG2	10:A:5250:HOH:O	1.99	0.62
1:B:422:LYS:HE3	1:B:432:ALA:HB2	1.82	0.61
1:B:736:ILE:HG21	1:B:842:PHE:HB2	1.82	0.61
1:A:1008:SER:HA	1:A:1081:VAL:HG11	1.83	0.61
1:B:495:SER:HA	1:B:509:ARG:HH12	1.64	0.61
1:A:264:ILE:HD11	6:A:3005:FAD:H3B	1.82	0.61
1:B:1286:THR:CG2	1:B:1287:ASN:H	2.08	0.61
1:B:914:PHE:HA	8:B:4007:ACY:H2	1.82	0.61
1:B:911:PHE:N	8:B:4007:ACY:H3	2.15	0.61
1:A:4:ASP:HB3	10:A:5500:HOH:O	2.00	0.60
1:B:325:GLU:HB2	1:B:412:SER:OG	2.01	0.60
1:B:3:ALA:HB3	1:B:20:ALA:N	2.15	0.60
1:A:376:SER:HB3	1:A:379:THR:OG1	2.01	0.60
1:B:736:ILE:HG23	1:B:736:ILE:O	2.02	0.60
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.84	0.60
1:A:3:ALA:HA	1:A:227:LEU:HD22	1.84	0.60
1:B:61:LEU:O	1:B:61:LEU:HD23	2.02	0.59
1:A:97:ARG:NH1	1:A:97:ARG:HB2	2.17	0.59
1:A:338:ALA:HA	1:A:429:ASP:OD1	2.01	0.59
1:B:721:LYS:O	1:B:725:GLU:HG3	2.02	0.59
1:B:1008:SER:HA	1:B:1081:VAL:HG11	1.83	0.59
1:B:336:TRP:HB3	1:B:427:ARG:O	2.02	0.59
1:B:241:THR:OG1	1:B:244:GLU:HG3	2.03	0.59
1:B:1286:THR:HG22	1:B:1287:ASN:ND2	2.17	0.59
1:B:512:THR:OG1	1:B:513:LEU:HD12	2.03	0.59
1:B:328:ARG:HG2	10:B:5538:HOH:O	2.03	0.59
1:A:346:ALA:HB1	6:A:3005:FAD:H4'	1.84	0.58
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.84	0.58
1:B:474:LEU:O	1:B:475:SER:HB2	2.03	0.58
1:A:1321:ALA:HB1	1:A:1325:CYS:HB2	1.85	0.58
1:B:720:LYS:HB2	1:B:720:LYS:NZ	2.20	0.57
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.40	0.57
1:A:237:ILE:HD12	1:A:277:MET:HE3	1.87	0.56
1:A:736:ILE:HG23	1:A:842:PHE:H	1.69	0.56
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.06	0.56
1:A:32:ARG:HH12	1:A:676:GLU:CD	2.14	0.56
1:A:818:LYS:HE2	10:A:5813:HOH:O	2.04	0.56
1:B:381:ARG:CG	1:B:381:ARG:HH11	2.19	0.56
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.06	0.55
1:A:1330:LEU:HD23	10:A:5762:HOH:O	2.05	0.55
1:B:948:LYS:HG2	1:B:951:ASP:OD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.07	0.55
1:A:555:ALA:HB3	1:A:1238:GLU:HG3	1.88	0.55
1:B:4:ASP:CB	10:B:5161:HOH:O	2.54	0.55
1:B:909:THR:O	8:B:4007:ACY:H1	2.06	0.54
1:A:154:ARG:HD2	10:A:5244:HOH:O	2.07	0.54
1:B:1207:THR:OG1	1:B:1208:LEU:HD13	2.06	0.54
1:A:3:ALA:HA	1:A:227:LEU:CD2	2.38	0.54
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.71	0.54
1:A:406:SER:C	1:A:407:ILE:HD12	2.32	0.54
1:A:430:ASP:HB2	1:A:1228:LYS:HE2	1.90	0.54
1:B:986:LYS:HA	1:B:989:LYS:HZ1	1.72	0.54
1:A:340:LYS:HE3	10:A:6067:HOH:O	2.08	0.53
1:A:407:ILE:HD12	1:A:407:ILE:N	2.23	0.53
1:A:885:MET:HE2	1:A:894:ILE:HD11	1.90	0.53
1:A:948:LYS:HG2	1:A:951:ASP:OD2	2.07	0.53
1:A:1203:LEU:HD13	1:A:1270:VAL:HG21	1.91	0.53
1:B:635:LEU:HD21	1:B:818:LYS:HG2	1.90	0.53
1:A:877:ILE:HD13	8:A:3007:ACY:H3	1.89	0.53
1:A:1001:ILE:CG1	1:A:1269:SER:HB3	2.39	0.53
1:B:875:HIS:O	1:B:879:GLU:HG3	2.09	0.53
1:A:1289:ASN:ND2	1:A:1292:GLU:HB2	2.22	0.52
1:B:612:ARG:NH1	1:B:689:TYR:HB2	2.23	0.52
1:B:1007:ILE:O	1:B:1008:SER:CB	2.57	0.52
1:B:604:PHE:HD2	9:B:5004:GOL:H11	1.74	0.52
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.43	0.52
1:B:256:LYS:HG3	1:B:275:PHE:CD2	2.44	0.52
1:A:1180:MET:HE3	1:A:1195:VAL:HG13	1.92	0.52
1:B:513:LEU:HD12	1:B:513:LEU:N	2.24	0.52
1:B:736:ILE:HG23	1:B:842:PHE:H	1.73	0.52
1:B:753:PRO:HD3	1:B:816:ALA:HB1	1.92	0.52
1:A:552:HIS:HB3	1:A:1237:THR:HG21	1.92	0.52
1:B:1007:ILE:O	1:B:1008:SER:HB3	2.08	0.52
1:B:5:GLU:HG3	10:B:5560:HOH:O	2.09	0.52
1:A:604:PHE:CD2	1:A:675:PRO:HG3	2.44	0.51
1:A:911:PHE:O	1:A:912:ARG:C	2.52	0.51
1:B:4:ASP:O	1:B:19:ASN:O	2.28	0.51
1:A:439:ARG:HH11	1:A:439:ARG:HB3	1.75	0.51
1:A:736:ILE:HG22	1:A:842:PHE:HB2	1.89	0.51
1:A:394:ARG:HD2	10:A:5374:HOH:O	2.09	0.51
1:A:719:LEU:HD13	1:A:860:GLU:OE2	2.10	0.51
1:B:3:ALA:C	10:B:5161:HOH:O	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:SER:HB2	4:A:3003:MTE:O3P	2.10	0.51
1:B:374:ILE:HB	1:B:381:ARG:HD3	1.91	0.51
1:A:1331:ARG:O	1:A:1332:VAL:HG12	2.11	0.51
1:A:622:VAL:O	1:A:626:GLN:HG3	2.10	0.51
1:A:624:GLU:HB2	1:A:684:VAL:HG12	1.91	0.51
1:B:381:ARG:HH11	1:B:381:ARG:HG2	1.75	0.51
1:A:541:THR:HG22	1:A:992:CYS:HB2	1.92	0.51
1:A:552:HIS:CG	1:A:553:PRO:HD2	2.46	0.51
1:A:875:HIS:O	1:A:879:GLU:HG3	2.10	0.50
1:A:1301:THR:HB	1:A:1302:PRO:HD2	1.93	0.50
1:B:310:LYS:O	1:B:314:GLU:HG3	2.10	0.50
1:B:1326:LYS:O	1:B:1326:LYS:HG3	2.11	0.50
1:A:506:GLU:CD	1:A:506:GLU:H	2.18	0.50
1:A:42:GLY:O	1:A:829:ARG:HD2	2.12	0.50
1:A:1007:ILE:O	1:A:1008:SER:CB	2.59	0.50
1:B:131:GLN:HE21	1:B:133:GLU:N	2.04	0.50
1:B:911:PHE:O	1:B:912:ARG:C	2.55	0.50
1:B:1314:THR:O	1:B:1318:VAL:HG13	2.11	0.50
1:A:323:LYS:HE2	1:A:411:TYR:HB3	1.92	0.50
1:A:358:ILE:HD11	10:A:5914:HOH:O	2.11	0.50
1:B:403:ILE:C	1:B:403:ILE:HD12	2.37	0.50
1:B:407:ILE:HD12	1:B:407:ILE:N	2.26	0.50
1:B:358:ILE:HD11	10:B:5893:HOH:O	2.12	0.50
1:B:338:ALA:HA	1:B:429:ASP:OD1	2.12	0.50
1:A:374:ILE:HD13	1:A:398:LEU:CD2	2.41	0.50
1:B:1289:ASN:CB	1:B:1292:GLU:HB2	2.37	0.50
1:A:1001:ILE:HG12	1:A:1269:SER:HB3	1.93	0.50
1:B:82:HIS:HA	1:B:216:LEU:HD21	1.94	0.50
1:B:424:ALA:HB1	1:B:430:ASP:OD2	2.12	0.50
1:B:3:ALA:O	1:B:19:ASN:O	2.30	0.49
1:A:509:ARG:HH11	1:A:1317:CYS:HB2	1.77	0.49
1:A:1319:THR:O	1:A:1319:THR:HG23	2.12	0.49
1:B:1191:ASP:O	1:B:1195:VAL:HG23	2.13	0.49
1:A:508:ARG:O	1:A:512:THR:HG23	2.13	0.49
1:A:1007:ILE:O	1:A:1008:SER:HB3	2.12	0.49
1:B:192:SER:HB3	10:B:5427:HOH:O	2.13	0.49
1:B:508:ARG:O	1:B:512:THR:HG23	2.13	0.49
1:A:1052:LYS:HD3	1:A:1254:TYR:CZ	2.48	0.49
1:B:719:LEU:HD11	1:B:895:ARG:CB	2.42	0.49
1:B:64:LYS:HG2	1:B:65:ILE:N	2.28	0.49
1:B:1287:ASN:O	1:B:1288:ASN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1324:ASN:O	1:B:1326:LYS:N	2.46	0.48
1:B:1287:ASN:H	1:B:1287:ASN:HD22	1.62	0.48
1:A:428:GLU:O	1:A:429:ASP:C	2.56	0.48
1:A:459:MET:HE2	1:A:512:THR:HG21	1.96	0.48
1:B:757:GLU:HB3	1:B:786:ARG:HE	1.78	0.48
1:A:337:PHE:C	1:A:337:PHE:CD2	2.91	0.48
1:B:606:ARG:CZ	1:B:679:GLU:HG3	2.43	0.48
1:B:394:ARG:HD2	10:B:5793:HOH:O	2.13	0.48
1:A:985:ASP:O	1:A:989:LYS:HG3	2.13	0.48
1:A:1207:THR:O	1:A:1208:LEU:HD12	2.14	0.48
1:B:1011:VAL:HG23	1:B:1011:VAL:O	2.13	0.48
1:A:986:LYS:HA	1:A:989:LYS:NZ	2.29	0.48
1:A:467:LEU:O	1:A:471:GLN:HG2	2.13	0.47
1:B:61:LEU:HD23	1:B:61:LEU:C	2.39	0.47
1:B:281:PRO:HB2	1:B:287:LEU:CD1	2.43	0.47
1:B:1078:ALA:HB1	5:B:4004:MOS:O1	2.14	0.47
1:B:217:LEU:O	1:B:220:LYS:HG2	2.14	0.47
1:A:116:CYS:O	1:A:120:ILE:HG13	2.14	0.47
1:A:1052:LYS:HE2	10:A:5520:HOH:O	2.14	0.47
1:B:124:MET:HE3	1:B:128:LEU:HG	1.95	0.47
1:B:509:ARG:O	1:B:513:LEU:CD1	2.58	0.47
1:A:736:ILE:CG2	1:A:736:ILE:O	2.61	0.47
1:A:964:VAL:HB	1:A:965:PRO:HD3	1.95	0.47
1:B:154:ARG:HD2	10:B:5205:HOH:O	2.15	0.47
1:B:1088:GLN:HG2	1:B:1133:TYR:CE1	2.48	0.47
1:A:225:LYS:C	1:A:225:LYS:HD3	2.40	0.47
1:A:503:GLY:C	1:A:505:ILE:HD12	2.40	0.47
1:A:856:ILE:HD12	1:A:856:ILE:N	2.29	0.47
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.30	0.47
1:B:1264:LEU:C	1:B:1264:LEU:HD23	2.40	0.47
1:A:144:GLN:HB2	1:A:339:GLY:HA2	1.97	0.47
1:B:3:ALA:HB1	1:B:20:ALA:O	2.15	0.47
1:B:379:THR:HG22	1:B:380:ARG:N	2.30	0.47
1:A:555:ALA:O	1:A:1238:GLU:HA	2.15	0.46
1:A:1252:ALA:HB3	1:A:1256:SER:O	2.15	0.46
1:B:216:LEU:HD13	1:B:216:LEU:O	2.15	0.46
1:B:152:GLY:HA2	1:B:1200:VAL:HG21	1.97	0.46
1:B:212:PHE:CZ	1:B:216:LEU:HD12	2.50	0.46
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.78	0.46
1:B:1315:THR:HG22	1:B:1315:THR:O	2.14	0.46
1:A:548:LEU:HD12	1:A:548:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:PHE:CD1	1:A:549:PHE:C	2.93	0.46
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.98	0.46
1:B:480:GLU:O	1:B:484:GLN:HG3	2.16	0.46
1:B:337:PHE:C	1:B:337:PHE:CD2	2.94	0.46
1:B:513:LEU:HD22	1:B:1317:CYS:SG	2.56	0.46
1:B:1082:SER:HB2	4:B:4003:MTE:O3P	2.15	0.46
1:B:325:GLU:N	1:B:412:SER:OG	2.48	0.46
1:B:389:PHE:O	1:B:391:PRO:HD3	2.16	0.46
1:B:1287:ASN:O	1:B:1288:ASN:CB	2.64	0.46
1:A:322:GLN:O	1:A:412:SER:HB3	2.16	0.46
1:A:752:ILE:CD1	1:A:822:PRO:HB3	2.45	0.46
1:B:264:ILE:HD11	6:B:4005:FAD:H3B	1.96	0.46
1:A:424:ALA:HB1	1:A:430:ASP:OD2	2.15	0.46
1:A:615:ALA:HB2	1:A:691:ASP:HA	1.97	0.46
1:A:721:LYS:HD2	1:A:721:LYS:C	2.41	0.46
1:A:570:GLU:CD	1:A:1057:PRO:HG3	2.40	0.46
1:B:459:MET:HE2	1:B:512:THR:HG21	1.98	0.46
1:B:713:LYS:HD2	1:B:895:ARG:NH1	2.30	0.46
1:A:225:LYS:HB2	1:A:225:LYS:NZ	2.30	0.45
1:A:1124:ARG:HD2	1:B:1134:ARG:HG3	1.98	0.45
1:B:1325:CYS:O	1:B:1326:LYS:HB3	2.15	0.45
1:A:651:ASP:CG	1:A:871:ARG:HH11	2.24	0.45
1:B:506:GLU:HG3	10:B:5340:HOH:O	2.16	0.45
1:A:529:LYS:O	1:A:530:ASP:HB2	2.16	0.45
1:A:1215:PRO:HD2	1:A:1216:GLU:OE2	2.17	0.45
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.31	0.45
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.45
1:B:135:THR:OG1	1:B:138:GLU:HG3	2.16	0.45
1:B:375:VAL:HG12	1:B:376:SER:N	2.31	0.45
1:A:540:PRO:C	1:A:542:TYR:H	2.25	0.45
1:B:381:ARG:CG	1:B:381:ARG:NH1	2.79	0.45
1:B:1207:THR:O	1:B:1208:LEU:HD12	2.17	0.45
1:A:480:GLU:O	1:A:484:GLN:HG3	2.16	0.45
1:A:599:TYR:HA	1:B:599:TYR:HA	1.97	0.45
1:A:605:LEU:HD23	1:A:605:LEU:C	2.41	0.45
1:A:877:ILE:CD1	8:A:3007:ACY:H3	2.47	0.45
1:B:473:GLN:O	1:B:476:LYS:HB2	2.17	0.45
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.81	0.45
1:A:117:THR:HB	1:A:118:PRO:HD3	1.98	0.45
1:A:650:ASN:ND2	1:A:778:LYS:HE3	2.25	0.45
1:A:907:SER:N	9:A:5001:GOL:O3	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:SER:OG	1:B:379:THR:HB	2.17	0.45
1:A:423:GLN:HB2	1:A:515:PHE:HZ	1.82	0.44
1:A:1001:ILE:HD11	1:A:1269:SER:HB3	1.98	0.44
1:B:3:ALA:HB3	1:B:19:ASN:CA	2.47	0.44
1:B:97:ARG:NH1	1:B:97:ARG:HB2	2.32	0.44
1:B:376:SER:O	1:B:377:ARG:C	2.60	0.44
1:B:628:VAL:HG21	1:B:681:ALA:HA	1.99	0.44
1:B:1279:ARG:HD3	10:B:5701:HOH:O	2.17	0.44
1:A:276:PRO:HG2	10:A:6037:HOH:O	2.17	0.44
1:B:4:ASP:HB3	10:B:5161:HOH:O	2.16	0.44
1:B:37:ARG:HG2	10:B:5115:HOH:O	2.17	0.44
1:B:116:CYS:O	1:B:120:ILE:HG13	2.17	0.44
1:B:257:LEU:O	6:B:4005:FAD:H2B	2.16	0.44
1:B:909:THR:OG1	1:B:910:ALA:N	2.49	0.44
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.49	0.44
1:A:509:ARG:HH12	1:A:1317:CYS:HA	1.82	0.44
1:B:986:LYS:O	1:B:990:GLU:HG3	2.18	0.44
1:A:337:PHE:C	1:A:337:PHE:HD2	2.26	0.44
1:B:605:LEU:C	1:B:605:LEU:HD23	2.43	0.44
1:A:358:ILE:HD12	1:A:358:ILE:C	2.41	0.44
1:A:734:LEU:HD21	1:A:921:PHE:CE2	2.53	0.44
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.17	0.44
1:B:572:THR:OG1	1:B:1048:GLN:HG2	2.18	0.44
1:A:725:GLU:HG3	1:A:857:VAL:HG11	2.00	0.44
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.82	0.44
1:A:152:GLY:HA2	1:A:1200:VAL:HG21	2.00	0.44
1:B:237:ILE:HD11	1:B:277:MET:HE2	2.00	0.44
1:B:322:GLN:O	1:B:412:SER:HB2	2.18	0.44
1:A:1017:ALA:HB1	1:A:1086:TYR:CD2	2.53	0.43
1:A:60:ARG:HG2	1:A:60:ARG:HH11	1.82	0.43
1:A:713:LYS:HD3	1:A:897:THR:HG22	2.00	0.43
1:A:1198:ALA:HB3	1:A:1263:PRO:HB2	2.00	0.43
1:B:164:ALA:O	1:B:165:LYS:HB3	2.17	0.43
1:B:406:SER:C	1:B:407:ILE:HD12	2.43	0.43
1:B:91:ILE:O	1:B:99:HIS:HB2	2.18	0.43
1:B:428:GLU:O	1:B:429:ASP:C	2.61	0.43
1:A:74:LEU:O	1:A:76:PRO:HD3	2.19	0.43
1:A:403:ILE:C	1:A:403:ILE:HD12	2.43	0.43
1:A:509:ARG:HH12	1:A:1317:CYS:CA	2.31	0.43
1:A:651:ASP:OD2	1:A:871:ARG:NH1	2.51	0.43
1:A:1207:THR:OG1	1:A:1208:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:ARG:HG2	10:A:5452:HOH:O	2.18	0.43
1:B:375:VAL:CG1	1:B:376:SER:N	2.82	0.43
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.53	0.43
1:A:549:PHE:HE1	1:A:551:LYS:HG2	1.84	0.43
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.32	0.43
1:B:670:VAL:HG11	1:B:681:ALA:HB3	2.00	0.43
1:B:752:ILE:CD1	1:B:822:PRO:HB3	2.48	0.43
1:B:985:ASP:O	1:B:989:LYS:HG3	2.18	0.43
1:A:624:GLU:HB3	1:A:684:VAL:HG11	2.00	0.43
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.54	0.43
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.88	0.43
1:A:618:LYS:HE3	1:A:618:LYS:HA	2.01	0.43
1:B:264:ILE:O	1:B:268:MET:HG2	2.19	0.43
1:B:1113:TRP:O	1:B:1117:VAL:HG23	2.18	0.43
1:B:346:ALA:HB1	6:B:4005:FAD:H4'	2.01	0.42
1:B:872:ASP:CG	1:B:873:LEU:H	2.25	0.42
1:A:1078:ALA:HB1	5:A:3004:MOS:O1	2.19	0.42
1:B:1187:ASN:CG	1:B:1190:ILE:HG13	2.44	0.42
1:B:1192:ILE:HA	1:B:1195:VAL:HB	2.01	0.42
1:A:97:ARG:HB2	1:A:97:ARG:CZ	2.50	0.42
1:B:555:ALA:O	1:B:1238:GLU:HA	2.20	0.42
1:B:1279:ARG:HG2	1:B:1294:PHE:HE2	1.84	0.42
1:A:909:THR:OG1	1:A:910:ALA:N	2.49	0.42
1:B:644:ASN:O	1:B:653:THR:HA	2.20	0.42
1:B:1011:VAL:CG2	1:B:1014:LEU:HD12	2.50	0.42
1:B:1312:LYS:HE3	1:B:1313:PHE:CZ	2.54	0.42
1:B:1176:THR:HG21	1:B:1199:PHE:CZ	2.55	0.42
1:B:505:ILE:HG22	1:B:506:GLU:N	2.34	0.42
1:B:899:ARG:HD2	1:B:899:ARG:HA	1.85	0.42
1:A:610:SER:HB2	1:A:660:VAL:HG11	2.01	0.42
1:A:1253:ILE:HD12	9:A:5007:GOL:H12	2.01	0.42
1:B:154:ARG:N	1:B:155:PRO:HD2	2.34	0.42
1:B:1259:VAL:HG22	1:B:1259:VAL:O	2.19	0.42
1:B:377:ARG:NH1	1:B:377:ARG:HG2	2.35	0.42
1:B:447:MET:HG2	1:B:527:LEU:HD13	2.02	0.42
1:B:1323:GLY:O	1:B:1324:ASN:C	2.63	0.42
1:A:197:ASN:O	1:A:200:GLU:HG2	2.20	0.42
1:B:657:LYS:O	1:B:658:ASP:HB2	2.18	0.42
1:B:880:ARG:HD2	1:B:914:PHE:O	2.20	0.42
1:B:1173:ASN:O	1:B:1236:PRO:HA	2.20	0.42
1:B:1253:ILE:HD12	9:B:5008:GOL:C1	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:PRO:O	1:A:541:THR:HB	2.18	0.42
1:A:651:ASP:OD1	1:A:871:ARG:HG3	2.20	0.42
1:A:1279:ARG:HD2	10:A:5671:HOH:O	2.20	0.41
1:B:58:TYR:CD2	1:B:220:LYS:HB2	2.54	0.41
1:A:100:PRO:O	1:A:104:ARG:HG3	2.20	0.41
1:A:428:GLU:N	1:A:428:GLU:CD	2.78	0.41
1:A:1046:MET:HA	1:A:1046:MET:HE2	2.03	0.41
1:A:3:ALA:O	1:A:4:ASP:C	2.63	0.41
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.55	0.41
1:B:1287:ASN:H	1:B:1287:ASN:ND2	2.17	0.41
1:A:736:ILE:HG22	1:A:842:PHE:CB	2.50	0.41
1:B:655:PHE:CE1	1:B:814:LEU:HD23	2.56	0.41
1:B:885:MET:HE2	1:B:894:ILE:HD11	2.01	0.41
1:A:193:PRO:HG2	1:A:560:PHE:CE1	2.55	0.41
1:B:615:ALA:HB2	1:B:691:ASP:HA	2.02	0.41
1:B:1289:ASN:O	1:B:1290:THR:HB	2.21	0.41
1:B:3:ALA:HB1	1:B:230:GLU:O	2.20	0.41
1:B:358:ILE:C	1:B:358:ILE:HD12	2.46	0.41
1:B:481:LYS:HE2	1:B:485:ASP:OD1	2.21	0.41
1:A:193:PRO:HB3	1:A:562:GLU:HG2	2.01	0.41
1:A:505:ILE:HD12	1:A:505:ILE:N	2.36	0.41
1:A:857:VAL:HG12	1:A:857:VAL:O	2.20	0.41
1:A:256:LYS:HE3	6:A:3005:FAD:O3B	2.21	0.41
1:A:401:GLU:HB2	10:A:6007:HOH:O	2.21	0.41
1:A:426:ARG:NH2	1:A:429:ASP:O	2.52	0.41
1:A:644:ASN:O	1:A:653:THR:HA	2.21	0.41
1:A:808:VAL:HG23	10:A:6039:HOH:O	2.21	0.41
1:B:3:ALA:CB	1:B:230:GLU:O	2.69	0.41
1:B:509:ARG:HH11	1:B:509:ARG:HG2	1.86	0.41
1:B:885:MET:SD	1:B:896:GLY:HA3	2.61	0.41
1:A:284:ILE:HA	1:A:285:PRO:HD2	1.89	0.41
1:A:60:ARG:HG2	1:A:60:ARG:NH1	2.36	0.40
1:A:509:ARG:NH1	1:A:1317:CYS:CB	2.80	0.40
1:B:59:ASP:O	1:B:63:ASP:N	2.53	0.40
1:B:229:PHE:HB2	1:B:236:TRP:HB3	2.03	0.40
1:B:570:GLU:CD	1:B:1057:PRO:HG3	2.47	0.40
1:A:389:PHE:O	1:A:391:PRO:HD3	2.21	0.40
1:B:502:GLY:HA3	10:B:5612:HOH:O	2.20	0.40
1:A:197:ASN:HA	1:A:198:PRO:HD3	1.92	0.40
1:B:513:LEU:N	1:B:513:LEU:CD1	2.84	0.40
1:A:986:LYS:O	1:A:990:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:GLU:CD	1:A:1216:GLU:H	2.28	0.40
1:B:275:PHE:HA	1:B:276:PRO:HD2	1.93	0.40
1:B:771:LYS:HA	1:B:771:LYS:HD3	1.87	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	1292/1332 (97%)	1235 (96%)	43 (3%)	14 (1%)	11	4
1	B	1290/1332 (97%)	1235 (96%)	42 (3%)	13 (1%)	12	5
All	All	2582/2664 (97%)	2470 (96%)	85 (3%)	27 (1%)	12	5

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	1008	SER
1	A	1322	PRO
1	B	4	ASP
1	B	5	GLU
1	B	1008	SER
1	B	1287	ASN
1	A	429	ASP
1	A	1319	THR
1	B	1139	GLY
1	A	61	LEU
1	A	338	ALA
1	A	539	ASP
1	A	912	ARG
1	A	1318	VAL

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Mol	Chain	Res	Type
1	B	20	ALA
1	B	429	ASP
1	B	912	ARG
1	A	529	LYS
1	B	1322	PRO
1	B	1325	CYS
1	B	1326	LYS
1	A	797	GLY
1	A	1139	GLY
1	B	797	GLY
1	A	1320	GLY
1	B	1323	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	1100/1128 (98%)	1075 (98%)	25 (2%)	44	33
1	B	1098/1128 (97%)	1080 (98%)	18 (2%)	55	46
All	All	2198/2256 (97%)	2155 (98%)	43 (2%)	48	39

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	89	GLU
1	A	154	ARG
1	A	225	LYS
1	A	256	LYS
1	A	281	PRO
1	A	312	LEU
1	A	328	ARG
1	A	337	PHE
1	A	348	LEU
1	A	439	ARG

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Mol	Chain	Res	Type
1	A	481	LYS
1	A	506	GLU
1	A	537	LYS
1	A	550	GLN
1	A	551	LYS
1	A	562	GLU
1	A	618	LYS
1	A	652	GLU
1	A	736	ILE
1	A	743	TYR
1	A	1072	PRO
1	A	1102	GLU
1	A	1216	GLU
1	A	1332	VAL
1	B	89	GLU
1	B	120	ILE
1	B	154	ARG
1	B	209	GLU
1	B	216	LEU
1	B	256	LYS
1	B	328	ARG
1	B	348	LEU
1	B	381	ARG
1	B	433	LYS
1	B	552	HIS
1	B	720	LYS
1	B	736	ILE
1	B	743	TYR
1	B	845	ARG
1	B	983	GLU
1	B	1002	PRO
1	B	1192	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	251	GLN
1	A	351	ASN
1	A	550	GLN
1	A	567	GLN
1	A	650	ASN

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Mol	Chain	Res	Type
1	A	705	ASN
1	A	976	GLN
1	A	1088	GLN
1	A	1145	ASN
1	A	1148	ASN
1	A	1284	GLN
1	A	1289	ASN
1	B	62	GLN
1	B	131	GLN
1	B	144	GLN
1	B	146	ASN
1	B	226	GLN
1	B	272	ASN
1	B	333	GLN
1	B	351	ASN
1	B	473	GLN
1	B	552	HIS
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	991	ASN
1	B	1145	ASN
1	B	1212	HIS
1	B	1220	HIS
1	B	1284	GLN
1	B	1287	ASN
1	B	1324	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 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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
9	GOL	B	5008	-	5,5,5	5.25	4 (80%)	5,5,5	6.77	3 (60%)
9	GOL	A	5003	-	5,5,5	5.24	4 (80%)	5,5,5	6.77	3 (60%)
3	FES	A	3002	1	0,4,4	-	-	-	-	-
9	GOL	A	5001	-	5,5,5	5.24	4 (80%)	5,5,5	6.77	3 (60%)
6	FAD	A	3005	-	58,58,58	1.76	16 (27%)	85,89,89	2.15	29 (34%)
9	GOL	B	5002	-	5,5,5	5.25	4 (80%)	5,5,5	6.77	3 (60%)
5	MOS	B	4004	4,7	0,3,3	-	-	-	-	-
3	FES	B	4002	1	0,4,4	-	-	-	-	-
8	ACY	A	3007	-	3,3,3	1.21	0	3,3,3	1.68	1 (33%)
4	MTE	A	3003	5	21,26,26	5.87	10 (47%)	19,40,40	3.16	10 (52%)
3	FES	A	3001	1	0,4,4	-	-	-	-	-
5	MOS	A	3004	4,7	0,3,3	-	-	-	-	-
8	ACY	B	4007	-	3,3,3	1.16	0	3,3,3	1.71	1 (33%)
9	GOL	A	5007	-	5,5,5	5.25	4 (80%)	5,5,5	6.77	3 (60%)
6	FAD	B	4005	-	58,58,58	1.73	15 (25%)	85,89,89	2.27	28 (32%)
7	FYX	B	4006	5	21,21,21	2.56	10 (47%)	27,28,28	2.97	14 (51%)
9	GOL	B	5006	-	5,5,5	5.25	4 (80%)	5,5,5	6.77	3 (60%)
9	GOL	A	5005	-	5,5,5	5.24	4 (80%)	5,5,5	6.77	3 (60%)
9	GOL	B	5004	-	5,5,5	5.25	4 (80%)	5,5,5	6.77	3 (60%)
4	MTE	B	4003	5	21,26,26	5.90	12 (57%)	19,40,40	3.02	9 (47%)
3	FES	B	4001	1	0,4,4	-	-	-	-	-
7	FYX	A	3006	5	21,21,21	2.59	11 (52%)	27,28,28	2.99	13 (48%)

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
9	GOL	B	5004	-	-	2/4/4/4	-
3	FES	A	3001	1	-	-	0/1/1/1
3	FES	B	4001	1	-	-	0/1/1/1
9	GOL	B	5008	-	-	2/4/4/4	-
9	GOL	A	5003	-	-	2/4/4/4	-
6	FAD	B	4005	-	-	2/34/50/50	0/6/6/6
9	GOL	A	5007	-	-	2/4/4/4	-
9	GOL	B	5002	-	-	2/4/4/4	-
7	FYX	B	4006	5	-	0/8/10/10	0/3/3/3
4	MTE	B	4003	5	-	3/6/34/34	0/3/3/3
3	FES	B	4002	1	-	-	0/1/1/1
9	GOL	A	5001	-	-	2/4/4/4	-
3	FES	A	3002	1	-	-	0/1/1/1
4	MTE	A	3003	5	-	3/6/34/34	0/3/3/3
7	FYX	A	3006	5	-	0/8/10/10	0/3/3/3
6	FAD	A	3005	-	-	1/34/50/50	0/6/6/6
9	GOL	B	5006	-	-	2/4/4/4	-
9	GOL	A	5005	-	-	2/4/4/4	-

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4003	MTE	C7-C6	19.33	1.69	1.53
4	A	3003	MTE	C7-C6	18.98	1.68	1.53
4	A	3003	MTE	C9-C10	13.54	1.61	1.38
4	B	4003	MTE	C9-C10	13.49	1.61	1.38
9	B	5006	GOL	C3-C2	-9.90	1.14	1.51
9	B	5002	GOL	C3-C2	-9.89	1.14	1.51
9	B	5004	GOL	C3-C2	-9.89	1.14	1.51
9	A	5007	GOL	C3-C2	-9.89	1.14	1.51
9	B	5008	GOL	C3-C2	-9.88	1.14	1.51
9	A	5001	GOL	C3-C2	-9.88	1.14	1.51
9	A	5005	GOL	C3-C2	-9.88	1.14	1.51
9	A	5003	GOL	C3-C2	-9.88	1.14	1.51
4	A	3003	MTE	C9-N5	7.57	1.55	1.37
4	B	4003	MTE	P-O4'	-6.74	1.39	1.60
4	A	3003	MTE	P-O4'	-6.55	1.39	1.60
4	B	4003	MTE	C9-N5	5.39	1.50	1.37
6	A	3005	FAD	C10-N1	5.10	1.43	1.33
4	B	4003	MTE	P-O3P	-4.98	1.36	1.54
4	A	3003	MTE	P-O3P	-4.98	1.36	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	4005	FAD	C10-N1	4.82	1.43	1.33
7	A	3006	FYX	NPN-NPL	-4.48	1.27	1.36
7	B	4006	FYX	CPH-CPK	-4.47	1.40	1.47
7	B	4006	FYX	NPN-NPL	-4.41	1.27	1.36
4	B	4003	MTE	C6-N5	4.40	1.51	1.46
7	A	3006	FYX	CPH-CPK	-4.29	1.40	1.47
7	B	4006	FYX	CPP-CPM	-4.09	1.39	1.47
4	A	3003	MTE	O4-C4	4.04	1.31	1.23
7	B	4006	FYX	CPB-NPC	3.99	1.23	1.14
7	A	3006	FYX	CPP-CPM	-3.95	1.40	1.47
9	B	5004	GOL	C1-C2	-3.90	1.36	1.51
9	A	5005	GOL	C1-C2	-3.89	1.37	1.51
9	B	5002	GOL	C1-C2	-3.89	1.37	1.51
9	A	5007	GOL	C1-C2	-3.88	1.37	1.51
9	A	5003	GOL	C1-C2	-3.88	1.37	1.51
9	B	5006	GOL	C1-C2	-3.88	1.37	1.51
9	A	5001	GOL	C1-C2	-3.87	1.37	1.51
7	A	3006	FYX	CPB-NPC	3.87	1.23	1.14
9	B	5008	GOL	C1-C2	-3.87	1.37	1.51
7	A	3006	FYX	CPK-NPL	3.85	1.38	1.32
4	B	4003	MTE	O4-C4	3.74	1.30	1.23
7	B	4006	FYX	CPK-NPL	3.65	1.37	1.32
6	B	4005	FAD	C4X-N5	3.58	1.38	1.30
6	A	3005	FAD	C4X-N5	3.55	1.38	1.30
9	B	5002	GOL	O2-C2	-3.54	1.33	1.43
9	A	5005	GOL	O2-C2	-3.54	1.33	1.43
9	B	5006	GOL	O2-C2	-3.54	1.33	1.43
9	B	5008	GOL	O2-C2	-3.54	1.33	1.43
9	A	5007	GOL	O2-C2	-3.53	1.33	1.43
9	A	5001	GOL	O2-C2	-3.53	1.33	1.43
9	B	5004	GOL	O2-C2	-3.52	1.33	1.43
9	A	5003	GOL	O2-C2	-3.51	1.33	1.43
9	A	5007	GOL	O1-C1	3.51	1.57	1.42
9	B	5008	GOL	O1-C1	3.50	1.57	1.42
9	A	5001	GOL	O1-C1	3.50	1.57	1.42
9	A	5003	GOL	O1-C1	3.50	1.57	1.42
9	B	5004	GOL	O1-C1	3.49	1.57	1.42
9	B	5002	GOL	O1-C1	3.49	1.57	1.42
9	B	5006	GOL	O1-C1	3.49	1.57	1.42
9	A	5005	GOL	O1-C1	3.47	1.57	1.42
6	A	3005	FAD	C10-N10	3.38	1.44	1.37
6	B	4005	FAD	C5A-N7A	-3.20	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	4005	FAD	C10-N10	3.20	1.44	1.37
4	A	3003	MTE	C10-N8	3.16	1.38	1.35
4	B	4003	MTE	C10-N8	3.13	1.38	1.35
6	A	3005	FAD	C5A-N7A	-3.10	1.33	1.39
6	A	3005	FAD	C9-C9A	3.04	1.44	1.39
6	B	4005	FAD	C6-C7	2.99	1.43	1.39
6	B	4005	FAD	C9A-C5X	2.94	1.45	1.41
7	A	3006	FYX	CPM-NPJ	2.91	1.38	1.33
6	B	4005	FAD	C4A-N3A	2.88	1.39	1.34
6	A	3005	FAD	C6-C7	2.88	1.43	1.39
6	A	3005	FAD	C9A-C5X	2.86	1.45	1.41
6	B	4005	FAD	C9-C9A	2.86	1.44	1.39
7	B	4006	FYX	CPM-NPJ	2.85	1.38	1.33
7	A	3006	FYX	CPQ-CPP	2.80	1.43	1.39
4	B	4003	MTE	C2-N1	2.79	1.39	1.33
6	A	3005	FAD	P-O1P	2.73	1.60	1.50
4	B	4003	MTE	O4'-C4'	-2.71	1.34	1.44
7	B	4006	FYX	CPQ-CPP	2.69	1.43	1.39
6	A	3005	FAD	C4A-N3A	2.65	1.39	1.34
6	B	4005	FAD	C9A-N10	2.65	1.45	1.41
4	A	3003	MTE	C2-N1	2.65	1.39	1.33
6	A	3005	FAD	C9A-N10	2.62	1.45	1.41
6	B	4005	FAD	PA-O1A	2.62	1.59	1.50
7	A	3006	FYX	CPG-CPH	2.58	1.43	1.39
6	B	4005	FAD	P-O1P	2.57	1.59	1.50
6	A	3005	FAD	PA-O1A	2.57	1.59	1.50
7	B	4006	FYX	CPG-CPH	2.53	1.43	1.39
6	B	4005	FAD	C6-C5X	2.40	1.43	1.40
7	A	3006	FYX	CPG-CPD	2.36	1.41	1.39
6	A	3005	FAD	C6-C5X	2.35	1.43	1.40
6	A	3005	FAD	C1'-C2'	2.35	1.55	1.52
6	A	3005	FAD	C4-N3	2.34	1.43	1.38
7	B	4006	FYX	CPM-NPN	2.29	1.38	1.34
7	A	3006	FYX	CPM-NPN	2.29	1.38	1.34
4	B	4003	MTE	P-O2P	-2.28	1.46	1.54
6	B	4005	FAD	C4-N3	2.26	1.43	1.38
4	A	3003	MTE	P-O2P	-2.25	1.46	1.54
7	A	3006	FYX	CPO-CPP	2.24	1.42	1.39
6	B	4005	FAD	C1'-C2'	2.21	1.55	1.52
4	A	3003	MTE	O4'-C4'	-2.18	1.36	1.44
7	B	4006	FYX	CPG-CPD	2.16	1.41	1.39
6	B	4005	FAD	C8M-C8	2.10	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4003	MTE	C4'-C3'	-2.07	1.49	1.51
6	A	3005	FAD	C8M-C8	2.03	1.54	1.51
6	A	3005	FAD	C8-C7	2.00	1.45	1.40

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	5008	GOL	O3-C3-C2	13.82	172.58	110.38
9	A	5003	GOL	O3-C3-C2	13.81	172.56	110.38
9	A	5001	GOL	O3-C3-C2	13.81	172.55	110.38
9	A	5007	GOL	O3-C3-C2	13.81	172.54	110.38
9	B	5002	GOL	O3-C3-C2	13.81	172.54	110.38
9	B	5006	GOL	O3-C3-C2	13.81	172.54	110.38
9	B	5004	GOL	O3-C3-C2	13.80	172.50	110.38
9	A	5005	GOL	O3-C3-C2	13.80	172.49	110.38
4	A	3003	MTE	C2-N1-C10	7.86	127.24	113.36
4	B	4003	MTE	C2-N1-C10	7.85	127.22	113.36
7	A	3006	FYX	NPL-CPK-NPJ	-6.82	104.46	114.17
6	A	3005	FAD	N3A-C2A-N1A	-6.81	118.28	128.58
7	B	4006	FYX	NPL-CPK-NPJ	-6.78	104.52	114.17
6	B	4005	FAD	N3A-C2A-N1A	-6.66	118.50	128.58
7	A	3006	FYX	CPF-NPE-CPD	6.24	124.94	116.51
7	B	4006	FYX	CPF-NPE-CPD	6.23	124.93	116.51
6	B	4005	FAD	C2B-C1B-N9A	5.90	127.97	113.30
6	A	3005	FAD	C5'-C4'-C3'	-5.44	101.95	112.22
4	B	4003	MTE	O4-C4-C9	-5.43	114.16	127.26
6	B	4005	FAD	O4'-C4'-C3'	5.35	121.77	109.25
9	B	5006	GOL	O2-C2-C3	5.31	131.16	109.18
9	A	5007	GOL	O2-C2-C3	5.30	131.14	109.18
9	B	5008	GOL	O2-C2-C3	5.30	131.11	109.18
9	B	5002	GOL	O2-C2-C3	5.30	131.10	109.18
9	A	5005	GOL	O2-C2-C3	5.29	131.10	109.18
9	B	5004	GOL	O2-C2-C3	5.29	131.10	109.18
9	A	5001	GOL	O2-C2-C3	5.29	131.09	109.18
4	A	3003	MTE	O4-C4-C9	-5.29	114.50	127.26
9	A	5003	GOL	O2-C2-C3	5.28	131.06	109.18
6	B	4005	FAD	C5'-C4'-C3'	-5.18	102.45	112.22
7	A	3006	FYX	CPI-CPF-NPE	-4.90	117.97	123.97
7	B	4006	FYX	CPI-CPF-NPE	-4.85	118.03	123.97
6	A	3005	FAD	C2B-C1B-N9A	4.74	125.09	113.30
6	B	4005	FAD	O2B-C2B-C3B	4.53	126.35	111.82
4	A	3003	MTE	O3'-C7-N8	-4.51	104.51	108.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	3005	FAD	O4'-C4'-C3'	4.51	119.80	109.25
4	B	4003	MTE	O3'-C7-N8	-4.46	104.56	108.61
6	B	4005	FAD	O2'-C2'-C3'	4.44	119.65	109.25
6	B	4005	FAD	C5A-C4A-N3A	-4.36	120.71	126.72
6	A	3005	FAD	C5A-C4A-N3A	-4.36	120.72	126.72
7	A	3006	FYX	CPK-NPL-NPN	4.35	110.99	102.97
7	B	4006	FYX	CPK-NPL-NPN	4.32	110.92	102.97
7	A	3006	FYX	CPM-NPJ-CPK	4.27	109.29	103.35
7	A	3006	FYX	CPT-NPS-CPR	4.14	126.32	116.86
7	B	4006	FYX	CPT-NPS-CPR	4.10	126.24	116.86
6	A	3005	FAD	O3'-C3'-C4'	4.06	118.16	108.93
6	A	3005	FAD	C2A-N3A-C4A	4.05	121.72	111.83
7	B	4006	FYX	CPM-NPJ-CPK	4.04	108.98	103.35
6	B	4005	FAD	C2A-N3A-C4A	3.98	121.55	111.83
6	B	4005	FAD	O5'-C5'-C4'	-3.97	98.78	109.36
4	A	3003	MTE	C4-C9-N5	3.92	126.96	116.27
6	A	3005	FAD	O2'-C2'-C3'	3.73	117.97	109.25
6	B	4005	FAD	C5X-N5-C4X	3.57	123.87	118.09
4	A	3003	MTE	O3'-C7-C6	-3.51	106.62	108.96
4	A	3003	MTE	N2-C2-N3	3.51	124.16	116.76
6	B	4005	FAD	C9A-C5X-N5	-3.49	118.75	122.45
4	B	4003	MTE	N2-C2-N3	3.46	124.07	116.76
6	A	3005	FAD	C5X-N5-C4X	3.46	123.68	118.09
4	B	4003	MTE	C4-C9-N5	3.43	125.62	116.27
6	A	3005	FAD	C9A-C5X-N5	-3.36	118.89	122.45
7	A	3006	FYX	CPO-CPR-NPS	-3.30	117.97	123.60
7	B	4006	FYX	CPO-CPR-NPS	-3.27	118.03	123.60
4	B	4003	MTE	C9-C4-N3	3.19	120.89	112.13
7	A	3006	FYX	NPN-CPM-NPJ	-3.18	104.55	110.32
4	A	3003	MTE	C9-C4-N3	3.14	120.76	112.13
6	B	4005	FAD	O3'-C3'-C4'	3.13	116.05	108.93
7	B	4006	FYX	NPN-CPM-NPJ	-3.12	104.67	110.32
7	A	3006	FYX	CPH-CPK-NPL	3.11	128.13	122.57
6	A	3005	FAD	N3A-C4A-N9A	3.07	132.40	127.17
4	A	3003	MTE	C7-C6-N5	3.06	110.87	107.87
6	B	4005	FAD	N3A-C4A-N9A	3.04	132.34	127.17
6	B	4005	FAD	C1'-N10-C9A	3.02	126.50	120.63
7	B	4006	FYX	CPG-CPD-NPE	-3.00	119.55	123.57
7	A	3006	FYX	CPG-CPD-NPE	-2.98	119.56	123.57
7	A	3006	FYX	CPQ-CPT-NPS	-2.92	118.61	123.60
7	B	4006	FYX	CPH-CPK-NPL	2.86	127.68	122.57
7	B	4006	FYX	CPQ-CPT-NPS	-2.86	118.73	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4003	MTE	O3'-C7-C6	-2.79	107.10	108.96
7	B	4006	FYX	CPH-CPK-NPJ	2.79	127.80	122.92
6	B	4005	FAD	C4-C4X-N5	2.76	122.02	118.21
6	A	3005	FAD	C4-C4X-N5	2.76	122.02	118.21
9	B	5004	GOL	O1-C1-C2	2.74	122.70	110.38
6	A	3005	FAD	C10-C4X-N5	-2.73	119.22	124.81
6	B	4005	FAD	C10-C4X-N5	-2.73	119.22	124.81
6	A	3005	FAD	C4X-C4-N3	2.73	120.21	113.25
9	B	5006	GOL	O1-C1-C2	2.73	122.68	110.38
9	A	5005	GOL	O1-C1-C2	2.73	122.67	110.38
9	A	5007	GOL	O1-C1-C2	2.73	122.66	110.38
9	B	5002	GOL	O1-C1-C2	2.73	122.65	110.38
9	B	5008	GOL	O1-C1-C2	2.72	122.64	110.38
6	B	4005	FAD	C4X-C4-N3	2.72	120.17	113.25
9	A	5001	GOL	O1-C1-C2	2.72	122.60	110.38
9	A	5003	GOL	O1-C1-C2	2.71	122.58	110.38
6	A	3005	FAD	C1'-N10-C9A	2.70	125.88	120.63
6	A	3005	FAD	C4-N3-C2	-2.67	120.89	125.64
6	B	4005	FAD	C4-N3-C2	-2.67	120.90	125.64
6	A	3005	FAD	O2B-C2B-C3B	2.66	120.36	111.82
4	B	4003	MTE	O4-C4-N3	2.57	124.95	120.11
7	A	3006	FYX	CPH-CPK-NPJ	2.56	127.40	122.92
6	B	4005	FAD	C4A-C5A-N7A	-2.52	107.70	110.58
6	A	3005	FAD	O3B-C3B-C4B	-2.52	103.84	111.08
6	B	4005	FAD	C5A-N7A-C8A	2.51	107.40	103.45
6	B	4005	FAD	C2A-N1A-C6A	2.49	122.82	118.73
6	A	3005	FAD	C4A-C5A-N7A	-2.46	107.77	110.58
4	A	3003	MTE	O4-C4-N3	2.46	124.74	120.11
6	A	3005	FAD	C5A-N7A-C8A	2.44	107.28	103.45
6	A	3005	FAD	C2A-N1A-C6A	2.44	122.73	118.73
6	B	4005	FAD	O3B-C3B-C4B	-2.42	104.12	111.08
6	A	3005	FAD	O5B-PA-O1A	2.42	118.51	108.94
6	A	3005	FAD	C8M-C8-C9	-2.39	115.36	119.57
6	A	3005	FAD	O4B-C1B-N9A	-2.38	103.51	108.09
6	B	4005	FAD	C4'-C3'-C2'	-2.35	109.66	113.57
6	B	4005	FAD	C8M-C8-C9	-2.32	115.49	119.57
8	B	4007	ACY	O-C-CH3	-2.31	113.06	122.53
7	B	4006	FYX	CPQ-CPP-CPO	2.29	121.48	118.57
6	A	3005	FAD	C3B-C2B-C1B	2.27	105.75	101.46
8	A	3007	ACY	O-C-CH3	-2.26	113.25	122.53
6	A	3005	FAD	O5'-P-O1P	2.15	117.45	108.94
7	B	4006	FYX	CPP-CPM-NPJ	2.14	128.22	124.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3006	FYX	CPQ-CPP-CPO	2.13	121.28	118.57
6	B	4005	FAD	C4X-C10-N10	2.13	119.53	116.48
4	A	3003	MTE	N3-C2-N1	-2.13	119.42	123.32
6	B	4005	FAD	N9A-C8A-N7A	-2.12	110.93	113.94
6	A	3005	FAD	C7M-C7-C6	-2.11	115.86	119.57
4	B	4003	MTE	N3-C2-N1	-2.10	119.48	123.32
6	A	3005	FAD	C4X-C10-N10	2.09	119.47	116.48
6	B	4005	FAD	C10-N1-C2	2.08	121.35	116.85
6	A	3005	FAD	C8M-C8-C7	2.05	124.94	120.76
6	B	4005	FAD	O2A-PA-O5B	2.02	116.72	107.57

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3003	MTE	C4'-O4'-P-O3P
4	B	4003	MTE	C4'-O4'-P-O2P
4	B	4003	MTE	C4'-O4'-P-O3P
9	A	5001	GOL	O2-C2-C3-O3
9	A	5003	GOL	O2-C2-C3-O3
9	A	5005	GOL	O2-C2-C3-O3
9	A	5007	GOL	O2-C2-C3-O3
9	B	5002	GOL	O2-C2-C3-O3
9	B	5004	GOL	O2-C2-C3-O3
9	B	5006	GOL	O2-C2-C3-O3
9	B	5008	GOL	O2-C2-C3-O3
9	A	5001	GOL	O1-C1-C2-O2
9	A	5003	GOL	O1-C1-C2-O2
9	A	5005	GOL	O1-C1-C2-O2
9	A	5007	GOL	O1-C1-C2-O2
9	B	5002	GOL	O1-C1-C2-O2
9	B	5004	GOL	O1-C1-C2-O2
9	B	5006	GOL	O1-C1-C2-O2
9	B	5008	GOL	O1-C1-C2-O2
4	A	3003	MTE	C3'-C4'-O4'-P
4	B	4003	MTE	C3'-C4'-O4'-P
4	A	3003	MTE	C4'-O4'-P-O2P
6	B	4005	FAD	O2'-C2'-C3'-C4'
6	B	4005	FAD	C5'-O5'-P-O1P
6	A	3005	FAD	C4'-C5'-O5'-P

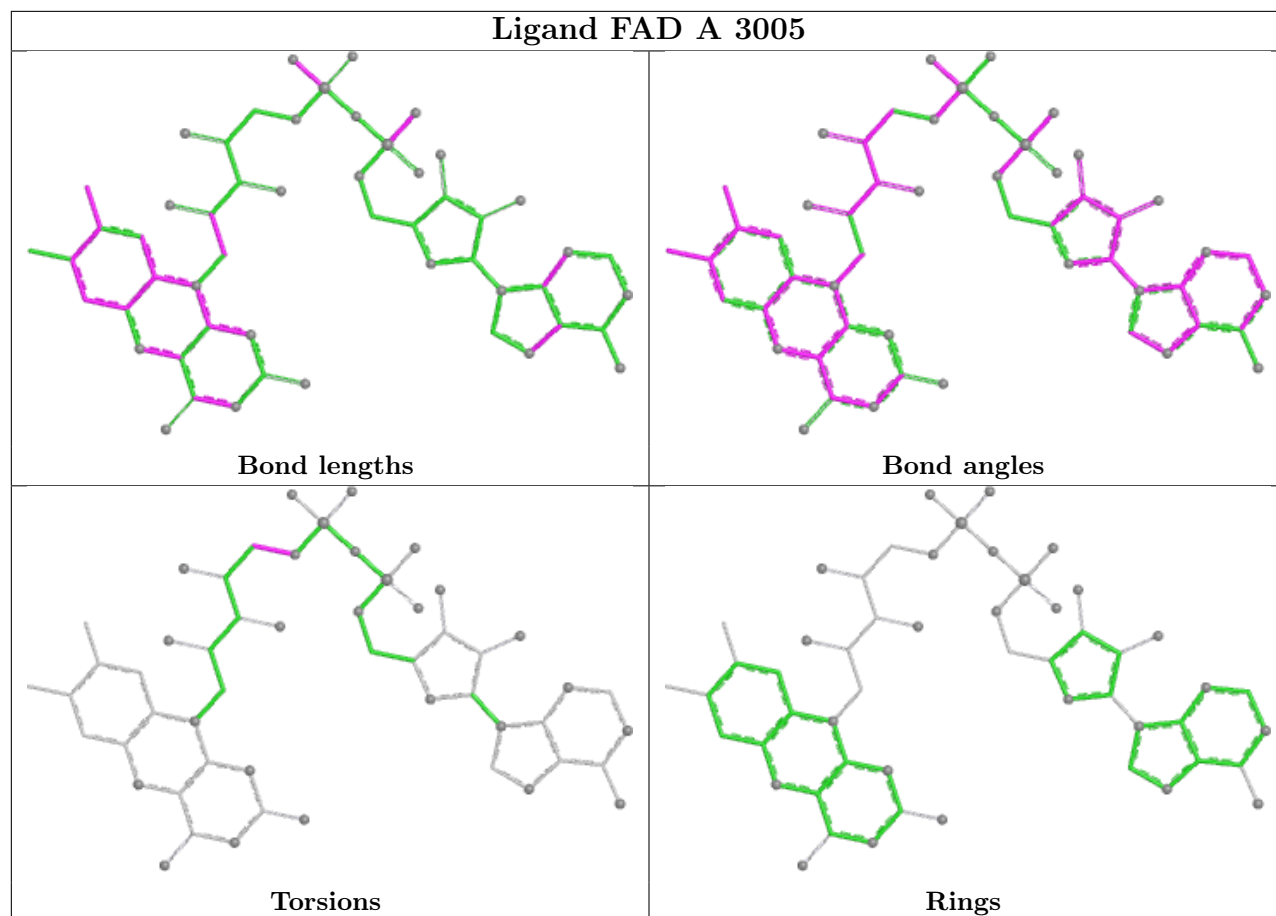
There are no ring outliers.

13 monomers are involved in 27 short contacts:

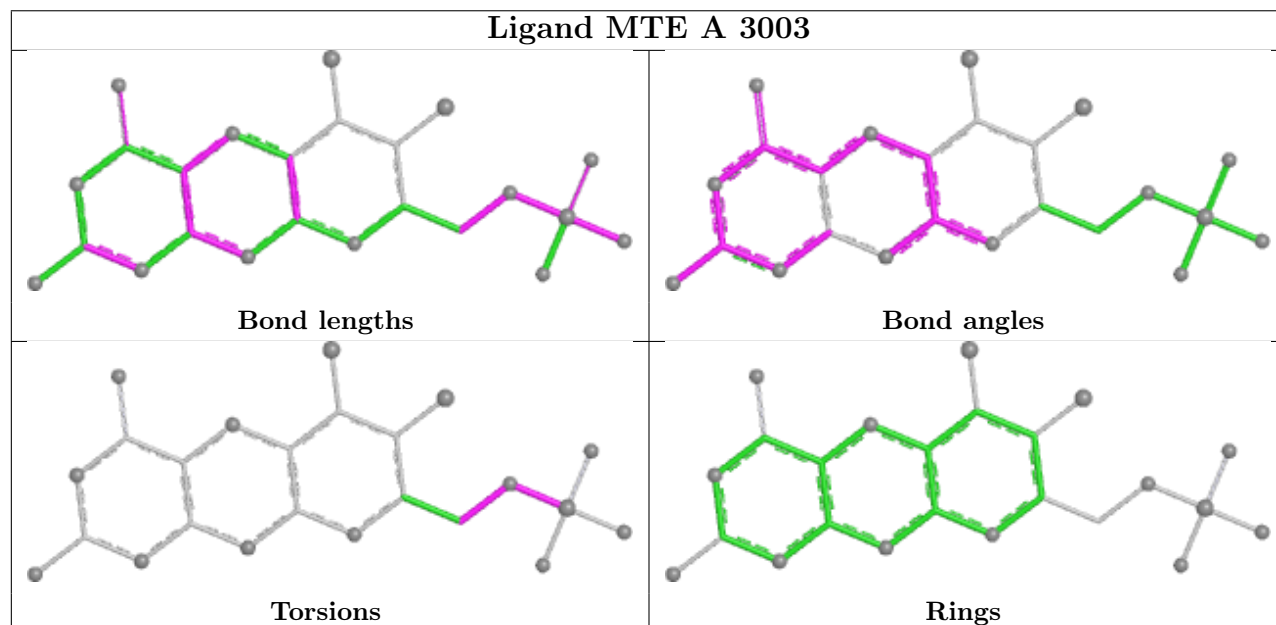
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	5008	GOL	2	0
9	A	5003	GOL	1	0
9	A	5001	GOL	1	0
6	A	3005	FAD	3	0
5	B	4004	MOS	2	0
8	A	3007	ACY	3	0
4	A	3003	MTE	1	0
5	A	3004	MOS	2	0
8	B	4007	ACY	4	0
9	A	5007	GOL	3	0
6	B	4005	FAD	3	0
9	B	5004	GOL	1	0
4	B	4003	MTE	1	0

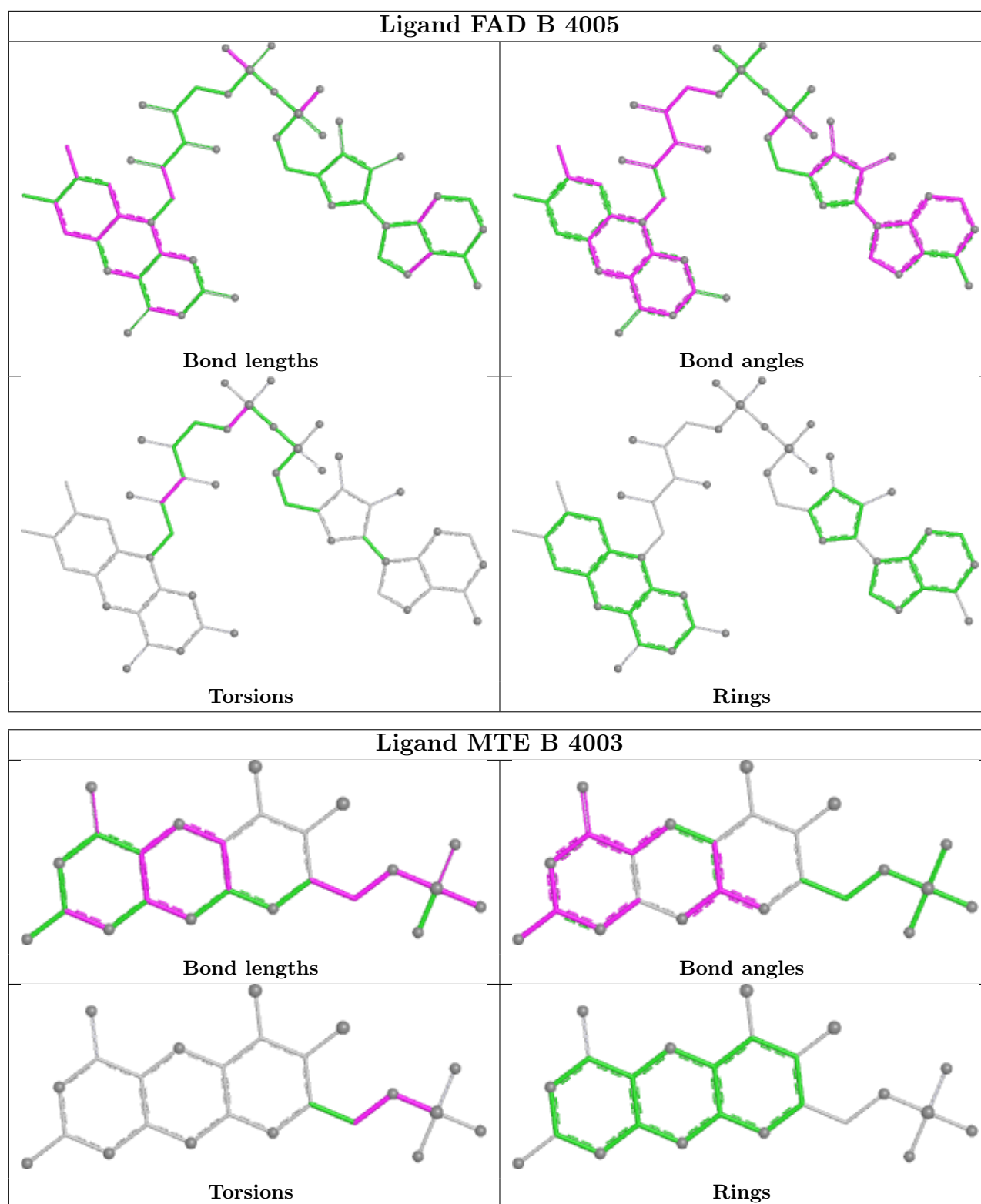
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 FAD A 3005



Ligand MTE A 3003





5.7 Other polymers [i](#)

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, 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	1298/1332 (97%)	0.01	76 (5%) 28 31	9, 18, 39, 61	0
1	B	1296/1332 (97%)	0.02	69 (5%) 32 36	9, 19, 38, 61	0
All	All	2594/2664 (97%)	0.02	145 (5%) 30 33	9, 18, 39, 61	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ALA	11.2
1	B	1322	PRO	8.0
1	A	431	ILE	8.0
1	A	1332	VAL	7.8
1	A	1318	VAL	7.7
1	B	1321	ALA	6.8
1	A	1321	ALA	6.8
1	A	1319	THR	6.8
1	B	1323	GLY	6.6
1	A	538	LEU	6.6
1	B	4	ASP	6.6
1	B	1325	CYS	6.5
1	A	1320	GLY	6.4
1	A	1322	PRO	6.3
1	A	1323	GLY	5.9
1	B	1320	GLY	5.9
1	A	1324	ASN	5.8
1	A	61	LEU	5.7
1	A	540	PRO	5.7
1	B	431	ILE	5.6
1	A	549	PHE	5.6
1	A	1317	CYS	5.5
1	B	1324	ASN	5.2
1	A	1325	CYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	1316	LEU	5.0
1	B	1318	VAL	4.9
1	A	1287	ASN	4.9
1	B	1287	ASN	4.9
1	B	5	GLU	4.8
1	B	528	GLY	4.7
1	B	551	LYS	4.6
1	B	336	TRP	4.3
1	B	552	HIS	4.3
1	B	1319	THR	4.2
1	A	432	ALA	4.2
1	A	530	ASP	4.0
1	B	1288	ASN	4.0
1	B	20	ALA	4.0
1	A	539	ASP	4.0
1	A	424	ALA	4.0
1	A	551	LYS	3.9
1	B	1317	CYS	3.9
1	A	4	ASP	3.9
1	B	19	ASN	3.8
1	A	3	ALA	3.8
1	A	336	TRP	3.8
1	A	433	LYS	3.8
1	B	1326	LYS	3.8
1	B	540	PRO	3.7
1	A	165	LYS	3.7
1	B	60	ARG	3.7
1	A	423	GLN	3.7
1	A	412	SER	3.7
1	A	552	HIS	3.7
1	A	430	ASP	3.7
1	B	538	LEU	3.6
1	A	548	LEU	3.5
1	B	165	LYS	3.5
1	A	1001	ILE	3.5
1	B	1316	LEU	3.4
1	A	555	ALA	3.4
1	B	1329	SER	3.4
1	A	429	ASP	3.3
1	B	425	SER	3.3
1	A	550	GLN	3.3
1	A	537	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1286	THR	3.2
1	A	651	ASP	3.2
1	B	1289	ASN	3.1
1	B	61	LEU	3.1
1	A	1288	ASN	3.1
1	B	548	LEU	3.0
1	A	565	ASN	3.0
1	B	543	THR	3.0
1	B	424	ALA	3.0
1	A	60	ARG	3.0
1	B	1332	VAL	3.0
1	B	550	GLN	3.0
1	A	428	GLU	2.9
1	A	543	THR	2.8
1	A	553	PRO	2.8
1	A	192	SER	2.8
1	B	433	LYS	2.8
1	B	216	LEU	2.8
1	B	565	ASN	2.7
1	A	544	SER	2.7
1	A	338	ALA	2.7
1	B	1286	THR	2.7
1	B	983	GLU	2.7
1	B	430	ASP	2.7
1	A	541	THR	2.6
1	A	509	ARG	2.6
1	A	425	SER	2.6
1	A	547	LEU	2.6
1	B	1330	LEU	2.6
1	A	684	VAL	2.6
1	B	724	SER	2.6
1	B	549	PHE	2.5
1	A	1143	GLU	2.5
1	B	554	PRO	2.5
1	A	542	TYR	2.5
1	A	272	ASN	2.5
1	A	426	ARG	2.5
1	B	1290	THR	2.5
1	A	989	LYS	2.5
1	B	378	GLY	2.4
1	A	337	PHE	2.4
1	B	1328	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	222	VAL	2.4
1	A	1331	ARG	2.4
1	B	377	ARG	2.4
1	B	140	GLU	2.4
1	B	412	SER	2.4
1	B	338	ALA	2.4
1	B	383	VAL	2.4
1	B	989	LYS	2.4
1	B	500	ALA	2.4
1	A	1315	THR	2.3
1	B	539	ASP	2.3
1	A	398	LEU	2.3
1	B	547	LEU	2.3
1	A	725	GLU	2.3
1	A	983	GLU	2.3
1	A	225	LYS	2.3
1	A	1326	LYS	2.3
1	B	337	PHE	2.2
1	B	553	PRO	2.2
1	B	564	PRO	2.2
1	B	537	LYS	2.2
1	A	545	ALA	2.2
1	A	529	LYS	2.2
1	A	1330	LEU	2.2
1	A	724	SER	2.2
1	B	497	SER	2.2
1	B	541	THR	2.1
1	B	129	ARG	2.1
1	A	500	ALA	2.1
1	A	546	THR	2.1
1	B	1327	PRO	2.1
1	A	64	LYS	2.0
1	A	497	SER	2.0
1	A	427	ARG	2.0
1	B	321	THR	2.0
1	B	546	THR	2.0
1	B	427	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

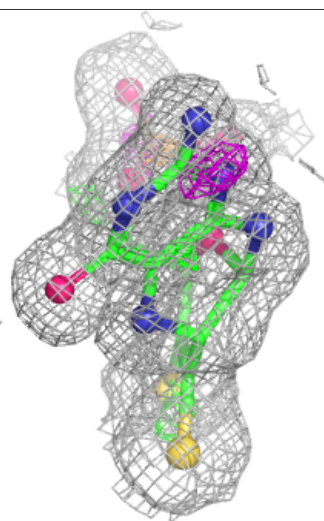
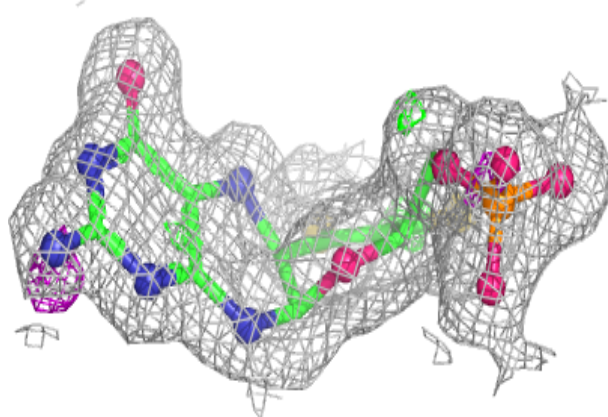
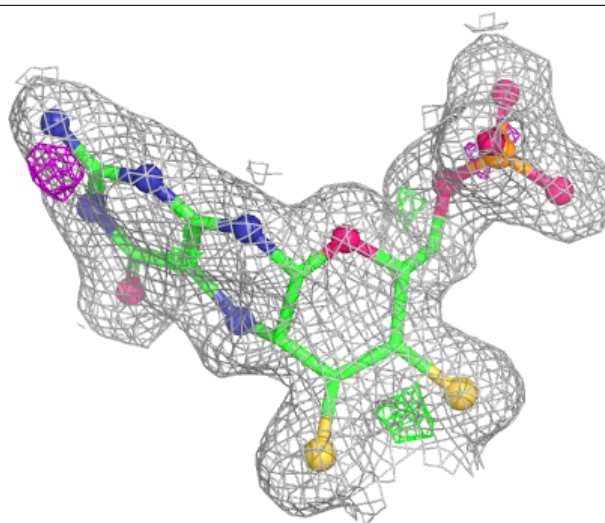
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
9	GOL	A	5007	6/6	0.65	0.22	40,42,43,45	0
9	GOL	B	5008	6/6	0.66	0.24	42,43,45,46	0
9	GOL	B	5004	6/6	0.71	0.23	34,38,41,42	0
9	GOL	B	5006	6/6	0.81	0.16	31,35,37,40	0
9	GOL	A	5001	6/6	0.81	0.16	23,29,30,36	0
9	GOL	A	5003	6/6	0.82	0.17	29,34,35,37	0
9	GOL	A	5005	6/6	0.82	0.15	29,34,38,41	0
9	GOL	B	5002	6/6	0.85	0.12	24,29,31,31	0
7	FYX	B	4006	19/19	0.93	0.08	14,18,24,27	0
7	FYX	A	3006	19/19	0.94	0.07	15,18,27,27	0
8	ACY	A	3007	4/4	0.96	0.05	4,9,13,13	0
8	ACY	B	4007	4/4	0.96	0.05	7,13,13,16	0
4	MTE	A	3003	24/24	0.97	0.06	8,12,15,17	0
6	FAD	A	3005	53/53	0.97	0.06	12,16,20,24	0
6	FAD	B	4005	53/53	0.97	0.06	12,17,21,23	0
4	MTE	B	4003	24/24	0.98	0.06	9,11,15,16	0
3	FES	A	3001	4/4	0.99	0.03	11,11,11,11	0
3	FES	A	3002	4/4	0.99	0.02	11,11,12,12	0
3	FES	B	4001	4/4	0.99	0.02	11,11,12,12	0
3	FES	B	4002	4/4	0.99	0.03	11,12,12,12	0
2	CA	A	3008	1/1	0.99	0.03	12,12,12,12	0
5	MOS	B	4004	4/4	1.00	0.02	10,13,14,15	0
2	CA	B	4008	1/1	1.00	0.02	16,16,16,16	0
5	MOS	A	3004	4/4	1.00	0.02	12,14,15,16	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.

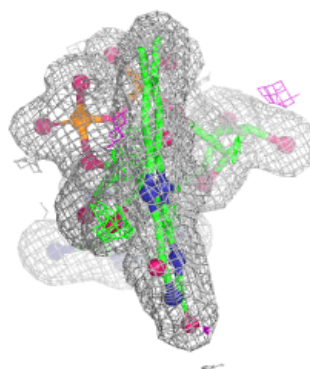
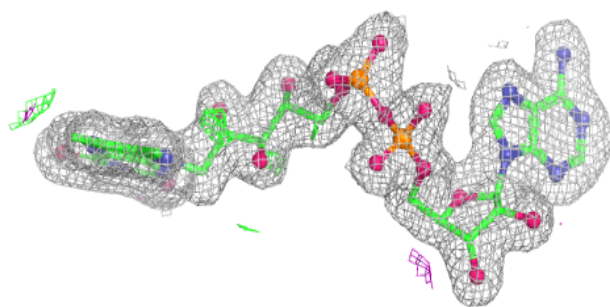
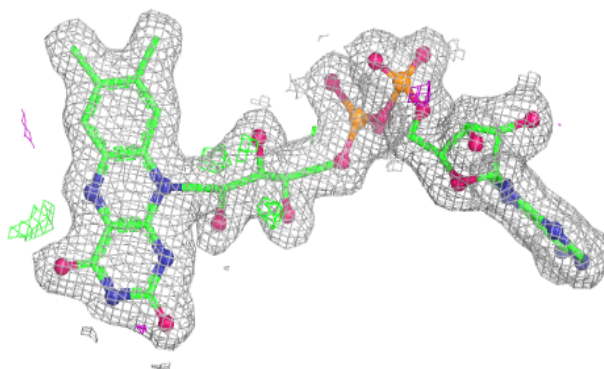
Electron density around MTE A 3003:

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

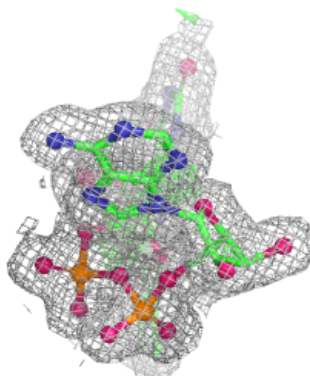
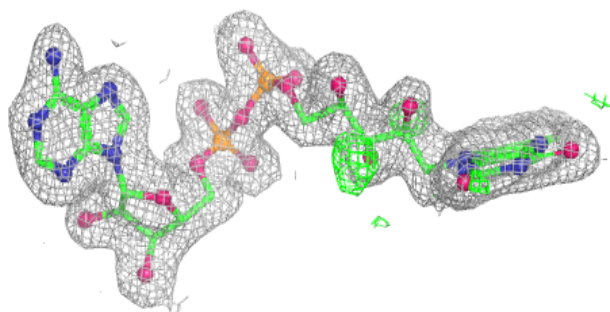
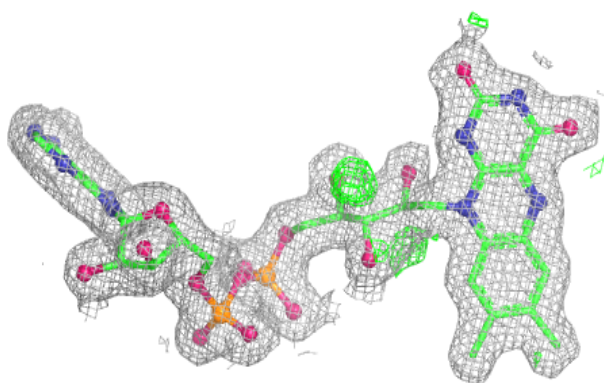


Electron density around FAD A 3005:

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

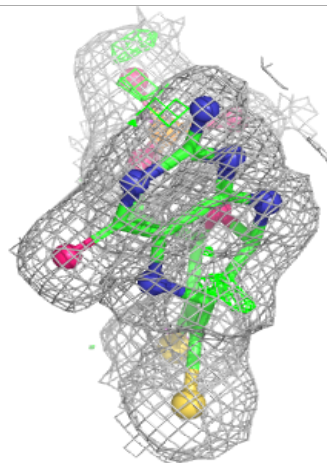
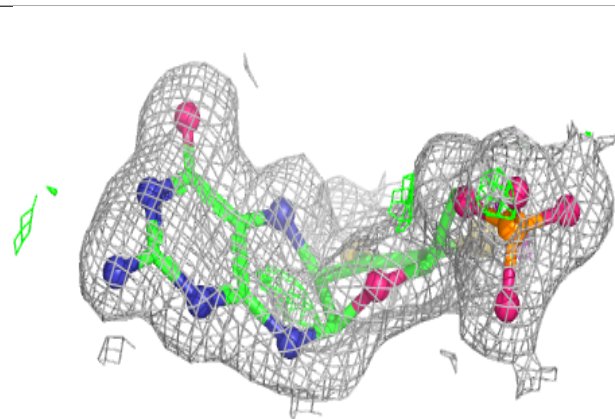
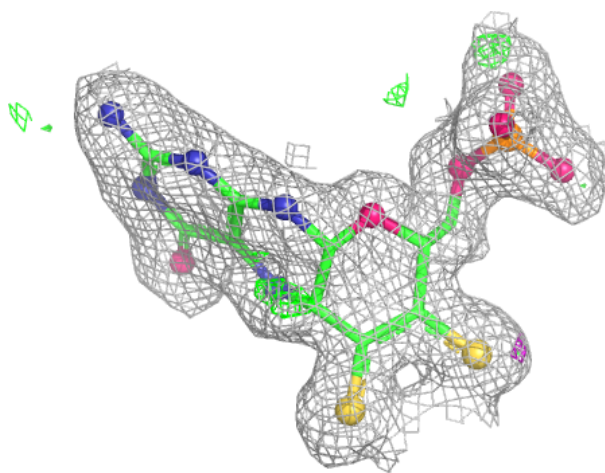
**Electron density around FAD B 4005:**

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



Electron density around MTE B 4003:

$2mF_o-DF_c$ (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.