



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:14 AM EDT

PDB ID : 1VDV / pdb_00001vdv
Title : Bovine Milk Xanthine Dehydrogenase Y-700 Bound Form
Authors : Fukunari, A.; Okamoto, K.; Nishino, T.; Eger, B.T.; Pai, E.F.; Kamezawa, M.; Yamada, I.; Kato, N.
Deposited on : 2004-03-25
Resolution : 1.98 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

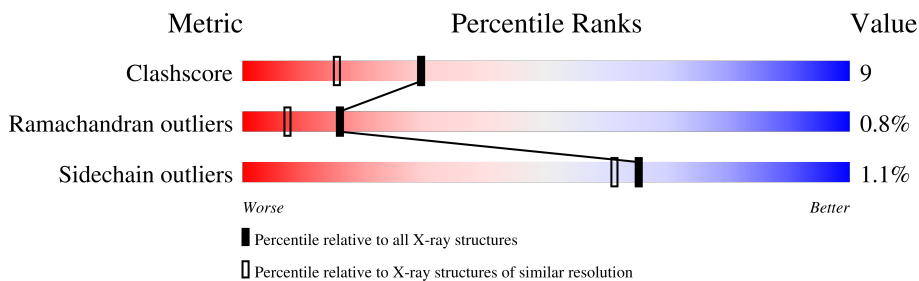
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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))
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1332	
1	B	1332	

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
7	ACY	A	5201	-	-	X	-
7	ACY	B	5202	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22610 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	1299	Total	C	N	O	S	0	0	0
			10077	6404	1728	1884	61			
1	B	1296	Total	C	N	O	S	0	0	0
			10054	6391	1724	1878	61			

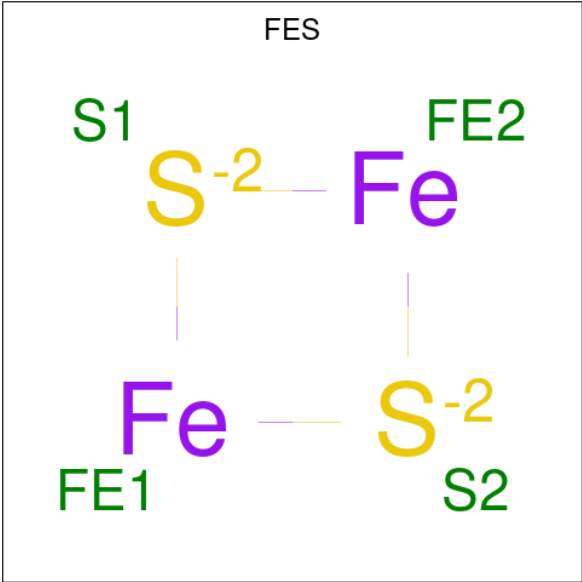
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P80457
B	1	MET	-	initiating methionine	UNP P80457

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

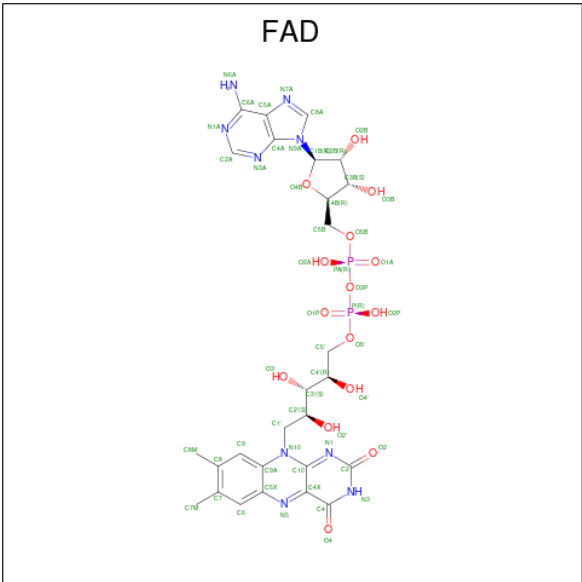
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

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



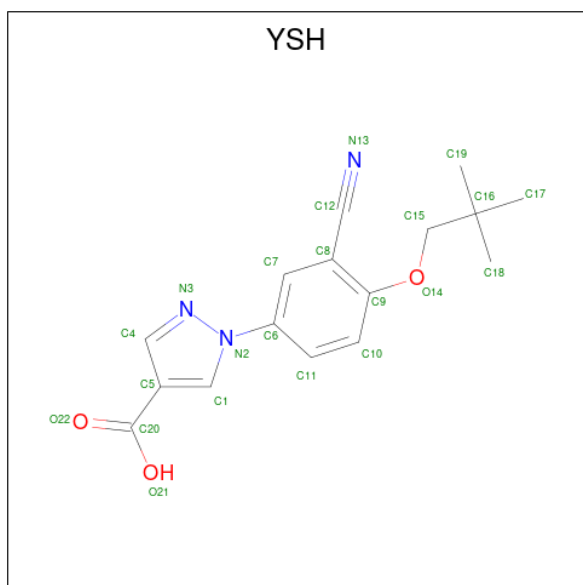
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 5 is 1-[3-CYANO-4-(NEOPENTYLOXY)PHENYL]-1H-PYRAZOLE-4-CARBOXYLIC ACID (CCD ID: YSH) (formula: C₁₆H₁₇N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			22	16	3	3		
5	B	1	Total	C	N	O	0	0
			22	16	3	3		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



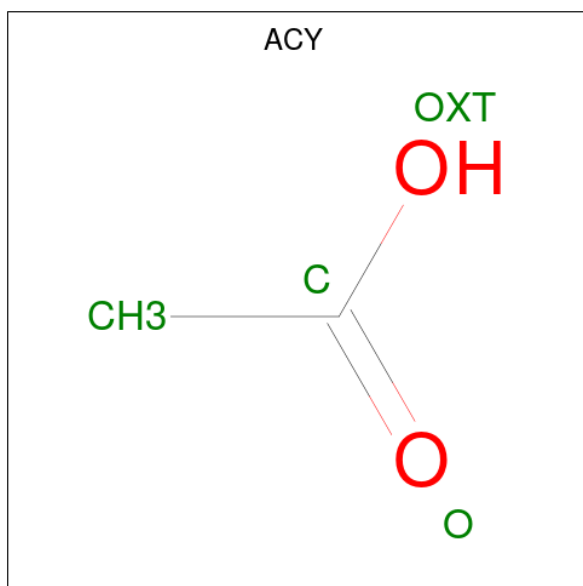
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total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

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

- Molecule 7 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 8 is Molybdopterin hydroxy-oxo-thiol-molybdenum (CCD ID: HOH) (formula: H_2O).

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	A	1	Total 28	C 10	Mo 1	N 5	O 8	P 1	S 3	0	0
8	B	1	Total 28	C 10	Mo 1	N 5	O 8	P 1	S 3	0	0

- Molecule 9 is water.

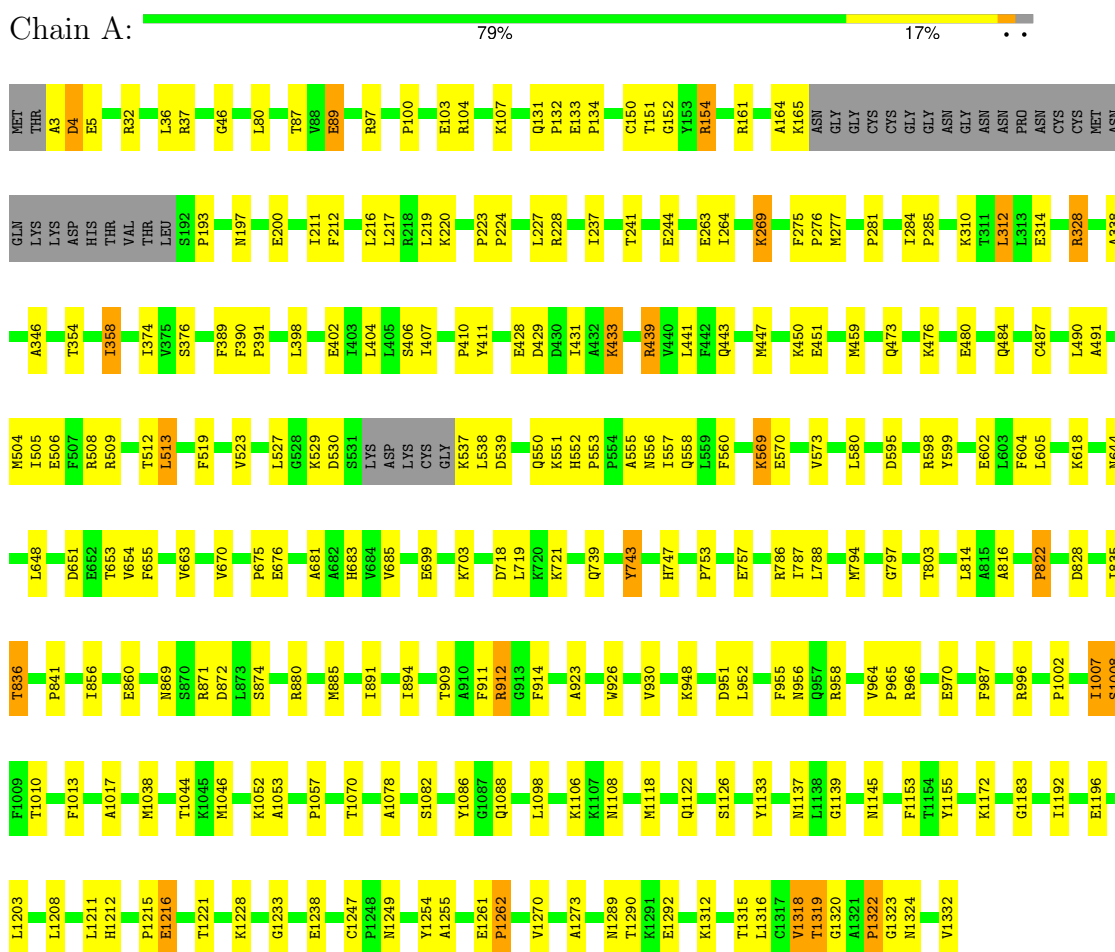
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1086	Total 1086	O 1086	0	0
9	B	1033	Total 1033	O 1033	0	0

3 Residue-property plots

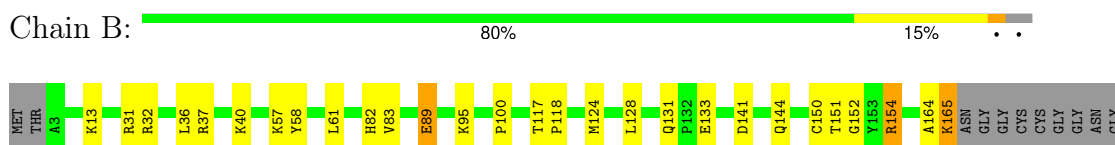
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: Xanthine dehydrogenase/oxidase



• Molecule 1: Xanthine dehydrogenase/oxidase





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.82Å 123.94Å 148.89Å 90.00° 91.16° 90.00°	Depositor
Resolution (Å)	20.00 – 1.98	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.98)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.178 , 0.215	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22610	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZXF, FES, CA, ACY, YSH, FAD

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	0.36	0/10298	0.91	41/13939 (0.3%)
1	B	0.36	0/10275	0.91	40/13909 (0.3%)
All	All	0.36	0/20573	0.91	81/27848 (0.3%)

There are no bond length outliers.

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	835	ILE	N-CA-C	10.79	123.01	111.58
1	A	835	ILE	N-CA-C	10.43	122.64	111.58
1	B	151	THR	N-CA-C	10.30	123.77	111.82
1	A	151	THR	N-CA-C	10.11	123.55	111.82
1	B	836	THR	N-CA-C	8.76	123.80	113.20
1	A	433	LYS	N-CA-C	-8.22	101.02	112.45
1	B	433	LYS	N-CA-C	-7.93	100.62	112.04
1	A	836	THR	N-CA-C	7.57	122.36	113.20
1	B	1262	PRO	N-CA-C	7.44	119.78	110.70
1	A	390	PHE	CA-C-N	7.42	126.69	118.97
1	A	390	PHE	C-N-CA	7.42	126.69	118.97
1	A	956	ASN	N-CA-C	7.35	121.65	112.24
1	A	1262	PRO	N-CA-C	7.22	119.50	110.70
1	B	956	ASN	N-CA-C	7.16	121.59	112.86
1	A	828	ASP	N-CA-C	-6.93	101.19	110.55
1	B	869	ASN	N-CA-C	6.92	121.16	113.21
1	A	654	VAL	N-CA-C	-6.90	103.47	111.00
1	A	1273	ALA	N-CA-C	-6.90	103.84	111.36
1	A	743	TYR	N-CA-C	-6.88	100.09	110.28
1	B	1108	ASN	CA-C-N	6.83	127.11	119.32
1	B	1108	ASN	C-N-CA	6.83	127.11	119.32
1	B	1085	ILE	N-CA-C	6.82	117.43	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	891	ILE	CA-C-N	6.78	126.30	119.24
1	B	891	ILE	C-N-CA	6.78	126.30	119.24
1	B	743	TYR	N-CA-C	-6.75	100.29	110.28
1	B	436	CYS	N-CA-C	6.58	118.21	108.60
1	B	1273	ALA	N-CA-C	-6.57	104.20	111.36
1	B	152	GLY	N-CA-C	-6.55	106.19	115.43
1	A	1323	GLY	N-CA-C	-6.53	107.21	115.31
1	B	828	ASP	N-CA-C	-6.44	101.86	110.55
1	B	654	VAL	N-CA-C	-6.38	104.04	111.00
1	A	663	VAL	N-CA-C	-6.29	101.43	109.30
1	A	450	LYS	N-CA-C	-6.23	105.70	113.55
1	A	411	TYR	N-CA-C	-6.20	101.31	110.48
1	B	505	ILE	N-CA-C	6.10	116.27	110.42
1	A	152	GLY	N-CA-C	-6.09	106.84	115.43
1	B	390	PHE	CA-C-N	6.03	125.24	118.97
1	B	390	PHE	C-N-CA	6.03	125.24	118.97
1	A	1108	ASN	CA-C-N	5.95	126.11	119.32
1	A	1108	ASN	C-N-CA	5.95	126.11	119.32
1	A	891	ILE	CA-C-N	5.95	125.42	119.24
1	A	891	ILE	C-N-CA	5.95	125.42	119.24
1	B	696	ILE	N-CA-C	5.82	117.20	111.67
1	A	80	LEU	N-CA-C	5.77	120.02	112.92
1	B	543	THR	N-CA-C	5.77	118.04	111.11
1	B	663	VAL	N-CA-C	-5.73	102.13	109.30
1	B	40	LYS	N-CA-C	5.73	119.02	110.14
1	A	872	ASP	CB-CA-C	-5.67	110.02	116.54
1	A	822	PRO	N-CA-C	-5.64	102.41	111.38
1	B	197	ASN	CA-C-N	5.62	125.46	119.28
1	B	197	ASN	C-N-CA	5.62	125.46	119.28
1	B	411	TYR	N-CA-C	-5.59	102.21	110.48
1	B	964	VAL	CB-CA-C	-5.57	108.41	113.70
1	A	1137	ASN	N-CA-C	5.53	118.88	111.24
1	A	358	ILE	N-CA-C	5.38	116.70	111.91
1	A	354	THR	N-CA-C	-5.36	105.55	111.71
1	A	841	PRO	N-CA-C	-5.36	102.86	111.38
1	A	410	PRO	N-CA-C	5.35	119.89	111.38
1	B	150	CYS	N-CA-C	5.35	119.80	112.68
1	B	1228	LYS	N-CA-C	5.33	117.67	107.75
1	B	787	ILE	N-CA-C	5.25	115.53	108.17
1	A	1007	ILE	N-CA-C	5.25	115.66	107.99
1	A	5	GLU	N-CA-C	5.23	117.75	109.96
1	B	410	PRO	N-CA-C	5.22	119.68	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	821	HIS	CA-C-N	-5.20	114.60	119.85
1	B	821	HIS	C-N-CA	-5.20	114.60	119.85
1	A	1070	THR	N-CA-C	-5.17	106.92	113.43
1	A	443	GLN	N-CA-C	-5.15	102.97	110.08
1	A	150	CYS	N-CA-C	5.14	119.44	112.04
1	A	685	VAL	N-CA-C	-5.14	102.88	109.30
1	B	841	PRO	N-CA-C	-5.12	103.23	111.38
1	B	450	LYS	N-CA-C	-5.11	105.89	112.68
1	A	269	LYS	N-CA-C	5.09	116.91	111.36
1	B	244	GLU	N-CA-C	-5.09	99.97	110.80
1	A	787	ILE	N-CA-C	5.07	115.27	108.17
1	B	31	ARG	N-CA-C	5.07	116.89	111.36
1	A	874	SER	N-CA-C	5.07	117.46	111.33
1	B	764	VAL	N-CA-C	5.07	115.95	108.45
1	A	447	MET	N-CA-C	-5.02	106.47	112.59
1	A	869	ASN	N-CA-C	5.02	118.98	113.21
1	A	1228	LYS	N-CA-C	5.00	117.05	107.75

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	10077	0	10076	182	0
1	B	10054	0	10053	167	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	8	0	0	1	0
3	B	8	0	0	0	0
4	A	53	0	31	3	0
4	B	53	0	31	2	0
5	A	22	0	16	3	0
5	B	22	0	16	3	0
6	A	66	0	88	8	0
6	B	60	0	80	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	4	0	3	4	0
7	B	4	0	3	4	0
8	A	28	0	0	0	0
8	B	28	0	0	0	0
9	A	1086	0	0	10	0
9	B	1033	0	0	9	0
All	All	22610	0	20397	351	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (351) 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)
5:B:5102:YSH:N2	5:B:5102:YSH:C1	1.70	1.52
5:A:5101:YSH:N2	5:A:5101:YSH:C1	1.68	1.51
1:A:3:ALA:HB1	1:A:228:ARG:H	1.20	1.06
1:A:537:LYS:HG2	1:A:538:LEU:H	1.28	0.98
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.30	0.97
1:B:1286:THR:HG22	1:B:1287:ASN:H	1.32	0.94
1:A:439:ARG:HH11	1:A:439:ARG:HB3	1.32	0.93
1:A:131:GLN:HE21	1:A:133:GLU:H	1.14	0.90
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.36	0.89
1:B:1321:ALA:HB1	1:B:1322:PRO:HD2	1.56	0.87
1:A:1211:LEU:HA	1:A:1221:THR:HG21	1.57	0.86
1:A:885:MET:HE2	1:A:894:ILE:HD11	1.57	0.86
1:B:404:LEU:HD21	1:B:407:ILE:HD11	1.57	0.86
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.57	0.84
1:A:3:ALA:HB1	1:A:228:ARG:N	1.93	0.83
1:B:131:GLN:HE21	1:B:133:GLU:H	1.26	0.83
1:B:1088:GLN:HG2	1:B:1133:TYR:CD1	2.15	0.82
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.45	0.80
1:B:551:LYS:NZ	1:B:551:LYS:HA	1.96	0.80
1:A:719:LEU:HD21	1:A:860:GLU:HG2	1.65	0.79
1:A:358:ILE:HD12	1:A:431:ILE:HG23	1.64	0.78
1:A:718:ASP:HB3	1:A:721:LYS:HE2	1.69	0.75
1:A:537:LYS:HG2	1:A:538:LEU:N	2.03	0.73
1:A:406:SER:C	1:A:407:ILE:HD12	2.13	0.73
1:B:551:LYS:HZ2	1:B:552:HIS:H	1.32	0.73
1:B:36:LEU:HD22	1:B:89:GLU:HG3	1.71	0.73
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:LYS:HA	1:B:551:LYS:HZ2	1.54	0.70
1:A:1118:MET:O	1:A:1122:GLN:HG2	1.92	0.70
1:B:1286:THR:HG22	1:B:1287:ASN:N	2.05	0.69
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	1.92	0.69
1:B:552:HIS:CE1	1:B:1172:LYS:HZ3	2.09	0.69
1:A:264:ILE:HD11	4:A:3005:FAD:H3B	1.75	0.68
1:B:1078:ALA:HB1	9:B:5304:ZXF:O1	1.94	0.68
1:A:217:LEU:O	1:A:220:LYS:HG2	1.93	0.68
1:A:911:PHE:H	7:A:5201:ACY:H3	1.59	0.67
1:A:441:LEU:HB3	1:A:451:GLU:HB2	1.76	0.66
1:B:376:SER:HB3	1:B:379:THR:OG1	1.95	0.66
1:B:719:LEU:HD11	1:B:895:ARG:HB2	1.78	0.66
1:A:948:LYS:HG2	1:A:951:ASP:OD2	1.95	0.65
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.96	0.65
1:B:948:LYS:HG2	1:B:951:ASP:OD2	1.97	0.65
1:A:538:LEU:HD12	6:A:5002:GOL:H31	1.77	0.65
1:A:193:PRO:HG2	1:A:560:PHE:CE1	2.32	0.65
1:A:428:GLU:OE2	1:A:1233:GLY:HA3	1.96	0.65
1:B:1312:LYS:O	1:B:1316:LEU:HD13	1.97	0.65
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.79	0.65
1:B:406:SER:O	1:B:407:ILE:HD12	1.97	0.65
1:A:131:GLN:HE21	1:A:133:GLU:N	1.92	0.64
1:A:439:ARG:HB3	1:A:439:ARG:NH1	2.09	0.64
1:B:551:LYS:HZ2	1:B:552:HIS:N	1.96	0.64
1:B:911:PHE:H	7:B:5202:ACY:H3	1.63	0.64
1:B:719:LEU:HD11	1:B:895:ARG:CB	2.28	0.63
1:A:580:LEU:HD13	1:A:1044:THR:HG23	1.80	0.63
1:A:358:ILE:CD1	1:A:431:ILE:HG23	2.28	0.63
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.63	0.63
1:A:217:LEU:HD12	1:A:220:LYS:HD3	1.82	0.62
1:A:164:ALA:O	1:A:165:LYS:HB2	2.00	0.61
1:B:1286:THR:CG2	1:B:1287:ASN:H	2.11	0.61
1:A:197:ASN:O	1:A:200:GLU:HG2	2.01	0.61
1:A:788:LEU:HB2	6:A:5011:GOL:H12	1.83	0.60
1:A:651:ASP:CG	1:A:871:ARG:HH11	2.09	0.60
1:B:757:GLU:HB3	1:B:786:ARG:HE	1.66	0.60
9:B:5304:ZXF:O2	9:B:5304:ZXF:MO	1.73	0.60
1:B:310:LYS:O	1:B:314:GLU:HG3	2.02	0.59
1:B:911:PHE:N	7:B:5202:ACY:H3	2.16	0.59
1:A:3:ALA:HA	1:A:227:LEU:HD22	1.83	0.59
1:A:4:ASP:HB3	9:A:5928:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:5101:YSH:C1	5:A:5101:YSH:C6	2.78	0.59
1:A:439:ARG:HH11	1:A:439:ARG:CB	2.13	0.59
1:A:911:PHE:N	7:A:5201:ACY:H3	2.18	0.59
1:A:328:ARG:HG2	9:A:5679:HOH:O	2.03	0.59
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.84	0.59
1:B:1318:VAL:HG22	1:B:1321:ALA:HB2	1.85	0.59
1:A:966:ARG:O	1:A:970:GLU:HG3	2.02	0.58
1:B:570:GLU:OE2	1:B:1057:PRO:HG3	2.03	0.58
1:A:3:ALA:HA	1:A:227:LEU:CD2	2.32	0.58
1:A:1010:THR:HG23	5:A:5101:YSH:O22	2.04	0.58
1:A:1203:LEU:HD13	1:A:1270:VAL:HG21	1.85	0.58
1:A:1172:LYS:HG3	6:A:5001:GOL:H31	1.87	0.57
1:B:1289:ASN:O	1:B:1290:THR:HB	2.05	0.57
1:B:372:LEU:HD23	1:B:407:ILE:HG13	1.86	0.57
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.05	0.57
1:B:32:ARG:HH12	1:B:676:GLU:CD	2.13	0.57
1:A:914:PHE:HA	7:A:5201:ACY:H2	1.87	0.56
1:B:473:GLN:O	1:B:476:LYS:HB2	2.05	0.56
1:B:713:LYS:HD3	1:B:897:THR:HG22	1.88	0.56
1:A:552:HIS:CG	1:A:553:PRO:HD2	2.40	0.56
1:A:1322:PRO:C	1:A:1324:ASN:H	2.12	0.56
1:B:346:ALA:HB1	4:B:4005:FAD:H4'	1.86	0.56
1:B:1326:LYS:HG3	9:B:5861:HOH:O	2.04	0.56
1:B:197:ASN:O	1:B:200:GLU:HG2	2.04	0.56
1:B:1287:ASN:O	1:B:1288:ASN:HB2	2.06	0.56
1:B:406:SER:C	1:B:407:ILE:HD12	2.30	0.56
1:A:154:ARG:HD2	9:A:5453:HOH:O	2.06	0.56
1:A:1312:LYS:O	1:A:1316:LEU:HD23	2.06	0.56
1:A:433:LYS:HE3	1:A:504:MET:SD	2.46	0.55
1:A:569:LYS:NZ	1:A:569:LYS:HB3	2.21	0.55
1:B:509:ARG:HH11	1:B:509:ARG:HG2	1.72	0.55
1:A:1318:VAL:HB	1:A:1322:PRO:HB3	1.88	0.55
1:B:404:LEU:HD21	1:B:407:ILE:CD1	2.33	0.55
1:B:699:GLU:H	1:B:699:GLU:CD	2.14	0.54
1:B:1323:GLY:O	1:B:1325:CYS:N	2.41	0.54
1:A:1212:HIS:H	1:A:1221:THR:HG22	1.72	0.54
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.90	0.54
1:A:909:THR:O	7:A:5201:ACY:H1	2.08	0.54
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.08	0.54
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.90	0.53
1:A:269:LYS:HE3	9:A:6386:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:NH1	1:A:97:ARG:HB2	2.23	0.53
1:A:527:LEU:C	1:A:529:LYS:H	2.17	0.53
1:B:1323:GLY:O	1:B:1324:ASN:C	2.51	0.53
1:B:1010:THR:HG23	5:B:5102:YSH:O22	2.08	0.53
1:A:87:THR:HG1	1:A:89:GLU:HG2	1.74	0.52
1:B:1312:LYS:HG2	9:B:6326:HOH:O	2.10	0.52
1:B:909:THR:O	7:B:5202:ACY:H1	2.08	0.52
1:A:473:GLN:O	1:A:476:LYS:HB2	2.09	0.52
1:A:599:TYR:HA	1:B:599:TYR:HA	1.91	0.52
1:A:131:GLN:NE2	1:A:133:GLU:H	1.96	0.52
1:B:521:LEU:HD22	1:B:538:LEU:HD11	1.91	0.52
1:B:264:ILE:HD11	4:B:4005:FAD:H3B	1.90	0.52
1:B:551:LYS:HA	1:B:551:LYS:HZ3	1.73	0.52
1:A:389:PHE:O	1:A:391:PRO:HD3	2.10	0.52
5:B:5102:YSH:C1	5:B:5102:YSH:C6	2.81	0.52
1:A:1082:SER:HB2	9:A:5305:ZXF:O1P	2.10	0.52
1:B:154:ARG:HD2	9:B:5493:HOH:O	2.08	0.52
1:B:164:ALA:O	1:B:165:LYS:HB2	2.09	0.52
1:B:911:PHE:O	1:B:912:ARG:C	2.53	0.51
1:A:338:ALA:HA	1:A:429:ASP:OD1	2.11	0.51
1:A:537:LYS:CG	1:A:538:LEU:H	2.12	0.51
1:A:1078:ALA:HB1	9:A:5305:ZXF:O1	2.09	0.51
1:A:1322:PRO:C	1:A:1324:ASN:N	2.68	0.51
1:B:237:ILE:HG13	1:B:277:MET:HE1	1.91	0.51
1:A:505:ILE:N	1:A:505:ILE:HD12	2.25	0.51
1:B:376:SER:HB2	1:B:402:GLU:HG2	1.92	0.51
1:A:1318:VAL:HG12	1:A:1319:THR:H	1.76	0.51
1:A:911:PHE:O	1:A:912:ARG:C	2.53	0.50
1:B:548:LEU:HA	6:B:5022:GOL:H12	1.93	0.50
1:A:404:LEU:HD21	1:A:407:ILE:HD11	1.92	0.50
1:A:1319:THR:HG23	1:A:1320:GLY:N	2.26	0.50
1:B:723:PHE:CD2	1:B:847:LYS:HE2	2.47	0.50
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.11	0.50
1:B:1281:ALA:O	1:B:1284:GLN:HB3	2.12	0.50
1:A:480:GLU:O	1:A:484:GLN:HG3	2.11	0.50
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.47	0.50
1:B:914:PHE:HA	7:B:5202:ACY:H2	1.92	0.50
1:A:1318:VAL:HG12	1:A:1319:THR:N	2.26	0.50
1:A:1289:ASN:HD22	1:A:1292:GLU:HB2	1.77	0.50
1:B:1289:ASN:HB3	1:B:1292:GLU:HB2	1.94	0.50
1:A:161:ARG:HD3	9:A:5307:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ARG:HG3	1:B:600:GLU:HG2	1.94	0.49
1:A:604:PHE:CD2	1:A:675:PRO:HG3	2.46	0.49
1:A:605:LEU:HD23	1:A:605:LEU:C	2.37	0.49
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.48	0.49
1:B:1172:LYS:HG3	6:B:5008:GOL:H31	1.95	0.49
1:B:58:TYR:CD2	1:B:220:LYS:HB2	2.47	0.49
1:B:551:LYS:HZ2	1:B:551:LYS:CA	2.23	0.49
1:A:1007:ILE:O	1:A:1008:SER:CB	2.61	0.49
1:B:165:LYS:HB2	1:B:165:LYS:NZ	2.27	0.49
1:B:1173:ASN:O	1:B:1236:PRO:HA	2.13	0.49
1:A:237:ILE:N	1:A:237:ILE:HD12	2.28	0.49
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.48	0.49
1:A:644:ASN:O	1:A:653:THR:HA	2.13	0.49
1:A:459:MET:HE2	1:A:512:THR:HG21	1.94	0.49
1:A:856:ILE:HD12	1:A:856:ILE:N	2.27	0.49
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.78	0.49
1:A:739:GLN:HG2	1:A:911:PHE:CE1	2.48	0.49
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.95	0.49
1:B:1324:ASN:O	1:B:1325:CYS:C	2.56	0.49
1:B:403:ILE:C	1:B:403:ILE:HD12	2.38	0.48
1:A:699:GLU:CD	1:A:699:GLU:H	2.21	0.48
1:A:1017:ALA:HB1	1:A:1086:TYR:CD2	2.47	0.48
1:A:1106:LYS:NZ	1:A:1106:LYS:HB3	2.27	0.48
1:A:508:ARG:O	1:A:512:THR:HG23	2.13	0.48
1:B:655:PHE:CE1	1:B:814:LEU:HD23	2.47	0.48
1:B:826:MET:HB3	6:B:5014:GOL:H31	1.94	0.48
1:B:1007:ILE:O	1:B:1008:SER:CB	2.61	0.48
1:B:1082:SER:HB2	9:B:5304:ZXF:O1P	2.13	0.48
1:B:719:LEU:HD13	1:B:860:GLU:OE2	2.14	0.48
1:B:885:MET:HE2	1:B:894:ILE:HD11	1.94	0.48
6:A:5011:GOL:O3	1:B:1030:LEU:HD22	2.14	0.48
1:A:211:ILE:HG12	1:A:212:PHE:N	2.29	0.48
1:A:346:ALA:HB1	4:A:3005:FAD:H4'	1.96	0.48
1:A:1318:VAL:HG21	1:A:1322:PRO:CB	2.44	0.48
1:B:726:ALA:HB2	1:B:857:VAL:CG2	2.44	0.48
1:B:1321:ALA:HB1	1:B:1322:PRO:CD	2.38	0.48
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.78	0.48
1:B:952:LEU:HD23	1:B:958:ARG:HA	1.94	0.48
1:B:61:LEU:C	1:B:61:LEU:HD23	2.38	0.47
1:A:310:LYS:O	1:A:314:GLU:HG3	2.14	0.47
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:PHE:HE2	6:A:5006:GOL:H31	1.79	0.47
1:B:433:LYS:HG3	9:B:5852:HOH:O	2.14	0.47
1:B:948:LYS:HG2	1:B:951:ASP:CG	2.39	0.47
1:A:1215:PRO:HD2	1:A:1216:GLU:OE2	2.15	0.47
1:A:555:ALA:HB3	1:A:1238:GLU:HG3	1.95	0.47
1:B:544:SER:HB2	1:B:994:LYS:HD2	1.97	0.47
1:A:374:ILE:HD13	1:A:398:LEU:CD2	2.45	0.47
1:A:529:LYS:O	1:A:530:ASP:HB2	2.14	0.47
1:A:505:ILE:HD12	1:A:505:ILE:H	1.80	0.47
1:A:1318:VAL:CB	1:A:1322:PRO:HB3	2.44	0.47
1:B:325:GLU:HB2	1:B:412:SER:HB3	1.96	0.47
1:A:987:PHE:CD2	1:A:996:ARG:HG3	2.50	0.47
1:B:459:MET:HE2	1:B:512:THR:HG21	1.96	0.47
1:B:1318:VAL:O	1:B:1320:GLY:N	2.47	0.47
1:A:558:GLN:HB3	1:A:1192:ILE:HD13	1.96	0.46
1:A:570:GLU:CD	1:A:1057:PRO:HG3	2.40	0.46
1:A:926:TRP:O	1:A:930:VAL:HG23	2.14	0.46
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.80	0.46
1:A:794:MET:HE3	1:A:1038:MET:HB3	1.97	0.46
1:B:328:ARG:HH11	1:B:328:ARG:CG	2.20	0.46
1:B:736:ILE:HG23	1:B:736:ILE:O	2.16	0.46
1:A:1052:LYS:HD3	1:A:1254:TYR:CZ	2.51	0.46
1:B:994:LYS:HE3	6:B:5008:GOL:O2	2.15	0.46
1:B:217:LEU:O	1:B:220:LYS:HG2	2.15	0.46
1:A:1046:MET:HA	1:A:1046:MET:HE2	1.98	0.46
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.86	0.46
1:B:117:THR:HB	1:B:118:PRO:HD3	1.97	0.46
1:B:1203:LEU:HD11	9:B:5736:HOH:O	2.14	0.46
1:A:32:ARG:HH12	1:A:676:GLU:CD	2.24	0.46
1:B:13:LYS:HD3	1:B:13:LYS:C	2.41	0.46
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.16	0.46
1:A:37:ARG:HD3	1:A:595:ASP:O	2.16	0.46
1:A:648:LEU:HD11	1:A:803:THR:HG21	1.97	0.46
1:B:726:ALA:HB2	1:B:857:VAL:HG21	1.98	0.46
1:B:635:LEU:HD21	1:B:818:LYS:HG2	1.97	0.45
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.80	0.45
1:A:1216:GLU:H	1:A:1216:GLU:CD	2.23	0.45
1:B:37:ARG:HD3	6:B:5013:GOL:O3	2.15	0.45
1:B:124:MET:HE3	1:B:128:LEU:HG	1.99	0.45
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.79	0.45
1:A:602:GLU:HA	1:A:822:PRO:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:HE2	1:B:83:VAL:HG22	1.98	0.45
1:B:1221:THR:HG22	1:B:1226:THR:HB	1.98	0.45
1:A:193:PRO:HG2	1:A:560:PHE:CZ	2.52	0.45
1:B:389:PHE:O	1:B:391:PRO:HD3	2.16	0.45
1:A:964:VAL:HB	1:A:965:PRO:HD3	1.98	0.45
1:A:1126:SER:HB2	1:B:1132:PHE:CD1	2.52	0.45
1:A:164:ALA:O	1:A:165:LYS:CB	2.64	0.45
1:B:736:ILE:HG13	1:B:1298:SER:HB3	1.99	0.45
1:B:987:PHE:CD2	1:B:996:ARG:HG3	2.52	0.45
1:B:508:ARG:O	1:B:512:THR:HG23	2.17	0.45
1:A:506:GLU:CD	1:A:506:GLU:H	2.24	0.45
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.45
1:A:1153:PHE:HB2	1:A:1155:TYR:CZ	2.52	0.45
1:A:952:LEU:HD23	1:A:958:ARG:HA	2.00	0.44
1:B:605:LEU:C	1:B:605:LEU:HD23	2.42	0.44
1:A:407:ILE:HD12	1:A:407:ILE:N	2.31	0.44
1:A:604:PHE:CE2	6:A:5006:GOL:H31	2.52	0.44
1:A:683:HIS:HA	6:A:5019:GOL:H12	1.99	0.44
1:A:573:VAL:HG21	1:A:1052:LYS:HD2	2.00	0.44
1:B:644:ASN:O	1:B:653:THR:HA	2.18	0.44
1:B:1046:MET:HE2	1:B:1046:MET:HA	2.00	0.44
1:A:161:ARG:HH12	1:A:556:ASN:ND2	2.16	0.43
1:B:95:LYS:HG3	1:B:589:GLU:OE1	2.18	0.43
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.19	0.43
1:B:1088:GLN:HG2	1:B:1133:TYR:CE1	2.52	0.43
1:B:1088:GLN:HG3	9:B:5797:HOH:O	2.18	0.43
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.53	0.43
1:A:911:PHE:HD2	1:A:912:ARG:N	2.17	0.43
1:B:723:PHE:CE2	1:B:847:LYS:HE2	2.52	0.43
1:B:871:ARG:HG3	1:B:871:ARG:HH11	1.83	0.43
1:A:374:ILE:HG21	1:A:398:LEU:HD22	2.00	0.43
1:B:154:ARG:CD	1:B:1196:GLU:OE2	2.65	0.43
1:B:1264:LEU:C	1:B:1264:LEU:HD23	2.43	0.43
1:B:141:ASP:O	1:B:144:GLN:HG3	2.18	0.43
1:A:328:ARG:HG3	9:A:5888:HOH:O	2.17	0.43
1:A:487:CYS:HB3	1:A:513:LEU:HD13	2.00	0.43
1:A:651:ASP:OD1	1:A:871:ARG:NH1	2.52	0.43
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.19	0.43
1:A:1315:THR:O	1:A:1318:VAL:HG22	2.19	0.43
1:B:926:TRP:O	1:B:930:VAL:HG23	2.19	0.43
1:B:955:PHE:CA	1:B:1145:ASN:HD21	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:CD2	1:A:407:ILE:HD11	2.49	0.43
1:B:430:ASP:CG	1:B:1228:LYS:HE2	2.44	0.43
1:B:826:MET:H	6:B:5014:GOL:C3	2.30	0.43
1:A:1290:THR:O	1:A:1290:THR:HG22	2.19	0.43
1:B:82:HIS:NE2	1:B:219:LEU:HD13	2.33	0.43
1:B:1199:PHE:CE1	1:B:1267:GLY:HA2	2.53	0.43
1:B:992:CYS:SG	1:B:1285:HIS:NE2	2.92	0.43
1:A:131:GLN:O	1:A:134:PRO:HD3	2.19	0.42
1:B:699:GLU:CD	1:B:699:GLU:N	2.76	0.42
1:A:100:PRO:O	1:A:104:ARG:HG3	2.19	0.42
1:A:216:LEU:HD23	1:A:219:LEU:HD12	2.00	0.42
1:B:909:THR:OG1	1:B:910:ALA:N	2.51	0.42
1:A:87:THR:OG1	1:A:89:GLU:HG2	2.19	0.42
1:A:491:ALA:O	1:A:509:ARG:NH2	2.52	0.42
1:B:753:PRO:HD3	1:B:816:ALA:HB1	2.01	0.42
1:B:1108:ASN:N	1:B:1109:PRO:HD3	2.34	0.42
1:A:651:ASP:CG	1:A:871:ARG:NH1	2.76	0.42
1:A:275:PHE:HA	1:A:276:PRO:HD2	1.91	0.42
1:B:257:LEU:HA	1:B:279:ILE:O	2.18	0.42
1:A:519:PHE:O	1:A:523:VAL:HG23	2.20	0.42
1:A:699:GLU:CD	1:A:699:GLU:N	2.77	0.42
1:A:1183:GLY:HA2	1:A:1247:CYS:O	2.19	0.42
1:B:249:LYS:HG3	1:B:403:ILE:CG2	2.50	0.42
1:B:572:THR:HA	1:B:575:ARG:HD2	2.01	0.42
1:B:719:LEU:HD11	1:B:895:ARG:HB3	2.00	0.42
1:A:103:GLU:HG3	1:A:107:LYS:HE2	2.02	0.42
1:A:237:ILE:HD13	1:A:277:MET:HE3	2.01	0.42
1:A:651:ASP:OD2	1:A:871:ARG:HG3	2.19	0.42
1:B:572:THR:OG1	1:B:1048:GLN:HG2	2.19	0.42
1:B:1207:THR:C	1:B:1208:LEU:HD12	2.44	0.42
1:A:703:LYS:NZ	1:A:703:LYS:HB3	2.35	0.42
1:B:727:ASP:OD2	1:B:851:MET:HE3	2.20	0.42
1:A:46:GLY:HA2	3:A:3002:FES:S1	2.60	0.42
1:A:376:SER:HB3	1:A:402:GLU:HG2	2.02	0.42
1:A:885:MET:HE2	1:A:894:ILE:CD1	2.40	0.42
1:B:316:VAL:HA	1:B:324:THR:HG21	2.01	0.42
1:B:325:GLU:HB2	1:B:412:SER:CB	2.50	0.42
1:B:473:GLN:HA	1:B:473:GLN:NE2	2.35	0.42
1:B:271:LYS:NZ	6:B:5020:GOL:H32	2.35	0.41
1:A:312:LEU:HD12	1:A:312:LEU:HA	1.89	0.41
1:A:3:ALA:O	1:A:4:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.93	0.41
1:B:551:LYS:NZ	1:B:552:HIS:H	2.09	0.41
1:A:1216:GLU:CD	1:A:1216:GLU:N	2.78	0.41
1:A:1319:THR:HG23	1:A:1320:GLY:H	1.85	0.41
1:B:505:ILE:HD12	1:B:505:ILE:N	2.36	0.41
1:B:518:LYS:HZ3	6:B:5022:GOL:C3	2.32	0.41
1:B:1325:CYS:C	1:B:1326:LYS:HG2	2.45	0.41
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.01	0.41
1:A:1318:VAL:HG11	1:A:1322:PRO:HA	2.02	0.41
1:B:244:GLU:O	1:B:248:LEU:HG	2.19	0.41
1:B:1325:CYS:O	1:B:1326:LYS:CB	2.67	0.41
1:B:552:HIS:HB2	1:B:1237:THR:HG21	2.03	0.41
1:B:1287:ASN:O	1:B:1288:ASN:CB	2.67	0.41
1:B:657:LYS:O	1:B:658:ASP:HB2	2.21	0.41
1:B:899:ARG:HD2	1:B:899:ARG:HA	1.87	0.41
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.36	0.41
1:A:1088:GLN:HG3	9:A:5686:HOH:O	2.19	0.41
1:B:992:CYS:HA	1:B:1284:GLN:HE21	1.86	0.41
1:B:1289:ASN:O	1:B:1290:THR:CB	2.69	0.41
1:A:433:LYS:HD3	1:A:433:LYS:HA	1.81	0.40
1:B:58:TYR:CZ	1:B:220:LYS:HD2	2.56	0.40
1:B:328:ARG:CG	1:B:328:ARG:NH1	2.79	0.40
1:B:1325:CYS:O	1:B:1326:LYS:HB3	2.20	0.40
1:A:284:ILE:HA	1:A:285:PRO:HD2	1.91	0.40
1:B:712:LEU:HD21	1:B:875:HIS:CE1	2.56	0.40
1:A:527:LEU:C	1:A:529:LYS:N	2.80	0.40
1:A:1013:PHE:CD1	1:A:1013:PHE:C	2.99	0.40
1:A:1212:HIS:H	1:A:1221:THR:CG2	2.34	0.40
1:A:3:ALA:HA	1:A:227:LEU:HD23	2.04	0.40
1:A:490:LEU:HB2	1:A:513:LEU:CD2	2.52	0.40
1:A:539:ASP:H	6:A:5002:GOL:C3	2.35	0.40
1:A:551:LYS:HE3	9:A:6123:HOH:O	2.21	0.40
1:A:556:ASN:O	1:A:557:ILE:HD13	2.21	0.40
1:A:655:PHE:CE1	1:A:814:LEU:HD23	2.57	0.40
1:A:131:GLN:HA	1:A:132:PRO:HD2	1.95	0.40
1:A:263:GLU:HB2	4:A:3005:FAD:H52A	2.02	0.40
1:B:254:GLU:H	1:B:254:GLU:CD	2.28	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	1293/1332 (97%)	1244 (96%)	41 (3%)	8 (1%)	21	12
1	B	1290/1332 (97%)	1234 (96%)	44 (3%)	12 (1%)	14	6
All	All	2583/2664 (97%)	2478 (96%)	85 (3%)	20 (1%)	16	7

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	1008	SER
1	B	1008	SER
1	B	1287	ASN
1	B	1324	ASN
1	B	1326	LYS
1	A	1319	THR
1	B	244	GLU
1	B	1325	CYS
1	A	912	ARG
1	A	1322	PRO
1	B	912	ARG
1	B	1139	GLY
1	B	1319	THR
1	A	797	GLY
1	A	1318	VAL
1	B	797	GLY
1	B	1322	PRO
1	B	1323	GLY
1	A	1139	GLY

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1101/1128 (98%)	1086 (99%)	15 (1%)	59	54
1	B	1098/1128 (97%)	1088 (99%)	10 (1%)	70	67
All	All	2199/2256 (98%)	2174 (99%)	25 (1%)	65	61

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	154	ARG
1	A	281	PRO
1	A	312	LEU
1	A	328	ARG
1	A	439	ARG
1	A	513	LEU
1	A	550	GLN
1	A	569	LYS
1	A	618	LYS
1	A	743	TYR
1	A	1002	PRO
1	A	1208	LEU
1	A	1216	GLU
1	A	1332	VAL
1	B	89	GLU
1	B	100	PRO
1	B	154	ARG
1	B	165	LYS
1	B	328	ARG
1	B	513	LEU
1	B	551	LYS
1	B	600	GLU
1	B	743	TYR
1	B	1002	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN

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Mol	Chain	Res	Type
1	A	131	GLN
1	A	226	GLN
1	A	252	HIS
1	A	272	ASN
1	A	333	GLN
1	A	448	GLN
1	A	473	GLN
1	A	556	ASN
1	A	565	ASN
1	A	626	GLN
1	A	1145	ASN
1	A	1212	HIS
1	A	1220	HIS
1	A	1284	GLN
1	A	1289	ASN
1	A	1324	ASN
1	B	71	ASN
1	B	131	GLN
1	B	146	ASN
1	B	252	HIS
1	B	351	ASN
1	B	448	GLN
1	B	471	GLN
1	B	473	GLN
1	B	484	GLN
1	B	556	ASN
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	683	HIS
1	B	705	ASN
1	B	869	ASN
1	B	875	HIS
1	B	976	GLN
1	B	1145	ASN
1	B	1212	HIS
1	B	1220	HIS
1	B	1284	GLN

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 37 ligands modelled in this entry, 4 are monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	FES	B	4002	1	0,4,4	-	-	-		
5	YSH	A	5101	-	23,23,23	7.30	13 (56%)	33,33,33	4.20	12 (36%)
6	GOL	A	5019	-	5,5,5	0.33	0	5,5,5	0.32	0
5	YSH	B	5102	-	23,23,23	7.44	15 (65%)	33,33,33	4.14	11 (33%)
6	GOL	B	5012	-	5,5,5	0.23	0	5,5,5	0.45	0
6	GOL	A	5005	-	5,5,5	0.31	0	5,5,5	0.36	0
6	GOL	A	5016	-	5,5,5	0.28	0	5,5,5	0.51	0
6	GOL	B	5022	-	5,5,5	0.23	0	5,5,5	0.39	0
7	ACY	B	5202	-	3,3,3	1.19	0	3,3,3	1.70	1 (33%)
6	GOL	A	5002	-	5,5,5	0.23	0	5,5,5	0.39	0
3	FES	B	4001	1	0,4,4	-	-	-		
4	FAD	B	4005	-	58,58,58	2.37	24 (41%)	85,89,89	2.07	31 (36%)
7	ACY	A	5201	-	3,3,3	1.09	0	3,3,3	1.76	1 (33%)
3	FES	A	3002	1	0,4,4	-	-	-		
6	GOL	B	5015	-	5,5,5	0.26	0	5,5,5	0.33	0
6	GOL	B	5009	-	5,5,5	0.32	0	5,5,5	0.32	0
4	FAD	A	3005	-	58,58,58	2.27	19 (32%)	85,89,89	2.09	29 (34%)
9	ZXF	B	5304	-	24,31,31	5.87	12 (50%)	22,52,52	4.58	13 (59%)
6	GOL	B	5013	-	5,5,5	0.23	0	5,5,5	0.32	0
6	GOL	B	5007	-	5,5,5	0.29	0	5,5,5	0.34	0
6	GOL	A	5003	-	5,5,5	0.32	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	B	5014	-	5,5,5	0.22	0	5,5,5	0.40	0
9	ZXF	A	5305	-	24,31,31	6.18	13 (54%)	22,52,52	4.53	13 (59%)
6	GOL	A	5017	-	5,5,5	0.28	0	5,5,5	0.34	0
6	GOL	A	5018	-	5,5,5	0.35	0	5,5,5	0.29	0
6	GOL	B	5021	-	5,5,5	0.28	0	5,5,5	0.42	0
6	GOL	A	5004	-	5,5,5	0.29	0	5,5,5	0.35	0
6	GOL	A	5006	-	5,5,5	0.25	0	5,5,5	0.44	0
6	GOL	A	5001	-	5,5,5	0.32	0	5,5,5	0.42	0
6	GOL	B	5008	-	5,5,5	0.27	0	5,5,5	0.42	0
6	GOL	B	5020	-	5,5,5	0.26	0	5,5,5	0.36	0
6	GOL	A	5011	-	5,5,5	0.21	0	5,5,5	0.40	0
3	FES	A	3001	1	0,4,4	-	-	-	-	-

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
5	YSH	A	5101	-	-	0/16/16/16	0/2/2/2
6	GOL	A	5019	-	-	0/4/4/4	-
3	FES	B	4002	1	-	-	0/1/1/1
5	YSH	B	5102	-	-	2/16/16/16	0/2/2/2
6	GOL	B	5012	-	-	0/4/4/4	-
6	GOL	A	5005	-	-	0/4/4/4	-
6	GOL	A	5016	-	-	0/4/4/4	-
6	GOL	B	5022	-	-	0/4/4/4	-
6	GOL	A	5002	-	-	0/4/4/4	-
3	FES	B	4001	1	-	-	0/1/1/1
4	FAD	B	4005	-	-	2/34/50/50	0/6/6/6
3	FES	A	3002	1	-	-	0/1/1/1
6	GOL	B	5015	-	-	0/4/4/4	-
6	GOL	B	5009	-	-	0/4/4/4	-
4	FAD	A	3005	-	-	4/34/50/50	0/6/6/6
9	ZXF	B	5304	-	-	6/6/46/46	0/4/4/4
6	GOL	B	5013	-	-	0/4/4/4	-
6	GOL	B	5007	-	-	0/4/4/4	-
6	GOL	A	5003	-	-	0/4/4/4	-
6	GOL	B	5014	-	-	0/4/4/4	-
9	ZXF	A	5305	-	-	4/6/46/46	0/4/4/4
6	GOL	A	5017	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	5018	-	-	0/4/4/4	-
6	GOL	B	5021	-	-	0/4/4/4	-
6	GOL	A	5004	-	-	0/4/4/4	-
6	GOL	A	5006	-	-	0/4/4/4	-
6	GOL	A	5001	-	-	0/4/4/4	-
6	GOL	B	5008	-	-	0/4/4/4	-
6	GOL	B	5020	-	-	0/4/4/4	-
6	GOL	A	5011	-	-	0/4/4/4	-
3	FES	A	3001	1	-	-	0/1/1/1

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5102	YSH	C1-C5	21.19	1.71	1.38
5	A	5101	YSH	C1-C5	20.87	1.71	1.38
5	B	5102	YSH	C1-N2	19.56	1.70	1.35
9	A	5305	ZXF	C7-C6	19.00	1.68	1.53
5	A	5101	YSH	C1-N2	18.95	1.68	1.35
9	B	5304	ZXF	C7-C6	18.55	1.68	1.53
9	A	5305	ZXF	C9-C10	13.62	1.61	1.38
9	B	5304	ZXF	C9-C10	13.60	1.61	1.38
5	B	5102	YSH	C11-C6	12.30	1.62	1.39
5	A	5101	YSH	C11-C6	12.22	1.62	1.39
9	A	5305	ZXF	C9-N5	10.30	1.62	1.37
9	B	5304	ZXF	C9-N5	10.14	1.61	1.37
9	A	5305	ZXF	C6-N5	-9.25	1.36	1.46
5	B	5102	YSH	C10-C9	8.86	1.57	1.39
5	A	5101	YSH	C10-C9	8.63	1.57	1.39
9	B	5304	ZXF	P-O4'	-7.09	1.37	1.60
5	A	5101	YSH	O22-C20	6.96	1.39	1.22
9	A	5305	ZXF	P-O4'	-6.93	1.38	1.60
5	B	5102	YSH	O22-C20	6.85	1.39	1.22
5	B	5102	YSH	C6-N2	6.47	1.55	1.43
5	A	5101	YSH	C8-C12	6.19	1.53	1.44
5	A	5101	YSH	C6-N2	6.01	1.54	1.43
5	B	5102	YSH	C8-C12	6.00	1.53	1.44
4	A	3005	FAD	C10-N1	5.94	1.45	1.33
4	B	4005	FAD	C10-N1	5.67	1.44	1.33
9	B	5304	ZXF	P-O1P	-5.23	1.35	1.54
9	A	5305	ZXF	P-O1P	-5.17	1.35	1.54
9	B	5304	ZXF	C6-N5	-4.92	1.40	1.46
4	B	4005	FAD	C9A-C5X	4.91	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5102	YSH	C4-N3	4.79	1.40	1.32
4	B	4005	FAD	C10-N10	4.74	1.47	1.37
5	A	5101	YSH	C4-N3	4.66	1.39	1.32
5	B	5102	YSH	O14-C9	4.63	1.46	1.37
4	B	4005	FAD	C9-C9A	4.43	1.46	1.39
4	B	4005	FAD	C4X-N5	4.42	1.40	1.30
4	A	3005	FAD	C9A-C5X	4.35	1.48	1.41
4	A	3005	FAD	C10-N10	4.35	1.46	1.37
4	B	4005	FAD	C1'-C2'	4.35	1.58	1.52
4	B	4005	FAD	C6-C7	4.35	1.45	1.39
4	A	3005	FAD	C9-C9A	4.31	1.46	1.39
9	B	5304	ZXF	C10-N8	4.29	1.40	1.35
9	B	5304	ZXF	C4'-C3'	-4.29	1.45	1.51
9	A	5305	ZXF	C10-N8	4.27	1.40	1.35
4	A	3005	FAD	C4X-N5	4.26	1.39	1.30
5	A	5101	YSH	O14-C9	4.20	1.45	1.37
9	A	5305	ZXF	C4'-C3'	-4.13	1.46	1.51
9	A	5305	ZXF	O4-C4	4.13	1.31	1.23
4	A	3005	FAD	C9A-N10	4.10	1.48	1.41
4	B	4005	FAD	C9A-N10	4.09	1.48	1.41
4	A	3005	FAD	C6-C7	4.06	1.45	1.39
4	A	3005	FAD	C1'-C2'	3.94	1.58	1.52
9	B	5304	ZXF	O4-C4	3.72	1.30	1.23
4	B	4005	FAD	C6-C5X	3.63	1.45	1.40
9	B	5304	ZXF	MO-S1'	3.63	2.44	2.39
4	A	3005	FAD	C6-C5X	3.62	1.45	1.40
4	B	4005	FAD	C4A-N3A	3.62	1.41	1.34
9	A	5305	ZXF	MO-S1'	3.57	2.44	2.39
4	A	3005	FAD	C4A-N3A	3.44	1.40	1.34
5	A	5101	YSH	C11-C10	-3.31	1.33	1.38
9	A	5305	ZXF	O4'-C4'	-3.30	1.32	1.44
4	B	4005	FAD	C4-N3	3.17	1.44	1.38
4	B	4005	FAD	C5A-N7A	-3.11	1.33	1.39
4	A	3005	FAD	C5A-N7A	-3.11	1.33	1.39
4	B	4005	FAD	C8-C7	3.10	1.48	1.40
4	A	3005	FAD	C8-C7	3.07	1.48	1.40
4	A	3005	FAD	C4-N3	3.05	1.44	1.38
9	A	5305	ZXF	C2-N1	3.02	1.40	1.33
4	A	3005	FAD	C2A-N1A	2.94	1.39	1.33
5	B	5102	YSH	O21-C20	-2.93	1.22	1.30
5	A	5101	YSH	O21-C20	-2.91	1.22	1.30
4	B	4005	FAD	C4'-C3'	2.85	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5102	YSH	O14-C15	2.84	1.53	1.43
4	B	4005	FAD	C5'-C4'	2.78	1.55	1.51
5	A	5101	YSH	O14-C15	2.77	1.53	1.43
4	B	4005	FAD	C2A-N1A	2.76	1.38	1.33
9	B	5304	ZXF	C2-N1	2.70	1.39	1.33
4	B	4005	FAD	C2'-C3'	2.63	1.58	1.53
5	B	5102	YSH	C11-C10	-2.51	1.34	1.38
4	A	3005	FAD	C4'-C3'	2.48	1.57	1.53
4	B	4005	FAD	P-O1P	2.38	1.59	1.50
4	B	4005	FAD	C9-C8	2.36	1.42	1.39
4	A	3005	FAD	PA-O1A	2.36	1.59	1.50
4	A	3005	FAD	C5A-C4A	2.34	1.43	1.39
4	A	3005	FAD	P-O1P	2.31	1.58	1.50
4	B	4005	FAD	PA-O1A	2.29	1.58	1.50
5	B	5102	YSH	N2-N3	-2.24	1.33	1.36
5	B	5102	YSH	C4-C5	-2.23	1.36	1.41
4	B	4005	FAD	C5A-C4A	2.23	1.43	1.39
5	A	5101	YSH	C4-C5	-2.21	1.36	1.41
4	A	3005	FAD	C5'-C4'	2.20	1.54	1.51
9	A	5305	ZXF	P-O2P	-2.20	1.46	1.54
4	B	4005	FAD	C8M-C8	2.19	1.55	1.51
9	B	5304	ZXF	P-O2P	-2.18	1.46	1.54
4	B	4005	FAD	C1'-N10	2.18	1.53	1.47
5	B	5102	YSH	C8-C9	2.06	1.44	1.40
4	B	4005	FAD	C2A-N3A	2.01	1.37	1.33

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5101	YSH	C5-C1-N2	-14.03	90.97	107.09
5	B	5102	YSH	C5-C1-N2	-13.97	91.05	107.09
9	B	5304	ZXF	C2'-C1'-S1'	13.58	127.86	120.15
9	A	5305	ZXF	C2'-C1'-S1'	13.21	127.65	120.15
5	B	5102	YSH	C4-N3-N2	12.88	114.44	104.19
5	A	5101	YSH	C4-N3-N2	12.44	114.09	104.19
5	A	5101	YSH	C1-C5-C4	9.21	112.35	104.22
9	B	5304	ZXF	C1'-C2'-S2'	-8.97	115.06	120.15
5	B	5102	YSH	C1-C5-C4	8.74	111.94	104.22
9	A	5305	ZXF	C1'-C2'-S2'	-8.69	115.22	120.15
9	B	5304	ZXF	C2-N1-C10	8.06	127.58	113.36
9	A	5305	ZXF	C2-N1-C10	7.85	127.21	113.36
4	A	3005	FAD	N3A-C2A-N1A	-7.21	117.67	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4005	FAD	N3A-C2A-N1A	-7.12	117.81	128.58
5	A	5101	YSH	C6-N2-C1	-6.90	119.15	129.12
5	B	5102	YSH	C6-N2-C1	-6.28	120.04	129.12
9	B	5304	ZXF	O4-C4-C9	-5.41	114.21	127.26
9	A	5305	ZXF	O4-C4-C9	-5.32	114.43	127.26
9	A	5305	ZXF	C4-C9-N5	5.12	130.22	116.27
9	B	5304	ZXF	C4-C9-N5	5.01	129.94	116.27
4	A	3005	FAD	C2B-C1B-N9A	4.75	125.10	113.30
4	B	4005	FAD	C2B-C1B-N9A	4.64	124.83	113.30
5	A	5101	YSH	C6-N2-N3	4.48	128.73	121.08
4	B	4005	FAD	O4'-C4'-C3'	4.17	119.01	109.25
4	A	3005	FAD	C2A-N3A-C4A	4.16	121.99	111.83
4	B	4005	FAD	C5A-C4A-N3A	-4.16	120.99	126.72
5	B	5102	YSH	C6-N2-N3	4.14	128.15	121.08
4	B	4005	FAD	C2A-N3A-C4A	4.12	121.89	111.83
4	A	3005	FAD	C5A-C4A-N3A	-4.10	121.07	126.72
4	A	3005	FAD	C5X-N5-C4X	4.09	124.71	118.09
4	A	3005	FAD	O4'-C4'-C3'	4.08	118.79	109.25
4	B	4005	FAD	C5X-N5-C4X	4.04	124.62	118.09
9	A	5305	ZXF	O3'-C7-N8	-3.77	105.19	108.61
5	A	5101	YSH	C1-C5-C20	-3.54	121.00	126.14
4	A	3005	FAD	C9A-C5X-N5	-3.53	118.70	122.45
9	B	5304	ZXF	N2-C2-N3	3.52	124.19	116.76
9	B	5304	ZXF	O3'-C7-C6	-3.48	106.64	108.96
5	A	5101	YSH	C10-C11-C6	-3.48	115.90	120.30
9	A	5305	ZXF	C7-C6-N5	3.44	111.25	107.87
4	B	4005	FAD	C9A-C5X-N5	-3.44	118.80	122.45
9	A	5305	ZXF	N2-C2-N3	3.41	123.96	116.76
4	A	3005	FAD	C5'-C4'-C3'	-3.40	105.80	112.22
5	B	5102	YSH	C10-C11-C6	-3.37	116.03	120.30
9	A	5305	ZXF	O3'-C7-C6	-3.36	106.73	108.96
9	B	5304	ZXF	C7-C6-N5	3.27	111.08	107.87
9	B	5304	ZXF	C9-C4-N3	3.23	120.99	112.13
5	A	5101	YSH	O22-C20-C5	-3.22	114.01	121.92
4	B	4005	FAD	C5'-C4'-C3'	-3.22	106.15	112.22
4	B	4005	FAD	C1'-N10-C9A	3.18	126.81	120.63
9	A	5305	ZXF	C9-C4-N3	3.16	120.81	112.13
4	A	3005	FAD	C1'-N10-C9A	3.14	126.73	120.63
4	B	4005	FAD	N3A-C4A-N9A	3.11	132.46	127.17
4	A	3005	FAD	N3A-C4A-N9A	3.11	132.46	127.17
5	B	5102	YSH	O22-C20-C5	-3.08	114.36	121.92
5	B	5102	YSH	C1-C5-C20	-3.05	121.70	126.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4005	FAD	C4-C4X-N5	3.02	122.38	118.21
4	A	3005	FAD	O3'-C3'-C4'	2.94	115.62	108.93
4	A	3005	FAD	C4-C4X-N5	2.92	122.24	118.21
4	A	3005	FAD	C4X-C4-N3	2.82	120.44	113.25
4	B	4005	FAD	C4X-C4-N3	2.79	120.35	113.25
9	B	5304	ZXF	O3'-C7-N8	-2.77	106.10	108.61
4	A	3005	FAD	C8M-C8-C9	-2.76	114.71	119.57
5	A	5101	YSH	O21-C20-C5	2.71	120.89	113.72
4	B	4005	FAD	C8M-C8-C9	-2.70	114.81	119.57
5	B	5102	YSH	O21-C20-C5	2.70	120.89	113.72
4	B	4005	FAD	C10-C4X-N5	-2.69	119.32	124.81
4	A	3005	FAD	C3B-C2B-C1B	2.65	106.47	101.46
4	A	3005	FAD	C10-C4X-N5	-2.63	119.45	124.81
4	B	4005	FAD	O3'-C3'-C4'	2.60	114.83	108.93
4	B	4005	FAD	C2A-N1A-C6A	2.54	122.90	118.73
4	A	3005	FAD	C2A-N1A-C6A	2.54	122.90	118.73
4	B	4005	FAD	C4-N3-C2	-2.54	121.14	125.64
4	A	3005	FAD	O3B-C3B-C4B	-2.53	103.80	111.08
4	B	4005	FAD	O3B-C3B-C4B	-2.53	103.81	111.08
4	B	4005	FAD	C3B-C2B-C1B	2.53	106.25	101.46
4	B	4005	FAD	C4A-C5A-N7A	-2.53	107.69	110.58
9	B	5304	ZXF	O4-C4-N3	2.50	124.81	120.11
4	A	3005	FAD	C4-N3-C2	-2.48	121.24	125.64
9	A	5305	ZXF	O4-C4-N3	2.47	124.76	120.11
4	B	4005	FAD	O2B-C2B-C3B	2.47	119.74	111.82
4	A	3005	FAD	C8M-C8-C7	2.45	125.77	120.76
4	A	3005	FAD	C5A-N7A-C8A	2.44	107.29	103.45
4	B	4005	FAD	C5A-N7A-C8A	2.42	107.25	103.45
4	A	3005	FAD	O5B-PA-O1A	2.41	118.47	108.94
4	A	3005	FAD	C7M-C7-C6	-2.40	115.34	119.57
7	A	5201	ACY	O-C-CH3	-2.40	112.69	122.53
4	A	3005	FAD	C4A-C5A-N7A	-2.38	107.86	110.58
5	A	5101	YSH	C11-C6-C7	2.35	123.78	119.12
4	A	3005	FAD	O4B-C1B-N9A	-2.34	103.59	108.09
4	B	4005	FAD	C8M-C8-C7	2.33	125.52	120.76
4	A	3005	FAD	O2B-C2B-C3B	2.32	119.27	111.82
4	B	4005	FAD	C10-N1-C2	2.31	121.85	116.85
7	B	5202	ACY	O-C-CH3	-2.30	113.10	122.53
9	B	5304	ZXF	O2P-P-O4'	2.30	112.66	106.67
4	B	4005	FAD	C7M-C7-C6	-2.27	115.58	119.57
9	A	5305	ZXF	O3'-C3'-C2'	2.25	112.27	109.09
4	B	4005	FAD	O5B-PA-O1A	2.24	117.83	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5101	YSH	C6-C7-C8	-2.20	118.60	120.94
5	B	5102	YSH	C11-C6-C7	2.19	123.48	119.12
5	B	5102	YSH	C7-C6-N2	-2.19	115.94	119.28
4	A	3005	FAD	O5'-P-O1P	2.15	117.45	108.94
4	A	3005	FAD	C10-N1-C2	2.13	121.45	116.85
4	A	3005	FAD	O2'-C2'-C3'	2.12	114.21	109.25
9	B	5304	ZXF	N3-C2-N1	-2.10	119.48	123.32
9	A	5305	ZXF	N3-C2-N1	-2.09	119.50	123.32
4	B	4005	FAD	O5'-P-O1P	2.07	117.13	108.94
4	B	4005	FAD	C6A-C5A-N7A	2.05	136.05	132.09
5	A	5101	YSH	C5-C4-N3	-2.04	110.47	112.09
4	B	4005	FAD	O2'-C2'-C3'	2.03	114.00	109.25
4	B	4005	FAD	C4X-C10-N1	-2.02	119.64	124.59
4	B	4005	FAD	C4X-C10-N10	2.01	119.36	116.48

There are no chirality outliers.

All (18) 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'
5	B	5102	YSH	N13-C12-C8-C9
9	A	5305	ZXF	C4'-O4'-P-O2P
9	A	5305	ZXF	C4'-O4'-P-O1P
9	B	5304	ZXF	C2'-C3'-C4'-O4'
9	B	5304	ZXF	O3'-C3'-C4'-O4'
9	B	5304	ZXF	C3'-C4'-O4'-P
9	B	5304	ZXF	C4'-O4'-P-O2P
9	B	5304	ZXF	C4'-O4'-P-O1P
9	A	5305	ZXF	C4'-O4'-P-O3P
9	B	5304	ZXF	C4'-O4'-P-O3P
9	A	5305	ZXF	C3'-C4'-O4'-P
4	A	3005	FAD	C2'-C3'-C4'-O4'
5	B	5102	YSH	C16-C15-O14-C9
4	A	3005	FAD	O3'-C3'-C4'-O4'

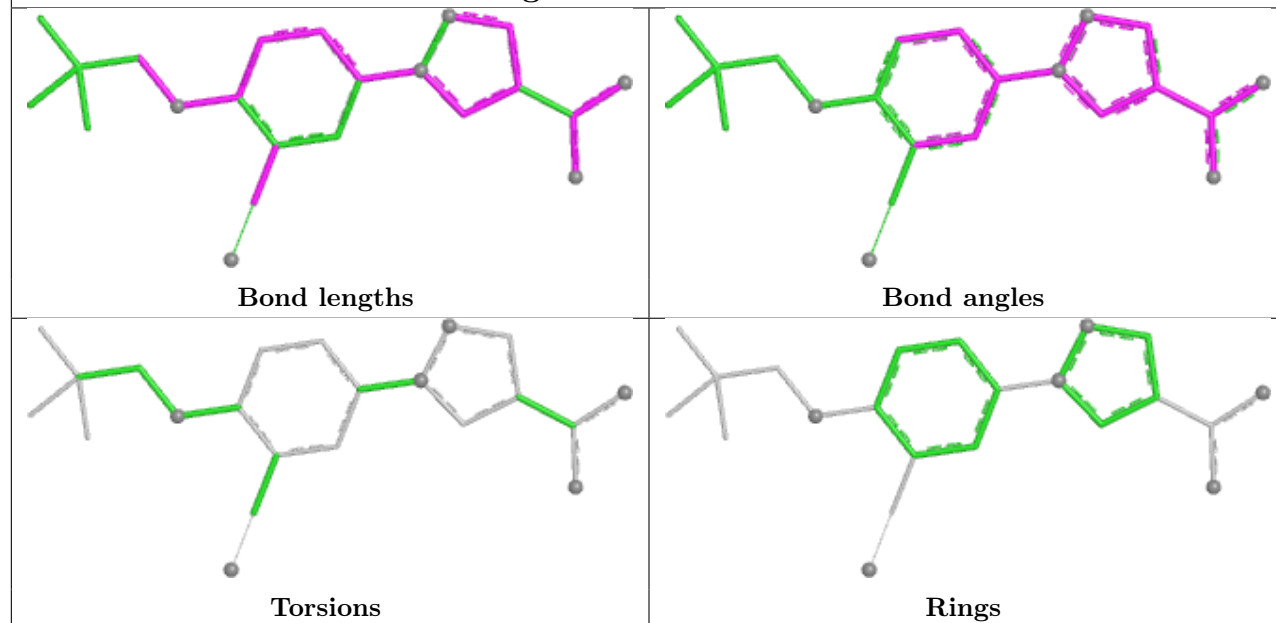
There are no ring outliers.

19 monomers are involved in 41 short contacts:

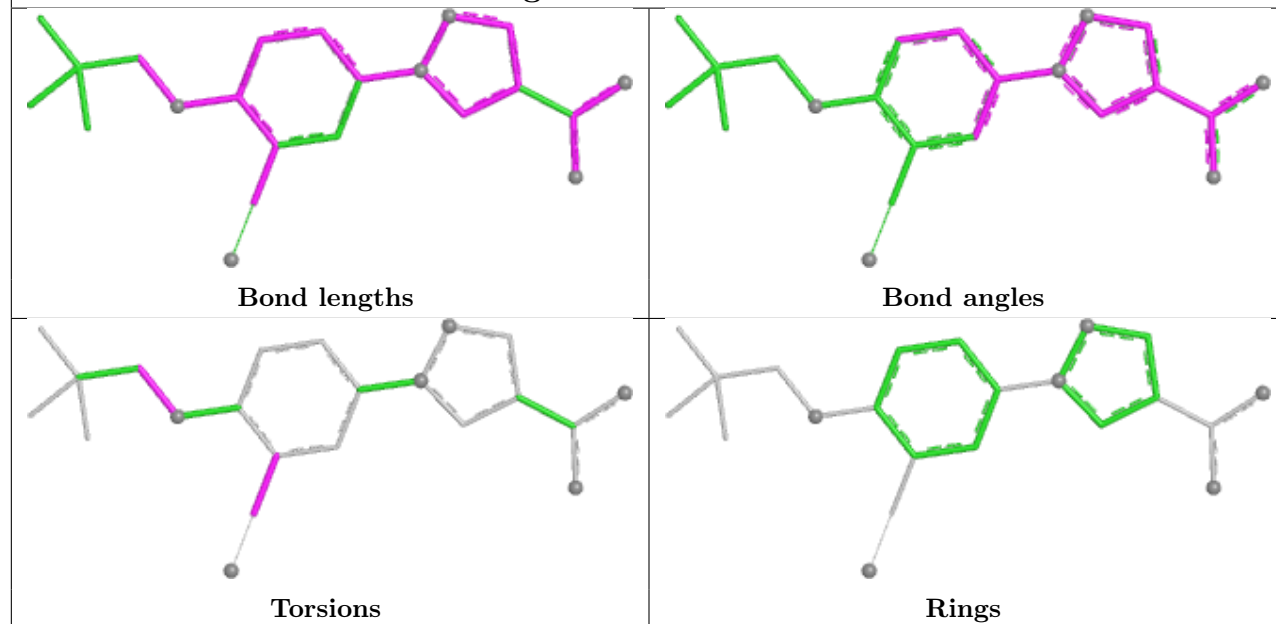
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5101	YSH	3	0
6	A	5019	GOL	1	0
5	B	5102	YSH	3	0
6	B	5022	GOL	2	0
7	B	5202	ACY	4	0
6	A	5002	GOL	2	0
4	B	4005	FAD	2	0
7	A	5201	ACY	4	0
3	A	3002	FES	1	0
4	A	3005	FAD	3	0
9	B	5304	ZXF	3	0
6	B	5013	GOL	1	0
6	B	5014	GOL	2	0
9	A	5305	ZXF	2	0
6	A	5006	GOL	2	0
6	A	5001	GOL	1	0
6	B	5008	GOL	2	0
6	B	5020	GOL	1	0
6	A	5011	GOL	2	0

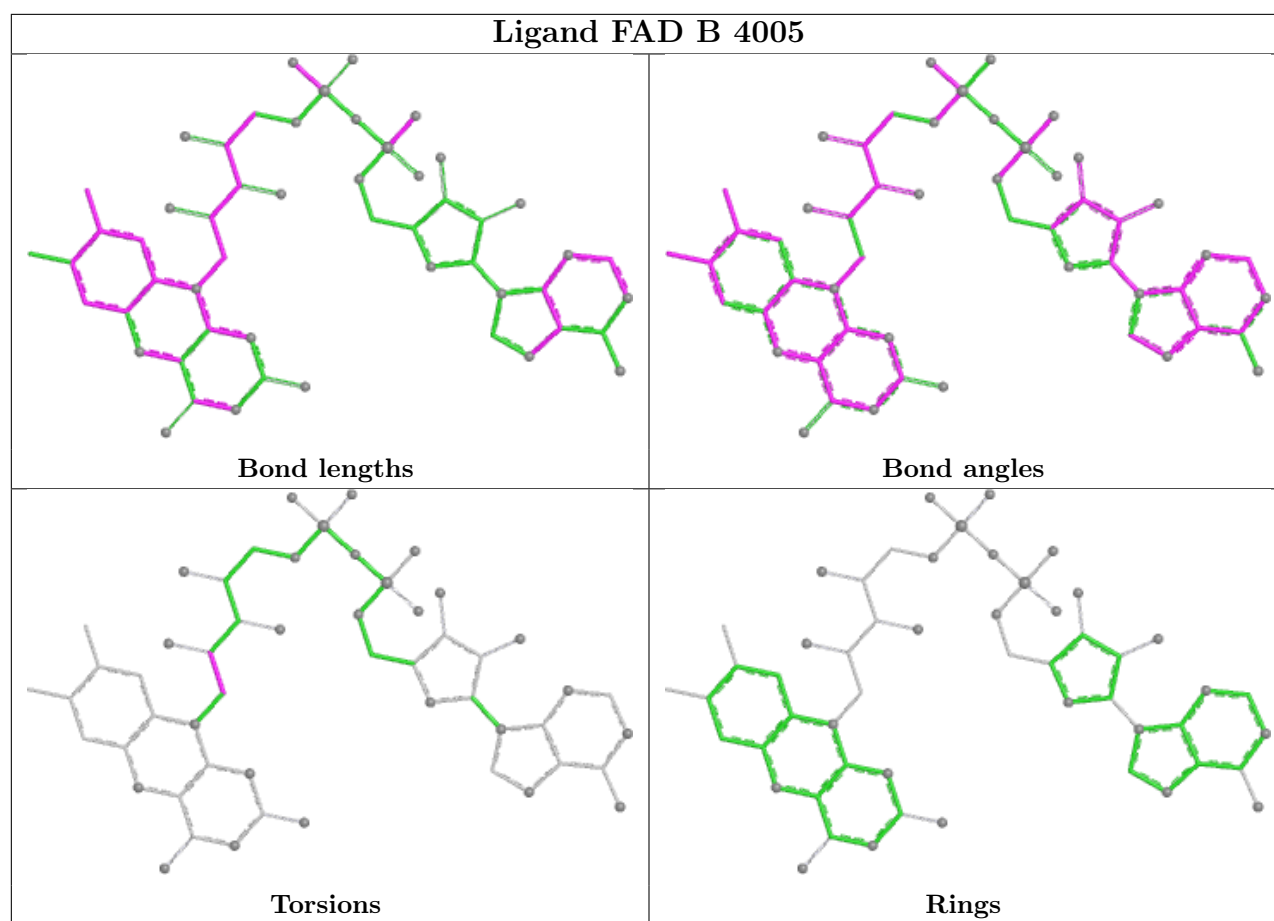
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

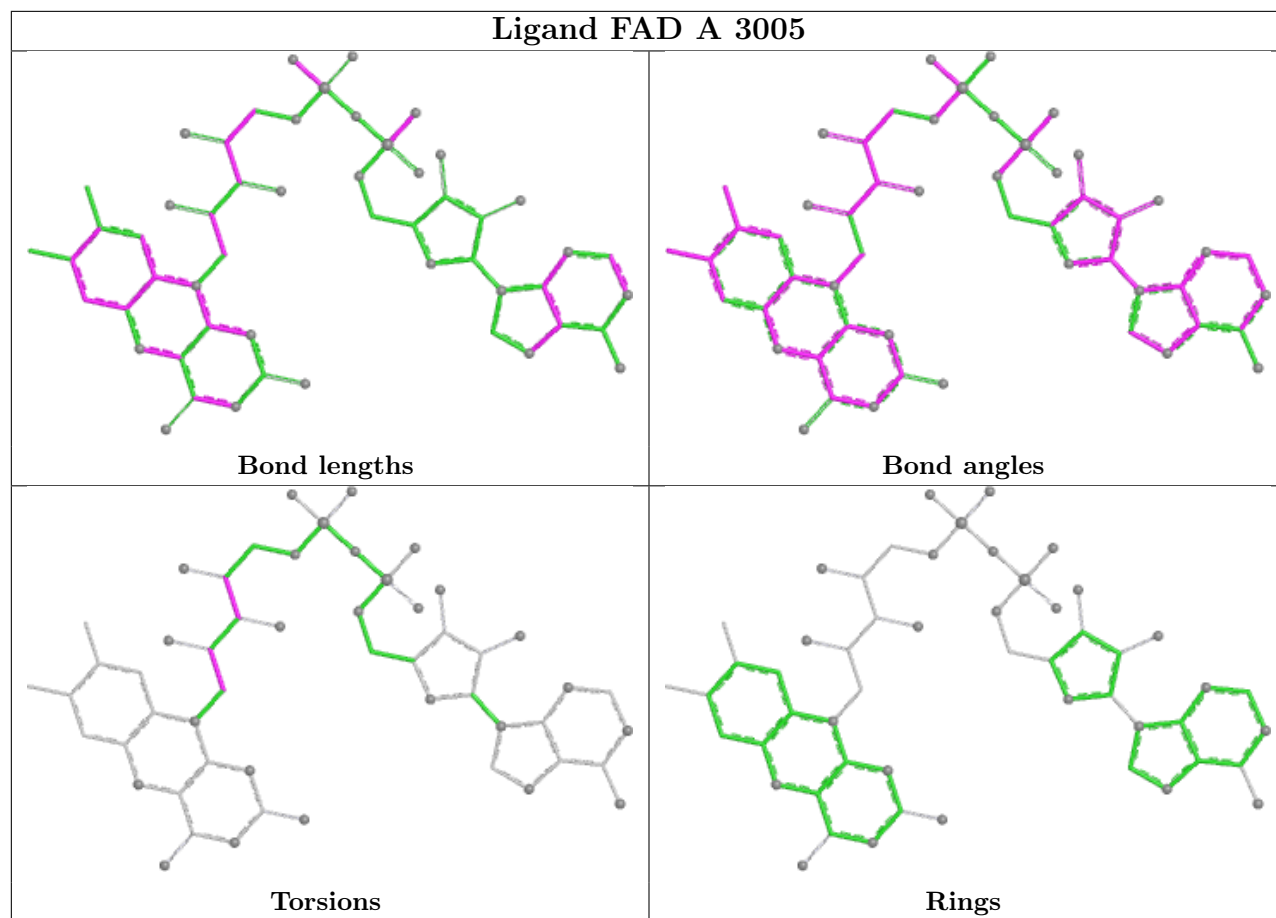
Ligand YSH A 5101

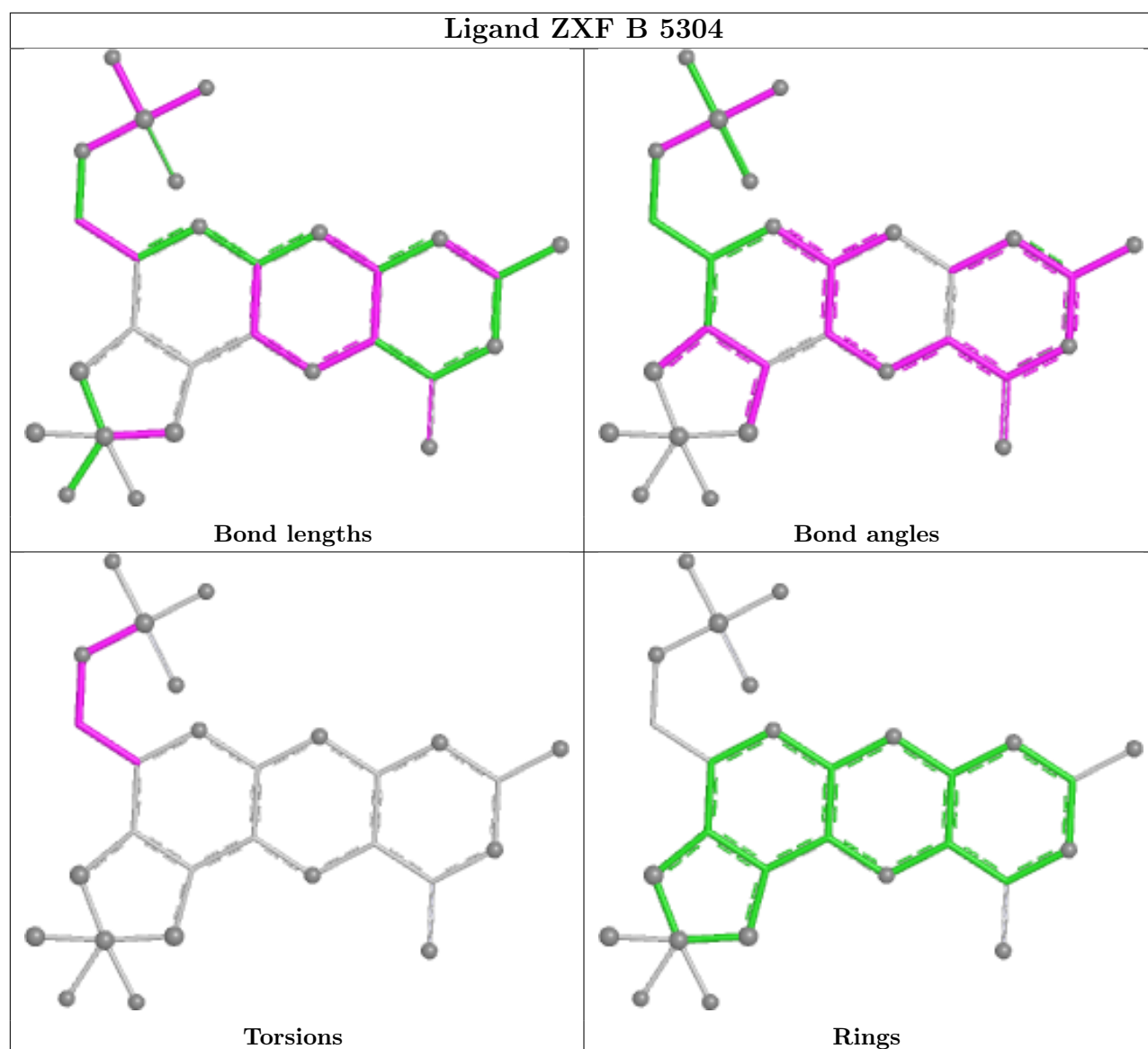


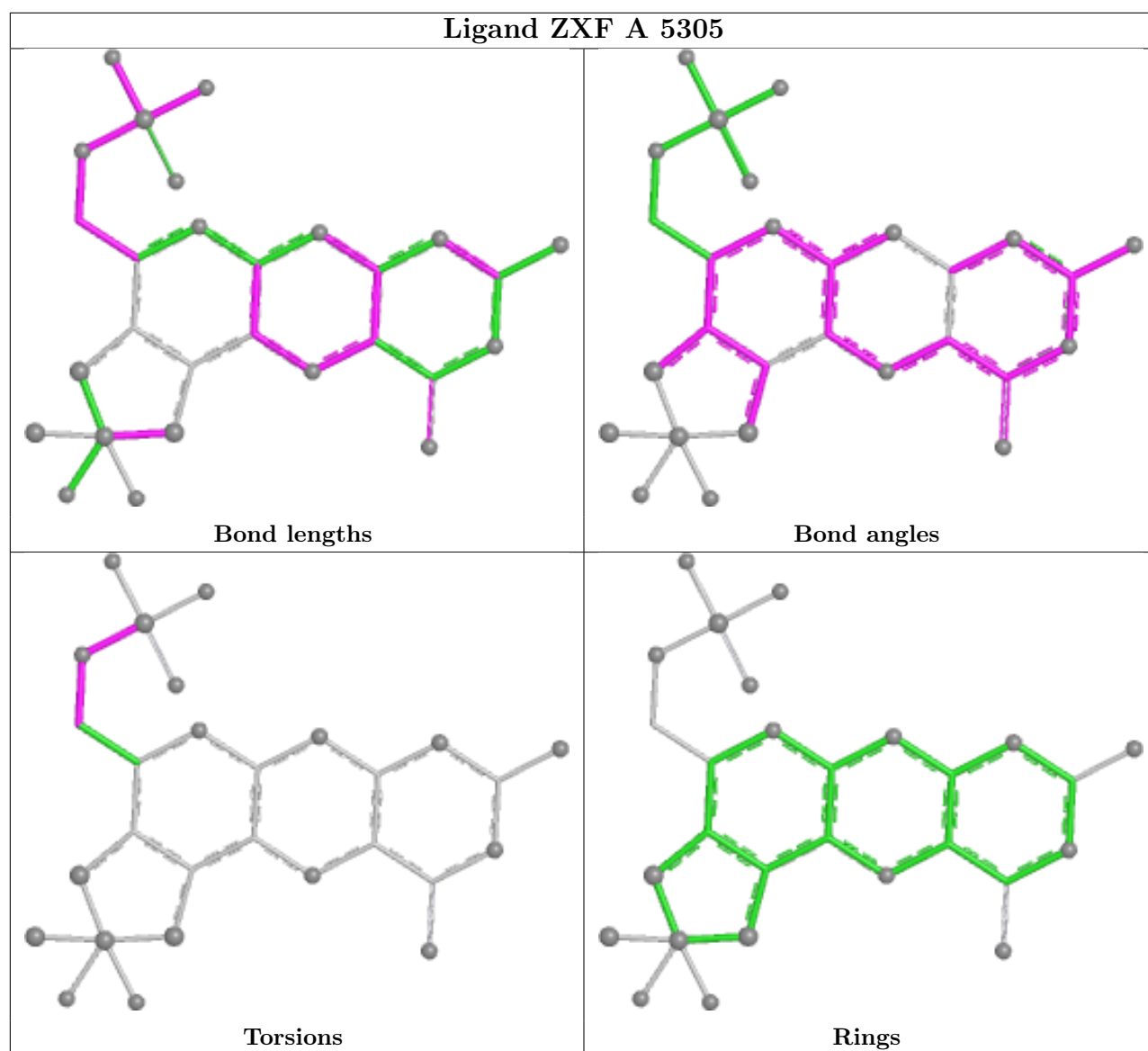
Ligand YSH B 5102











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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.