



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:54 AM EDT

PDB ID : 1FO4 / pdb_00001fo4
Title : CRYSTAL STRUCTURE OF XANTHINE DEHYDROGENASE ISOLATED FROM BOVINE MILK
Authors : Enroth, C.; Eger, B.T.; Okamoto, K.; Nishino, T.; Nishino, T.; Pai, E.F.
Deposited on : 2000-08-24
Resolution : 2.10 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

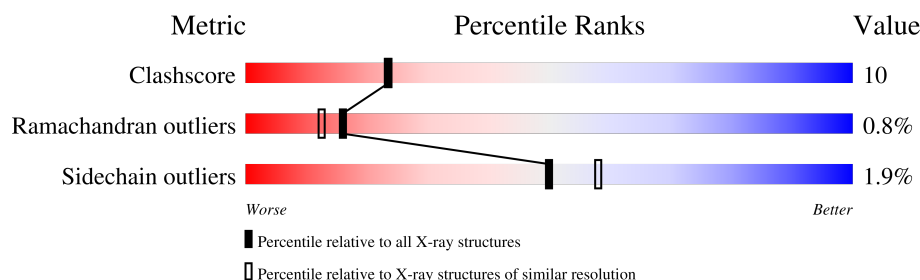
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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
5	FAD	A	3006	X	-	-	-
5	FAD	B	4006	X	-	-	-
6	GOL	A	3007	-	X	X	-
6	GOL	A	3008	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	B	4007	-	X	X	-
6	GOL	B	4008	-	X	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 22402 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.

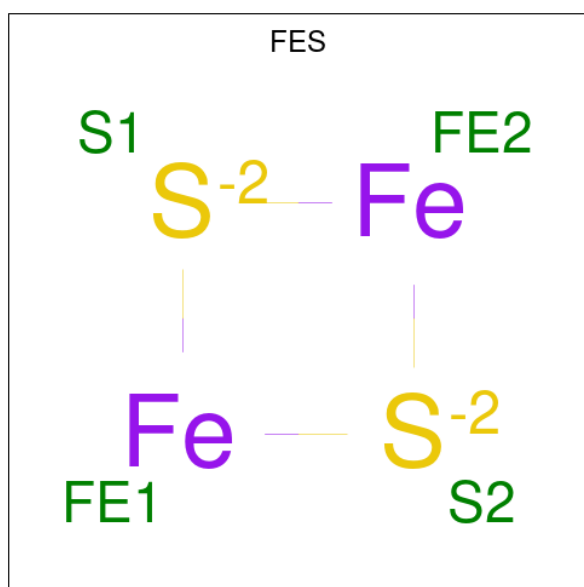
- Molecule 1 is a protein called XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	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			

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

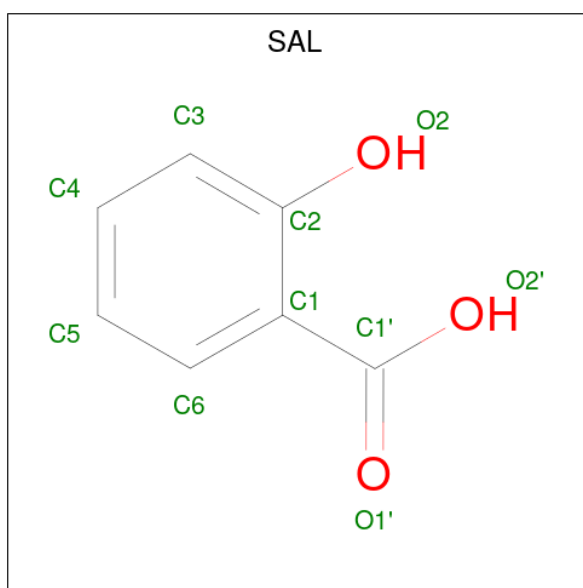
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

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



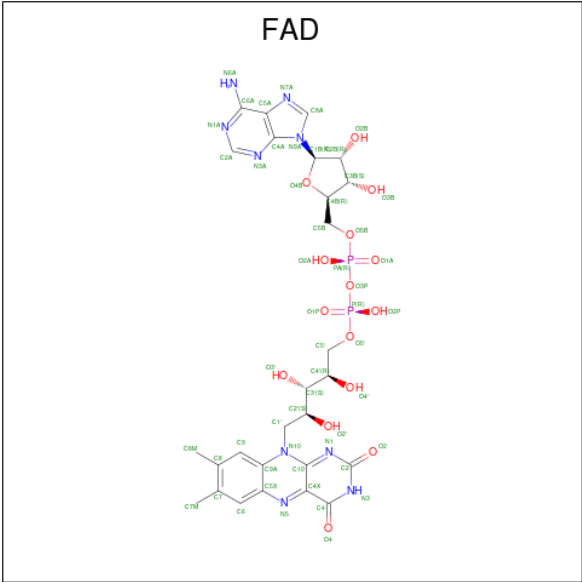
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: $C_7H_6O_3$).



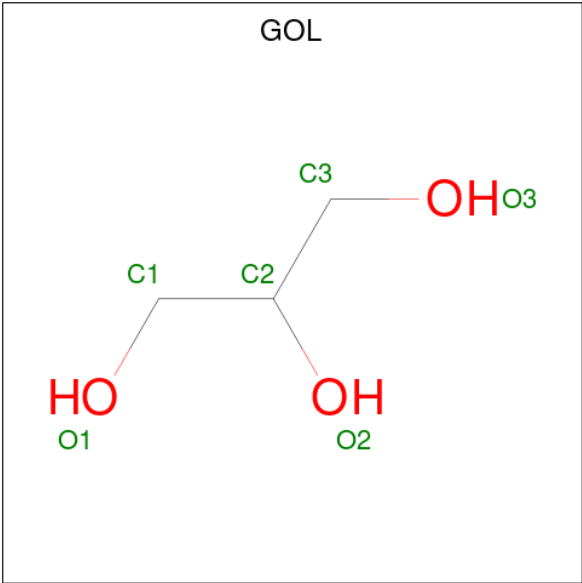
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	7	3		
4	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- 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		

Continued on next page...

Continued from previous page...

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		

- Molecule 7 is Molybdopterin dihydroxy-thioxo-molybdenum (CCD ID: HOH) (formula: H₂O).

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

- Molecule 8 is water.

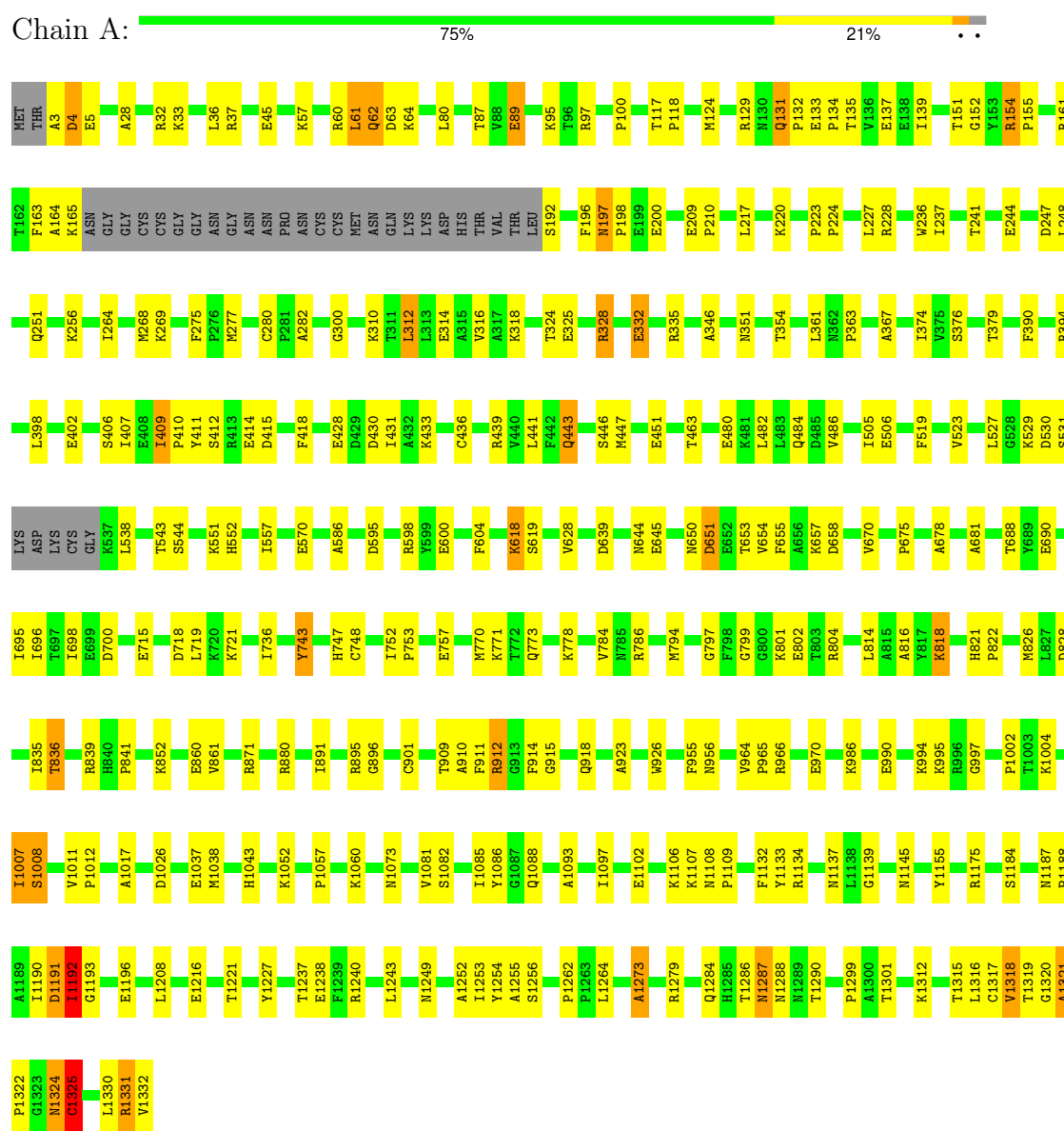
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1047	Total	O	0	0
			1047	1047		
8	B	1000	Total	O	0	0
			1000	1000		

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.

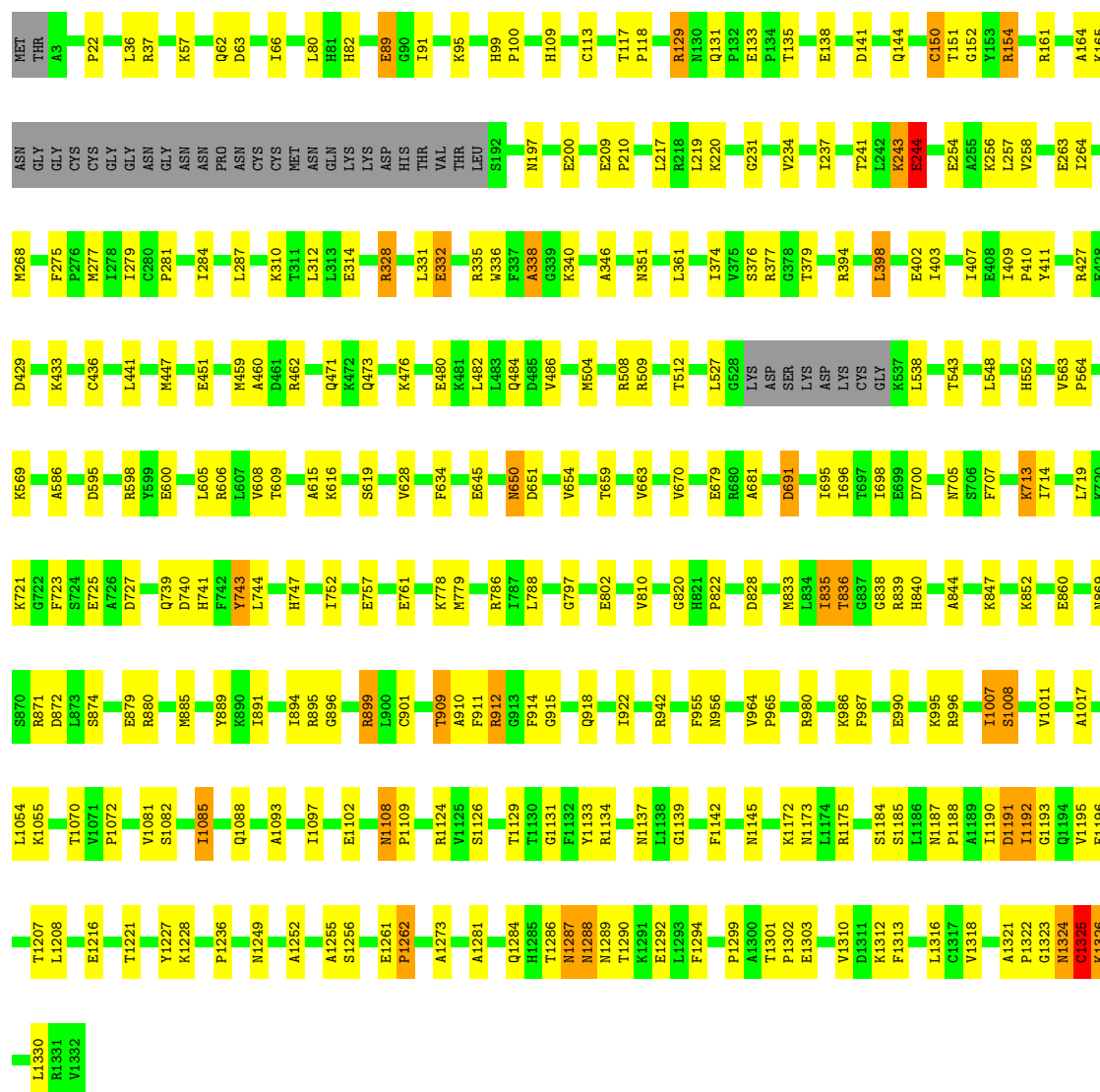
Note EDS was not executed.

• Molecule 1: XANTHINE DEHYDROGENASE



• Molecule 1: XANTHINE DEHYDROGENASE

76% 19% . .



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	169.45Å 124.49Å 148.33Å 90.00° 90.94° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10	Depositor
% Data completeness (in resolution range)	86.9 (25.00-2.10)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22402	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: SAL, FAD, GOL, FES, CA, ZW9

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	0.41	0/10298	0.96	48/13939 (0.3%)
1	B	0.42	0/10275	0.96	50/13909 (0.4%)
All	All	0.42	0/20573	0.96	98/27848 (0.4%)

There are no bond length outliers.

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	835	ILE	N-CA-C	12.48	122.93	110.82
1	A	835	ILE	N-CA-C	11.20	123.45	111.58
1	B	151	THR	N-CA-C	10.01	123.43	111.82
1	A	151	THR	N-CA-C	9.70	123.07	111.82
1	A	1191	ASP	N-CA-C	-9.66	96.89	110.50
1	A	836	THR	N-CA-C	8.33	123.10	113.19
1	B	243	LYS	N-CA-C	-8.32	97.49	109.96
1	B	836	THR	N-CA-C	8.27	123.03	113.19
1	B	696	ILE	N-CA-C	8.22	118.63	111.56
1	B	1191	ASP	N-CA-C	-8.11	98.48	110.48
1	A	1262	PRO	N-CA-C	7.87	120.31	110.70
1	B	743	TYR	N-CA-C	-7.83	98.69	110.28
1	B	1324	ASN	N-CA-C	-7.53	101.00	111.39
1	A	433	LYS	N-CA-C	-7.50	102.25	111.40
1	A	696	ILE	N-CA-C	7.46	118.76	111.67
1	B	433	LYS	N-CA-C	-7.45	102.31	111.40
1	B	1193	GLY	N-CA-C	-7.39	103.87	112.73
1	A	1193	GLY	N-CA-C	-7.36	103.35	112.77
1	A	828	ASP	N-CA-C	-7.13	100.92	110.55
1	B	654	VAL	N-CA-C	-7.12	103.24	111.00
1	B	828	ASP	N-CA-C	-7.12	100.94	110.55
1	A	956	ASN	N-CA-C	6.75	120.88	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1325	CYS	N-CA-C	6.75	121.91	107.67
1	B	1262	PRO	N-CA-C	6.74	118.92	110.70
1	B	1011	VAL	N-CA-C	-6.54	101.08	107.55
1	A	300	GLY	N-CA-C	-6.53	104.42	111.93
1	B	869	ASN	N-CA-C	6.50	120.69	113.21
1	A	654	VAL	N-CA-C	-6.47	103.94	111.00
1	A	1273	ALA	N-CA-C	-6.39	104.40	111.82
1	A	743	TYR	N-CA-C	-6.39	100.82	110.28
1	A	1011	VAL	N-CA-C	-6.39	101.22	107.55
1	B	1273	ALA	N-CA-C	-6.39	104.39	111.36
1	B	436	CYS	N-CA-C	6.38	118.47	108.96
1	A	62	GLN	N-CA-C	-6.34	105.55	113.28
1	A	1108	ASN	CA-C-N	6.30	125.80	119.24
1	A	1108	ASN	C-N-CA	6.30	125.80	119.24
1	A	543	THR	N-CA-C	6.28	118.13	111.28
1	B	663	VAL	N-CA-C	-6.28	101.45	109.30
1	A	152	GLY	N-CA-C	-6.26	106.60	115.43
1	B	956	ASN	N-CA-C	6.21	120.12	111.74
1	A	1287	ASN	CA-C-O	6.14	121.50	117.94
1	B	80	LEU	N-CA-C	6.07	119.64	112.72
1	A	411	TYR	N-CA-C	-5.94	101.69	110.48
1	B	234	VAL	N-CA-C	5.92	117.00	108.48
1	B	1228	LYS	N-CA-C	5.90	118.72	107.75
1	A	1287	ASN	CB-CA-C	-5.89	108.59	117.07
1	B	1007	ILE	N-CA-C	5.88	116.33	107.80
1	B	1085	ILE	N-CA-C	5.88	117.40	111.00
1	A	80	LEU	N-CA-C	5.78	120.03	112.92
1	B	650	ASN	N-CA-C	5.78	119.53	111.90
1	B	338	ALA	CB-CA-C	-5.75	109.92	116.54
1	A	891	ILE	CA-C-N	5.73	125.20	119.24
1	A	891	ILE	C-N-CA	5.73	125.20	119.24
1	A	390	PHE	CA-C-N	5.71	124.91	118.97
1	A	390	PHE	C-N-CA	5.71	124.91	118.97
1	B	713	LYS	N-CA-C	5.70	117.77	108.76
1	B	113	CYS	N-CA-C	-5.65	105.26	111.82
1	B	410	PRO	N-CA-C	5.63	120.34	111.38
1	A	1026	ASP	N-CA-C	-5.61	106.10	113.17
1	A	1137	ASN	N-CA-C	5.59	119.10	111.39
1	A	447	MET	N-CA-C	-5.56	105.18	112.41
1	B	409	ILE	CA-C-N	5.56	125.47	119.85
1	B	409	ILE	C-N-CA	5.56	125.47	119.85
1	A	821	HIS	CA-C-N	-5.51	114.28	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	821	HIS	C-N-CA	-5.51	114.28	119.85
1	B	152	GLY	N-CA-C	-5.51	107.64	115.30
1	B	1108	ASN	CA-C-N	5.51	126.72	119.84
1	B	1108	ASN	C-N-CA	5.51	126.72	119.84
1	B	691	ASP	N-CA-C	5.44	117.31	110.24
1	B	244	GLU	N-CA-C	-5.41	99.28	110.80
1	A	409	ILE	CA-C-N	5.40	125.33	119.76
1	A	409	ILE	C-N-CA	5.40	125.33	119.76
1	A	1007	ILE	N-CA-C	5.38	115.84	107.99
1	B	889	TYR	N-CA-C	5.37	118.16	109.40
1	B	150	CYS	N-CA-C	5.34	119.73	112.04
1	A	354	THR	N-CA-C	-5.32	105.60	111.71
1	B	909	THR	N-CA-C	5.29	115.37	108.07
1	A	197	ASN	CA-C-N	5.26	124.93	119.56
1	A	197	ASN	C-N-CA	5.26	124.93	119.56
1	B	411	TYR	N-CA-C	-5.24	102.72	110.48
1	B	835	ILE	CB-CA-C	-5.24	105.17	112.04
1	B	1137	ASN	N-CA-C	5.23	118.60	111.39
1	B	874	SER	N-CA-C	5.22	116.66	111.07
1	A	841	PRO	N-CA-C	-5.22	103.08	111.38
1	A	443	GLN	N-CA-C	-5.20	102.90	110.08
1	B	820	GLY	N-CA-C	-5.18	108.10	115.30
1	B	1070	THR	N-CA-C	-5.17	107.04	113.55
1	B	1131	GLY	N-CA-C	-5.16	103.01	110.90
1	A	436	CYS	N-CA-C	5.16	116.64	108.96
1	B	891	ILE	CA-C-N	5.15	126.28	119.84
1	B	891	ILE	C-N-CA	5.15	126.28	119.84
1	A	1085	ILE	N-CA-C	5.12	116.58	111.00
1	A	33	LYS	N-CA-C	5.10	116.69	111.03
1	A	282	ALA	N-CA-C	5.10	117.50	111.33
1	A	131	GLN	CA-C-N	5.04	124.70	119.56
1	A	131	GLN	C-N-CA	5.04	124.70	119.56
1	B	263	GLU	N-CA-C	-5.03	106.28	112.72
1	B	543	THR	N-CA-C	5.01	117.13	111.11

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	10075	219	0
1	B	10054	0	10054	194	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	10	0	4	0	0
4	B	10	0	4	1	0
5	A	53	0	29	2	0
5	B	53	0	30	2	0
6	A	12	0	5	7	0
6	B	12	0	7	11	0
7	A	28	0	0	0	0
7	B	28	0	0	0	0
8	A	1047	0	0	24	0
8	B	1000	0	0	16	0
All	All	22402	0	20208	414	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 (414) 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)
6:A:3008:GOL:O1	6:A:3008:GOL:C1	1.68	1.39
6:B:4008:GOL:O1	6:B:4008:GOL:C1	1.71	1.36
1:A:3:ALA:HB1	1:A:228:ARG:H	1.19	1.07
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.19	1.07
8:B:4020:ZW9:S	8:B:4020:ZW9:MO	1.66	1.06
1:B:243:LYS:O	1:B:244:GLU:HB2	1.62	0.99
1:B:1286:THR:HG22	1:B:1287:ASN:H	1.25	0.98
1:B:1321:ALA:HB1	1:B:1322:PRO:HD2	1.50	0.94
1:A:506:GLU:HG3	1:A:1319:THR:HB	1.47	0.93
8:A:4010:ZW9:S	8:A:4010:ZW9:MO	1.82	0.90
1:B:1312:LYS:O	1:B:1316:LEU:HD13	1.74	0.88
1:A:719:LEU:HD11	1:A:895:ARG:HB2	1.58	0.85
1:B:719:LEU:HD11	1:B:895:ARG:HB2	1.57	0.85
1:B:131:GLN:HE21	1:B:133:GLU:H	1.23	0.84
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.40	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1088:GLN:HG2	1:B:1133:TYR:CD1	2.14	0.81
1:B:264:ILE:HG22	1:B:268:MET:HE2	1.61	0.81
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.43	0.81
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.47	0.80
1:B:1191:ASP:O	1:B:1192:ILE:HB	1.78	0.80
1:B:719:LEU:HD11	1:B:895:ARG:CB	2.13	0.77
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	1.85	0.77
1:B:839:ARG:HG3	6:B:4007:GOL:H11	1.67	0.76
1:A:1191:ASP:O	1:A:1192:ILE:HB	1.85	0.75
1:A:131:GLN:HE21	1:A:133:GLU:H	1.34	0.75
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.87	0.74
1:A:1331:ARG:O	1:A:1332:VAL:O	2.05	0.74
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.22	0.74
1:B:36:LEU:HD22	1:B:89:GLU:HG3	1.67	0.74
1:B:376:SER:HB3	1:B:379:THR:OG1	1.86	0.74
1:B:885:MET:HE2	1:B:894:ILE:HD11	1.70	0.74
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.52	0.74
1:B:1207:THR:O	1:B:1208:LEU:HD12	1.89	0.72
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.53	0.71
1:A:506:GLU:CG	1:A:1319:THR:HB	2.20	0.71
1:A:1330:LEU:O	1:A:1331:ARG:HG2	1.89	0.71
1:B:164:ALA:O	1:B:165:LYS:HB2	1.89	0.71
1:A:3:ALA:HA	1:A:227:LEU:HD22	1.73	0.70
1:B:645:GLU:CG	1:B:650:ASN:HD22	2.01	0.70
1:B:1326:LYS:HD2	1:B:1326:LYS:N	2.06	0.70
1:B:264:ILE:HD11	5:B:4006:FAD:H3B	1.74	0.70
1:B:719:LEU:HD13	1:B:860:GLU:OE2	1.91	0.69
1:A:1324:ASN:C	1:A:1324:ASN:HD22	2.00	0.69
1:A:3:ALA:HB1	1:A:228:ARG:N	2.01	0.69
1:A:600:GLU:CD	1:B:598:ARG:HG2	2.17	0.68
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.57	0.68
1:B:37:ARG:HD3	1:B:595:ASP:O	1.93	0.68
1:B:241:THR:OG1	1:B:243:LYS:O	2.12	0.67
1:B:918:GLN:HE22	6:B:4007:GOL:H12	1.60	0.66
1:A:719:LEU:HD11	1:A:895:ARG:CB	2.25	0.66
1:A:598:ARG:HG2	1:B:600:GLU:OE2	1.95	0.66
1:B:761:GLU:HG3	1:B:788:LEU:HD23	1.78	0.65
1:B:1191:ASP:O	1:B:1192:ILE:CB	2.44	0.65
1:B:1318:VAL:HG23	1:B:1321:ALA:HB2	1.78	0.65
1:B:721:LYS:O	1:B:725:GLU:HG3	1.96	0.65
1:A:619:SER:HB3	1:A:688:THR:OG1	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1088:GLN:HG2	1:B:1133:TYR:CE1	2.31	0.65
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.78	0.65
1:A:264:ILE:HD11	5:A:3006:FAD:H3B	1.78	0.65
1:A:1332:VAL:HG22	1:A:1332:VAL:OXT	1.96	0.64
1:B:645:GLU:HG2	1:B:650:ASN:ND2	2.03	0.64
1:A:752:ILE:CD1	1:A:822:PRO:HB3	2.28	0.63
1:B:1017:ALA:HB2	1:B:1085:ILE:HD12	1.81	0.62
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.82	0.62
1:A:376:SER:HB3	1:A:379:THR:OG1	1.99	0.62
1:A:164:ALA:O	1:A:165:LYS:HB2	1.99	0.62
1:A:1322:PRO:HG2	1:A:1324:ASN:CG	2.25	0.62
1:B:552:HIS:CE1	1:B:1172:LYS:NZ	2.68	0.61
1:B:131:GLN:HE21	1:B:133:GLU:N	1.96	0.61
1:B:552:HIS:CE1	1:B:1172:LYS:HZ3	2.17	0.61
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.82	0.61
1:A:527:LEU:C	1:A:529:LYS:H	2.08	0.60
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.84	0.60
1:B:980:ARG:NH1	1:B:1175:ARG:HD3	2.16	0.60
1:A:237:ILE:HD12	1:A:277:MET:HE2	1.83	0.60
1:A:570:GLU:OE2	1:A:1057:PRO:HG3	2.02	0.59
1:B:707:PHE:CD2	1:B:899:ARG:HG3	2.37	0.59
1:A:264:ILE:HG22	1:A:268:MET:HE2	1.84	0.59
1:A:441:LEU:HB3	1:A:451:GLU:HB2	1.85	0.59
1:A:197:ASN:O	1:A:200:GLU:HG2	2.03	0.59
1:A:557:ILE:HD12	1:A:1240:ARG:NE	2.18	0.59
1:A:1188:PRO:O	1:A:1191:ASP:O	2.21	0.58
1:B:129:ARG:HG3	1:B:129:ARG:HH11	1.67	0.58
1:B:1188:PRO:O	1:B:1191:ASP:O	2.20	0.58
1:A:1330:LEU:HD12	1:A:1331:ARG:N	2.18	0.58
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.38	0.58
1:A:1191:ASP:O	1:A:1192:ILE:CB	2.51	0.58
1:B:1184:SER:HB3	6:B:4008:GOL:H11	1.84	0.57
1:B:281:PRO:HB2	1:B:287:LEU:CD1	2.34	0.57
1:A:406:SER:C	1:A:407:ILE:HD12	2.29	0.57
1:A:618:LYS:HD2	1:A:690:GLU:OE1	2.05	0.57
1:B:209:GLU:HG3	1:B:210:PRO:HD2	1.86	0.57
1:B:1286:THR:CG2	1:B:1287:ASN:H	2.04	0.57
1:A:314:GLU:O	1:A:318:LYS:HD3	2.05	0.57
1:A:394:ARG:HD2	8:A:4326:HOH:O	2.05	0.57
1:A:480:GLU:O	1:A:484:GLN:HG3	2.05	0.57
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:VAL:HG21	1:B:681:ALA:HA	1.87	0.56
1:B:1289:ASN:HB3	1:B:1292:GLU:HB2	1.87	0.56
1:B:217:LEU:O	1:B:220:LYS:HG2	2.05	0.56
1:B:340:LYS:HE3	8:B:4667:HOH:O	2.04	0.56
1:A:217:LEU:O	1:A:220:LYS:HG2	2.04	0.56
1:B:1325:CYS:HB2	1:B:1326:LYS:HD2	1.86	0.56
1:A:217:LEU:HD12	1:A:220:LYS:HD3	1.88	0.56
1:A:418:PHE:CD1	1:A:439:ARG:HB2	2.41	0.56
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.05	0.56
1:A:986:LYS:O	1:A:990:GLU:HG3	2.06	0.56
1:B:258:VAL:HG22	1:B:264:ILE:HG13	1.87	0.56
1:B:197:ASN:O	1:B:200:GLU:HG2	2.06	0.56
1:A:192:SER:HB2	8:A:4669:HOH:O	2.07	0.55
1:B:459:MET:HE2	1:B:512:THR:HG21	1.88	0.55
1:A:1312:LYS:O	1:A:1316:LEU:HD23	2.06	0.55
1:B:1221:THR:HG22	1:B:1227:TYR:HB2	1.87	0.55
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.04	0.55
1:B:1326:LYS:N	1:B:1326:LYS:CD	2.69	0.55
1:B:1287:ASN:O	1:B:1288:ASN:HB2	2.07	0.55
1:B:374:ILE:HD13	1:B:398:LEU:HD22	1.89	0.55
1:B:723:PHE:CE2	1:B:847:LYS:HE2	2.42	0.55
1:A:604:PHE:CD2	1:A:675:PRO:HG3	2.41	0.55
1:A:1082:SER:HB2	8:A:4010:ZW9:O1P	2.07	0.55
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.42	0.55
1:A:1330:LEU:HD12	1:A:1331:ARG:H	1.70	0.55
1:A:3:ALA:CB	1:A:228:ARG:H	2.06	0.54
1:A:1315:THR:O	1:A:1318:VAL:HG13	2.08	0.54
1:B:1286:THR:HG22	1:B:1287:ASN:N	2.09	0.54
1:B:616:LYS:HA	1:B:659:THR:HG22	1.88	0.54
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.89	0.54
1:B:1312:LYS:HE3	1:B:1313:PHE:CZ	2.42	0.54
1:A:95:LYS:HE2	8:A:4796:HOH:O	2.06	0.54
1:A:443:GLN:HB2	1:A:446:SER:OG	2.07	0.54
1:B:1185:SER:O	6:B:4008:GOL:H12	2.08	0.54
1:A:752:ILE:HD13	1:A:822:PRO:HB3	1.90	0.54
1:A:1221:THR:HG22	1:A:1227:TYR:HB2	1.89	0.54
1:A:1008:SER:HA	1:A:1081:VAL:HG11	1.90	0.53
1:B:284:ILE:HB	1:B:287:LEU:HD12	1.90	0.53
1:A:799:GLY:HA2	8:A:4010:ZW9:S	2.49	0.53
1:A:552:HIS:HB3	1:A:1237:THR:HG21	1.90	0.53
1:A:1093:ALA:O	1:A:1097:ILE:HG12	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1294:PHE:HB2	8:B:4880:HOH:O	2.07	0.53
1:A:1012:PRO:HB2	8:A:4688:HOH:O	2.09	0.53
1:B:918:GLN:HE22	6:B:4007:GOL:C1	2.22	0.53
1:A:3:ALA:O	1:A:4:ASP:HB3	2.08	0.53
1:A:529:LYS:O	1:A:531:SER:N	2.42	0.53
1:A:1320:GLY:O	1:A:1321:ALA:C	2.52	0.53
1:A:137:GLU:HG3	1:A:551:LYS:HZ2	1.73	0.53
1:A:430:ASP:OD1	1:A:431:ILE:N	2.42	0.53
6:A:3008:GOL:C1	6:A:3008:GOL:HO1	2.12	0.53
1:A:1324:ASN:C	1:A:1324:ASN:ND2	2.68	0.52
1:B:802:GLU:OE1	4:B:4005:SAL:H4	2.09	0.52
1:A:316:VAL:HA	1:A:324:THR:HG21	1.92	0.52
6:B:4008:GOL:C1	6:B:4008:GOL:HO1	2.14	0.52
1:B:57:LYS:HE2	1:B:66:ILE:HD11	1.90	0.52
1:A:911:PHE:O	1:A:912:ARG:C	2.52	0.52
1:B:131:GLN:NE2	1:B:133:GLU:H	2.00	0.52
1:A:3:ALA:HA	1:A:227:LEU:CD2	2.40	0.52
1:B:1326:LYS:O	1:B:1326:LYS:HD3	2.10	0.52
1:B:1007:ILE:O	1:B:1008:SER:CB	2.58	0.52
1:B:164:ALA:O	1:B:165:LYS:CB	2.57	0.51
1:A:1279:ARG:NH2	1:A:1290:THR:O	2.43	0.51
1:A:1332:VAL:OXT	1:A:1332:VAL:CG2	2.57	0.51
1:B:1287:ASN:O	1:B:1288:ASN:CB	2.58	0.51
1:A:552:HIS:HB2	8:A:4617:HOH:O	2.09	0.51
1:A:137:GLU:HG3	1:A:551:LYS:NZ	2.25	0.51
1:A:966:ARG:HG3	8:A:4860:HOH:O	2.11	0.51
1:B:504:MET:HE2	1:B:1303:GLU:OE1	2.10	0.51
1:B:695:ILE:HG23	1:B:700:ASP:HB3	1.93	0.51
1:A:407:ILE:HD12	1:A:407:ILE:N	2.26	0.51
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.11	0.51
1:A:918:GLN:HE22	6:A:3007:GOL:C1	2.23	0.51
1:B:117:THR:HB	1:B:118:PRO:HD3	1.92	0.51
1:B:154:ARG:HD2	8:B:4305:HOH:O	2.11	0.50
1:A:374:ILE:HD13	1:A:398:LEU:CD2	2.41	0.50
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.93	0.50
1:B:1187:ASN:CG	1:B:1190:ILE:HG12	2.36	0.50
1:A:60:ARG:O	1:A:61:LEU:HB2	2.09	0.50
1:A:839:ARG:NH1	6:A:3007:GOL:O1	2.44	0.50
1:B:1324:ASN:O	1:B:1326:LYS:N	2.44	0.50
1:A:506:GLU:CD	1:A:506:GLU:H	2.19	0.50
1:B:268:MET:HE1	8:B:4719:HOH:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:SER:HA	1:B:1081:VAL:HG11	1.92	0.50
1:A:346:ALA:HB1	5:A:3006:FAD:H4'	1.92	0.50
1:A:45:GLU:HG2	8:A:4719:HOH:O	2.12	0.50
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.77	0.50
1:A:752:ILE:HD12	1:A:822:PRO:HB3	1.93	0.50
1:B:1097:ILE:HD11	1:B:1129:THR:HG22	1.92	0.50
1:A:351:ASN:ND2	1:A:361:LEU:HB2	2.27	0.50
1:A:1322:PRO:HG2	1:A:1324:ASN:ND2	2.26	0.50
1:B:141:ASP:O	1:B:144:GLN:HG3	2.11	0.50
1:A:645:GLU:OE2	1:A:650:ASN:HB3	2.12	0.50
1:A:1317:CYS:O	1:A:1318:VAL:C	2.55	0.49
1:B:879:GLU:HG2	1:B:1142:PHE:CZ	2.46	0.49
1:A:964:VAL:HB	1:A:965:PRO:HD3	1.94	0.49
1:A:994:LYS:HE3	8:A:4560:HOH:O	2.12	0.49
1:B:885:MET:SD	1:B:896:GLY:HA3	2.52	0.49
1:A:135:THR:O	1:A:139:ILE:HG13	2.12	0.49
1:A:374:ILE:HG21	1:A:398:LEU:HD22	1.94	0.49
1:A:1007:ILE:O	1:A:1008:SER:CB	2.60	0.49
1:B:336:TRP:CZ3	1:B:427:ARG:HG2	2.48	0.49
1:B:713:LYS:HG3	1:B:714:ILE:N	2.26	0.49
1:A:5:GLU:HB2	8:A:4797:HOH:O	2.12	0.49
1:A:117:THR:HB	1:A:118:PRO:HD3	1.93	0.49
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.47	0.49
1:A:1184:SER:HB3	6:A:3008:GOL:H11	1.94	0.49
1:B:980:ARG:HD2	8:B:4566:HOH:O	2.12	0.49
1:A:256:LYS:HG3	1:A:275:PHE:CD2	2.48	0.49
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.13	0.49
1:A:570:GLU:CD	1:A:1057:PRO:HG3	2.37	0.49
1:A:955:PHE:CA	1:A:1145:ASN:HD21	2.21	0.49
1:B:840:HIS:N	6:B:4007:GOL:O3	2.38	0.49
1:A:915:GLY:H	6:A:3007:GOL:C1	2.26	0.49
1:B:154:ARG:CD	1:B:1196:GLU:OE2	2.59	0.49
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.93	0.49
1:B:839:ARG:NH1	6:B:4007:GOL:O1	2.46	0.49
1:A:312:LEU:O	1:A:316:VAL:HG23	2.13	0.48
1:A:1192:ILE:HG13	1:A:1243:LEU:HD11	1.95	0.48
1:A:1320:GLY:C	1:A:1322:PRO:HD3	2.38	0.48
1:A:418:PHE:HD1	1:A:439:ARG:HB2	1.78	0.48
1:A:651:ASP:OD1	1:A:871:ARG:NH1	2.45	0.48
1:B:1323:GLY:O	1:B:1324:ASN:C	2.57	0.48
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:PRO:HG3	1:A:463:THR:HG23	1.94	0.48
1:A:1320:GLY:O	1:A:1322:PRO:N	2.47	0.48
1:A:600:GLU:OE2	1:B:598:ARG:HG2	2.13	0.48
1:A:367:ALA:O	1:A:439:ARG:HD3	2.14	0.48
1:A:3:ALA:HB2	1:A:227:LEU:HA	1.95	0.48
1:A:64:LYS:HE2	8:A:4653:HOH:O	2.14	0.48
1:B:117:THR:CG2	1:B:586:ALA:HA	2.44	0.48
1:B:129:ARG:HG3	1:B:129:ARG:NH1	2.29	0.48
1:A:909:THR:OG1	1:A:910:ALA:N	2.45	0.47
1:A:1017:ALA:HB1	1:A:1086:TYR:CD2	2.48	0.47
1:B:62:GLN:O	1:B:63:ASP:C	2.58	0.47
1:B:150:CYS:SG	8:B:4020:ZW9:N2	2.87	0.47
1:A:544:SER:HB2	1:A:994:LYS:HD2	1.95	0.47
1:A:794:MET:HE3	1:A:1038:MET:HB3	1.96	0.47
1:A:1107:LYS:C	1:A:1109:PRO:HD3	2.39	0.47
1:A:161:ARG:HD3	8:A:4840:HOH:O	2.13	0.47
1:A:719:LEU:CD1	1:A:895:ARG:HD3	2.44	0.47
1:A:325:GLU:HB2	1:A:412:SER:OG	2.14	0.47
1:A:657:LYS:O	1:A:658:ASP:HB2	2.15	0.47
1:B:739:GLN:HG2	1:B:911:PHE:CE1	2.50	0.47
1:B:332:GLU:CG	1:B:548:LEU:HD13	2.45	0.47
1:B:473:GLN:O	1:B:476:LYS:HB2	2.14	0.47
1:B:911:PHE:O	1:B:912:ARG:C	2.58	0.47
1:A:861:VAL:O	1:A:896:GLY:HA2	2.14	0.47
1:A:131:GLN:O	1:A:134:PRO:HD3	2.15	0.47
1:B:129:ARG:NE	1:B:209:GLU:HG2	2.30	0.47
1:B:376:SER:HB2	1:B:402:GLU:HG2	1.96	0.47
1:A:1330:LEU:O	1:A:1331:ARG:CG	2.59	0.46
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.80	0.46
1:B:911:PHE:HD2	1:B:912:ARG:N	2.13	0.46
1:A:1318:VAL:HG23	1:A:1318:VAL:O	2.16	0.46
1:B:256:LYS:HG3	1:B:275:PHE:CD2	2.51	0.46
1:B:1207:THR:C	1:B:1208:LEU:HD12	2.40	0.46
1:A:698:ILE:HG23	1:A:901:CYS:SG	2.55	0.46
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.31	0.46
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.27	0.46
1:A:527:LEU:C	1:A:529:LYS:N	2.71	0.46
1:B:1321:ALA:O	1:B:1322:PRO:C	2.58	0.46
1:A:1134:ARG:HD3	1:B:1124:ARG:O	2.16	0.46
1:B:237:ILE:HD11	1:B:277:MET:HE2	1.97	0.46
1:B:312:LEU:HB2	1:B:331:LEU:HD21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LEU:O	1:A:486:VAL:HG23	2.16	0.46
1:A:688:THR:HG23	8:A:4422:HOH:O	2.14	0.46
1:A:914:PHE:HA	6:A:3007:GOL:O2	2.15	0.46
1:B:1175:ARG:HG2	8:B:4751:HOH:O	2.16	0.46
1:B:135:THR:OG1	1:B:138:GLU:HG3	2.16	0.46
1:B:482:LEU:C	1:B:482:LEU:HD23	2.41	0.46
1:A:1175:ARG:HG3	1:A:1238:GLU:HB2	1.98	0.46
1:A:237:ILE:CD1	1:A:277:MET:HE2	2.46	0.45
1:A:997:GLY:HA3	1:A:1273:ALA:O	2.15	0.45
1:A:747:HIS:CE1	1:A:801:LYS:HG2	2.51	0.45
1:B:915:GLY:H	6:B:4007:GOL:C1	2.29	0.45
1:A:718:ASP:HB3	1:A:721:LYS:HE3	1.97	0.45
1:B:705:ASN:HA	1:B:707:PHE:CE1	2.52	0.45
1:A:644:ASN:O	1:A:653:THR:HA	2.17	0.45
1:A:310:LYS:O	1:A:314:GLU:HG3	2.17	0.45
1:B:757:GLU:HB3	1:B:786:ARG:HE	1.82	0.45
1:B:1216:GLU:N	1:B:1216:GLU:CD	2.75	0.45
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.79	0.45
1:A:995:LYS:NZ	1:A:1284:GLN:NE2	2.64	0.45
1:B:37:ARG:HG2	1:B:37:ARG:HH11	1.82	0.45
1:B:1310:VAL:HG13	8:B:4809:HOH:O	2.16	0.45
1:A:519:PHE:O	1:A:523:VAL:HG23	2.17	0.44
1:B:377:ARG:HH11	1:B:377:ARG:HG2	1.82	0.44
1:B:740:ASP:OD2	1:B:833:MET:HG2	2.16	0.44
1:A:1330:LEU:O	1:A:1331:ARG:CB	2.66	0.44
1:B:779:MET:HG3	1:B:810:VAL:CG1	2.46	0.44
1:A:651:ASP:CG	1:A:871:ARG:HH11	2.25	0.44
1:A:695:ILE:HG23	1:A:700:ASP:HB3	1.98	0.44
1:A:37:ARG:HG2	1:A:595:ASP:HA	1.99	0.44
1:B:346:ALA:HB1	5:B:4006:FAD:H4'	1.99	0.44
1:B:1299:PRO:HG2	1:B:1301:THR:HG23	1.99	0.44
1:A:247:ASP:O	1:A:251:GLN:HG3	2.18	0.44
1:A:1322:PRO:C	1:A:1324:ASN:H	2.25	0.44
1:B:1108:ASN:N	1:B:1109:PRO:HD3	2.33	0.44
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.28	0.44
1:B:82:HIS:CE1	1:B:219:LEU:HD13	2.52	0.44
1:B:909:THR:OG1	1:B:910:ALA:N	2.47	0.44
1:B:1192:ILE:HA	1:B:1195:VAL:HB	1.98	0.44
1:A:557:ILE:HB	1:A:1240:ARG:HG2	1.99	0.44
1:A:1286:THR:HG22	1:A:1287:ASN:N	2.32	0.44
1:B:480:GLU:O	1:B:484:GLN:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:MET:HE2	1:A:163:PHE:CD1	2.52	0.43
1:A:1253:ILE:HG23	1:A:1253:ILE:O	2.18	0.43
8:A:4946:HOH:O	1:B:95:LYS:HE2	2.18	0.43
1:B:332:GLU:HG2	1:B:548:LEU:HD13	2.01	0.43
1:B:1082:SER:HB2	8:B:4020:ZW9:O2P	2.19	0.43
1:A:62:GLN:O	1:A:63:ASP:C	2.61	0.43
1:A:209:GLU:HG3	1:A:210:PRO:HD2	1.99	0.43
1:A:628:VAL:HG21	1:A:681:ALA:HA	2.00	0.43
1:A:1299:PRO:HG2	1:A:1301:THR:HG23	2.00	0.43
1:A:1325:CYS:HA	8:A:4966:HOH:O	2.17	0.43
1:B:914:PHE:HA	6:B:4007:GOL:O2	2.18	0.43
1:A:269:LYS:HE3	8:A:4958:HOH:O	2.18	0.43
1:B:91:ILE:O	1:B:99:HIS:HB2	2.19	0.43
1:B:563:VAL:O	1:B:564:PRO:C	2.62	0.43
1:B:606:ARG:HG2	1:B:679:GLU:HA	2.00	0.43
1:B:698:ILE:HG23	1:B:901:CYS:SG	2.58	0.43
1:A:715:GLU:CG	1:A:895:ARG:HG3	2.48	0.43
8:A:4908:HOH:O	1:B:1134:ARG:HD2	2.18	0.43
1:B:36:LEU:HD22	1:B:89:GLU:CG	2.44	0.43
1:B:509:ARG:HH11	1:B:509:ARG:HG2	1.84	0.43
1:B:407:ILE:HD12	1:B:407:ILE:N	2.33	0.43
1:B:1321:ALA:HB1	1:B:1322:PRO:CD	2.35	0.43
1:A:1324:ASN:C	8:A:4966:HOH:O	2.60	0.43
1:A:1175:ARG:NH2	1:A:1240:ARG:NH1	2.67	0.43
1:A:1187:ASN:CG	1:A:1190:ILE:HG12	2.43	0.43
1:A:482:LEU:C	1:A:482:LEU:HD23	2.44	0.43
1:B:508:ARG:O	1:B:512:THR:HG23	2.19	0.43
1:A:505:ILE:N	1:A:505:ILE:HD12	2.35	0.42
1:A:715:GLU:HG3	1:A:895:ARG:HG3	2.01	0.42
1:B:609:THR:HG21	1:B:835:ILE:HD11	2.00	0.42
1:B:1281:ALA:O	1:B:1284:GLN:HB3	2.18	0.42
1:A:966:ARG:O	1:A:970:GLU:HB2	2.19	0.42
1:A:1060:LYS:HA	8:A:4504:HOH:O	2.18	0.42
1:A:1252:ALA:HB3	1:A:1256:SER:O	2.19	0.42
1:B:752:ILE:CD1	1:B:822:PRO:HB3	2.48	0.42
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.85	0.42
1:A:237:ILE:HG21	1:A:248:LEU:HD11	2.01	0.42
1:A:1132:PHE:CD1	1:B:1126:SER:HB2	2.54	0.42
1:B:482:LEU:O	1:B:486:VAL:HG23	2.20	0.42
1:B:844:ALA:HB2	1:B:922:ILE:HD13	2.02	0.42
1:B:1316:LEU:HD11	8:B:4974:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:TRP:CZ2	1:A:280:CYS:HB2	2.55	0.42
1:A:639:ASP:HB3	1:A:818:LYS:HE3	2.01	0.42
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.85	0.42
8:B:4020:ZW9:S	8:B:4020:ZW9:O1	2.78	0.42
1:A:719:LEU:HD12	1:A:895:ARG:HD3	2.02	0.42
1:A:748:CYS:HB2	1:A:826:MET:HG3	2.01	0.42
1:A:1322:PRO:C	1:A:1324:ASN:N	2.76	0.42
1:B:608:VAL:HG21	1:B:634:PHE:HE1	1.84	0.42
1:B:942:ARG:HD2	8:B:4351:HOH:O	2.20	0.42
1:B:1054:LEU:O	1:B:1055:LYS:HB2	2.20	0.42
1:A:131:GLN:HA	1:A:132:PRO:HD2	1.92	0.42
1:A:137:GLU:OE2	1:A:551:LYS:HD2	2.20	0.42
1:B:338:ALA:HA	1:B:429:ASP:OD1	2.20	0.42
1:B:964:VAL:HB	1:B:965:PRO:HD3	2.02	0.42
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.84	0.42
1:A:154:ARG:N	1:A:155:PRO:HD2	2.34	0.42
1:A:1132:PHE:CG	1:B:1126:SER:HB2	2.55	0.42
1:B:117:THR:HG22	1:B:586:ALA:HA	2.01	0.42
1:A:196:PHE:CE1	1:A:198:PRO:HG3	2.54	0.41
1:A:995:LYS:HZ1	1:A:1284:GLN:NE2	2.18	0.41
1:B:403:ILE:C	1:B:403:ILE:HD12	2.45	0.41
1:B:447:MET:HG2	1:B:527:LEU:HD13	2.02	0.41
1:A:771:LYS:HD3	1:A:771:LYS:HA	1.92	0.41
1:B:779:MET:SD	1:B:779:MET:C	3.03	0.41
1:A:87:THR:HG1	1:A:89:GLU:HG2	1.84	0.41
1:A:268:MET:HE1	8:A:4726:HOH:O	2.20	0.41
1:B:254:GLU:CD	1:B:254:GLU:H	2.27	0.41
1:A:414:GLU:O	1:A:415:ASP:HB2	2.20	0.41
1:B:161:ARG:HD3	8:B:4822:HOH:O	2.20	0.41
1:B:605:LEU:C	1:B:605:LEU:HD23	2.45	0.41
1:A:117:THR:CG2	1:A:586:ALA:HA	2.50	0.41
1:A:770:MET:HE3	1:A:1073:ASN:HA	2.03	0.41
1:B:727:ASP:OD2	1:B:852:LYS:HG2	2.20	0.41
1:B:1252:ALA:HB3	1:B:1256:SER:O	2.20	0.41
1:A:28:ALA:O	1:A:32:ARG:HG2	2.20	0.41
1:A:409:ILE:HA	1:A:410:PRO:HD3	1.83	0.41
1:A:1106:LYS:O	1:A:1109:PRO:HD3	2.21	0.41
1:B:22:PRO:HD2	1:B:231:GLY:HA3	2.02	0.41
1:B:257:LEU:HA	1:B:279:ILE:O	2.20	0.41
1:B:310:LYS:O	1:B:314:GLU:HG3	2.20	0.41
1:B:871:ARG:O	1:B:872:ASP:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:HG22	1:A:586:ALA:HA	2.03	0.41
1:A:129:ARG:NE	1:A:209:GLU:HG2	2.35	0.41
1:B:109:HIS:HA	8:B:4182:HOH:O	2.19	0.41
1:B:351:ASN:ND2	1:B:361:LEU:HB2	2.36	0.41
1:B:670:VAL:HG11	1:B:681:ALA:HB3	2.02	0.41
1:B:1173:ASN:O	1:B:1236:PRO:HA	2.21	0.41
1:B:741:HIS:CE1	1:B:838:GLY:HA2	2.56	0.41
1:B:1289:ASN:O	1:B:1290:THR:HB	2.20	0.41
1:A:97:ARG:HB2	1:A:97:ARG:NH1	2.35	0.41
1:A:376:SER:HB2	1:A:402:GLU:HG2	2.03	0.41
1:A:428:GLU:CD	1:A:428:GLU:N	2.79	0.41
1:A:678:ALA:HB3	8:A:4714:HOH:O	2.20	0.41
1:A:719:LEU:HD13	1:A:860:GLU:OE2	2.21	0.41
1:B:394:ARG:HD2	8:B:4345:HOH:O	2.20	0.41
1:A:1004:LYS:HB2	1:A:1155:TYR:CE2	2.56	0.41
1:A:1052:LYS:HD3	1:A:1254:TYR:CZ	2.55	0.41
1:B:332:GLU:O	1:B:335:ARG:HB3	2.21	0.41
1:B:460:ALA:C	1:B:462:ARG:H	2.28	0.41
1:B:1301:THR:HB	1:B:1302:PRO:HD2	2.03	0.41
1:A:773:GLN:HG2	1:A:784:VAL:HG13	2.02	0.40
1:A:804:ARG:HG2	1:A:909:THR:HG21	2.02	0.40
1:A:1264:LEU:HD23	1:A:1264:LEU:C	2.46	0.40
1:B:986:LYS:O	1:B:990:GLU:HG3	2.22	0.40
1:B:1093:ALA:O	1:B:1097:ILE:HG12	2.20	0.40
1:A:332:GLU:O	1:A:335:ARG:HB3	2.22	0.40
1:A:644:ASN:HB2	8:A:4771:HOH:O	2.21	0.40
1:A:852:LYS:HB3	1:A:852:LYS:HE2	1.79	0.40
1:B:569:LYS:HE2	1:B:569:LYS:HB3	1.91	0.40
1:B:615:ALA:HB2	1:B:691:ASP:HA	2.04	0.40
1:B:987:PHE:CD2	1:B:996:ARG:HG3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1293/1332 (97%)	1228 (95%)	54 (4%)	11 (1%)	14	10
1	B	1290/1332 (97%)	1236 (96%)	45 (4%)	9 (1%)	18	15
All	All	2583/2664 (97%)	2464 (95%)	99 (4%)	20 (1%)	16	12

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	A	1331	ARG
1	B	244	GLU
1	B	1008	SER
1	B	1287	ASN
1	A	61	LEU
1	A	1192	ILE
1	A	1288	ASN
1	B	1192	ILE
1	B	1288	ASN
1	A	530	ASP
1	A	797	GLY
1	A	912	ARG
1	A	1318	VAL
1	B	912	ARG
1	B	1139	GLY
1	B	1325	CYS
1	A	1321	ALA
1	B	797	GLY
1	A	1139	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1101/1128 (98%)	1079 (98%)	22 (2%)	48	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1098/1128 (97%)	1079 (98%)	19 (2%)	53	62
All	All	2199/2256 (98%)	2158 (98%)	41 (2%)	50	58

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	57	LYS
1	A	89	GLU
1	A	100	PRO
1	A	154	ARG
1	A	312	LEU
1	A	328	ARG
1	A	332	GLU
1	A	538	LEU
1	A	618	LYS
1	A	651	ASP
1	A	736	ILE
1	A	743	TYR
1	A	802	GLU
1	A	818	LYS
1	A	1002	PRO
1	A	1102	GLU
1	A	1192	ILE
1	A	1208	LEU
1	A	1216	GLU
1	A	1324	ASN
1	A	1325	CYS
1	B	89	GLU
1	B	100	PRO
1	B	129	ARG
1	B	154	ARG
1	B	328	ARG
1	B	332	GLU
1	B	398	LEU
1	B	471	GLN
1	B	538	LEU
1	B	619	SER
1	B	651	ASP
1	B	743	TYR
1	B	744	LEU
1	B	899	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1072	PRO
1	B	1102	GLU
1	B	1325	CYS
1	B	1326	LYS
1	B	1330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	131	GLN
1	A	144	GLN
1	A	226	GLN
1	A	251	GLN
1	A	261	ASN
1	A	351	ASN
1	A	550	GLN
1	A	556	ASN
1	A	626	GLN
1	A	650	ASN
1	A	683	HIS
1	A	1145	ASN
1	A	1212	HIS
1	A	1284	GLN
1	A	1289	ASN
1	A	1324	ASN
1	B	131	GLN
1	B	146	ASN
1	B	351	ASN
1	B	473	GLN
1	B	556	ASN
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	875	HIS
1	B	925	ASN
1	B	1145	ASN
1	B	1220	HIS
1	B	1284	GLN
1	B	1287	ASN
1	B	1288	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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	A	3002	1	0,4,4	-	-	-		
6	GOL	B	4007	-	5,5,5	6.83	5 (100%)	5,5,5	6.37	4 (80%)
3	FES	B	4001	1	0,4,4	-	-	-		
5	FAD	B	4006	-	58,58,58	4.52	37 (63%)	85,89,89	2.07	23 (27%)
8	ZW9	B	4020	-	21,31,31	7.39	12 (57%)	22,52,52	4.47	14 (63%)
6	GOL	B	4008	-	5,5,5	4.45	3 (60%)	5,5,5	6.53	3 (60%)
8	ZW9	A	4010	-	21,31,31	7.29	16 (76%)	22,52,52	4.35	14 (63%)
5	FAD	A	3006	-	58,58,58	4.47	39 (67%)	85,89,89	2.07	23 (27%)
4	SAL	A	3005	-	10,10,10	2.07	5 (50%)	13,13,13	2.14	4 (30%)
4	SAL	B	4005	-	10,10,10	2.04	5 (50%)	13,13,13	2.20	4 (30%)
6	GOL	A	3007	-	5,5,5	7.26	5 (100%)	5,5,5	6.46	4 (80%)
6	GOL	A	3008	-	5,5,5	4.57	4 (80%)	5,5,5	6.40	3 (60%)
3	FES	B	4002	1	0,4,4	-	-	-		
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
3	FES	A	3001	1	-	-	0/1/1/1
6	GOL	B	4007	-	-	2/4/4/4	-
3	FES	A	3002	1	-	-	0/1/1/1
5	FAD	B	4006	-	2/2/9/9	3/34/50/50	0/6/6/6
3	FES	B	4001	1	-	-	0/1/1/1
8	ZW9	B	4020	-	-	1/6/46/46	0/4/4/4
8	ZW9	A	4010	-	-	1/6/46/46	0/4/4/4
4	SAL	A	3005	-	-	0/4/4/4	0/1/1/1
4	SAL	B	4005	-	-	0/4/4/4	0/1/1/1
6	GOL	A	3007	-	-	2/4/4/4	-
3	FES	B	4002	1	-	-	0/1/1/1
6	GOL	A	3008	-	-	2/4/4/4	-
6	GOL	B	4008	-	-	2/4/4/4	-
5	FAD	A	3006	-	2/2/9/9	2/34/50/50	0/6/6/6

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	4020	ZW9	C7-C6	23.94	1.72	1.53
8	A	4010	ZW9	C7-C6	22.52	1.71	1.53
8	B	4020	ZW9	C9-C10	17.85	1.69	1.38
8	A	4010	ZW9	C9-C10	16.44	1.66	1.38
6	A	3007	GOL	C3-C2	-13.47	1.00	1.51
5	B	4006	FAD	P-O3P	-12.82	1.45	1.59
6	B	4007	GOL	C3-C2	-12.57	1.03	1.51
5	B	4006	FAD	C9A-C5X	11.15	1.59	1.41
5	A	3006	FAD	C9A-C5X	10.36	1.57	1.41
5	A	3006	FAD	P-O3P	-9.93	1.48	1.59
5	A	3006	FAD	C5'-C4'	-9.83	1.38	1.51
8	A	4010	ZW9	C6-N5	8.63	1.56	1.46
5	B	4006	FAD	C9A-N10	8.51	1.55	1.41
8	B	4020	ZW9	C6-N5	8.30	1.55	1.46
5	B	4006	FAD	C5'-C4'	-8.20	1.40	1.51
5	A	3006	FAD	C9A-N10	7.92	1.54	1.41
5	A	3006	FAD	C4A-N3A	7.92	1.49	1.34
5	B	4006	FAD	C8-C7	7.65	1.59	1.40
5	A	3006	FAD	C9-C9A	7.62	1.51	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4006	FAD	C2A-N1A	7.33	1.47	1.33
5	B	4006	FAD	C4A-N3A	7.33	1.48	1.34
5	A	3006	FAD	C5A-C4A	7.29	1.52	1.39
5	A	3006	FAD	C5A-C6A	7.28	1.61	1.41
5	A	3006	FAD	C2A-N1A	7.22	1.46	1.33
6	A	3008	GOL	C3-C2	-7.19	1.24	1.51
5	A	3006	FAD	C8-C7	7.10	1.58	1.40
6	B	4008	GOL	O1-C1	6.80	1.71	1.42
5	B	4006	FAD	C5A-C6A	6.76	1.59	1.41
8	A	4010	ZW9	C4'-C3'	-6.66	1.42	1.51
5	B	4006	FAD	C5A-C4A	6.61	1.50	1.39
5	B	4006	FAD	C6-C5X	6.57	1.50	1.40
5	B	4006	FAD	PA-O3P	6.48	1.66	1.59
6	B	4008	GOL	C3-C2	-6.46	1.27	1.51
5	A	3006	FAD	C2A-N3A	6.28	1.45	1.33
6	A	3008	GOL	O1-C1	6.25	1.68	1.42
8	A	4010	ZW9	C9-N5	6.24	1.52	1.37
8	B	4020	ZW9	C10-N8	6.14	1.41	1.35
5	B	4006	FAD	C9-C9A	6.13	1.49	1.39
8	A	4010	ZW9	P-O4'	-6.01	1.41	1.60
8	A	4010	ZW9	P-O1P	-5.99	1.32	1.54
8	B	4020	ZW9	P-O4'	-5.65	1.42	1.60
5	A	3006	FAD	C6-C7	5.65	1.47	1.39
5	A	3006	FAD	C1'-C2'	5.51	1.60	1.52
6	A	3007	GOL	C1-C2	-5.49	1.30	1.51
8	B	4020	ZW9	C9-N5	5.24	1.50	1.37
6	B	4007	GOL	O2-C2	-5.11	1.28	1.43
6	A	3007	GOL	O2-C2	-5.08	1.28	1.43
5	B	4006	FAD	PA-O5B	-4.84	1.40	1.59
5	A	3006	FAD	C5A-N7A	-4.82	1.30	1.39
5	B	4006	FAD	C6-C7	4.79	1.46	1.39
5	A	3006	FAD	C2-N3	4.79	1.49	1.39
5	B	4006	FAD	O5B-C5B	-4.77	1.26	1.44
5	B	4006	FAD	O4B-C4B	4.73	1.55	1.45
6	A	3007	GOL	O3-C3	-4.67	1.22	1.42
8	A	4010	ZW9	O3'-C7	4.62	1.50	1.43
5	A	3006	FAD	O4B-C4B	4.62	1.55	1.45
8	B	4020	ZW9	C4'-C3'	-4.57	1.45	1.51
8	B	4020	ZW9	P-O1P	-4.52	1.38	1.54
8	A	4010	ZW9	C10-N8	4.51	1.40	1.35
5	A	3006	FAD	C6A-N6A	-4.49	1.22	1.34
5	A	3006	FAD	O3'-C3'	4.42	1.53	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	4007	GOL	O3-C3	-4.32	1.24	1.42
5	B	4006	FAD	C4X-N5	4.32	1.40	1.30
5	B	4006	FAD	C4X-C10	4.30	1.56	1.44
5	B	4006	FAD	C5A-N7A	-4.27	1.31	1.39
5	A	3006	FAD	O5B-C5B	-4.27	1.28	1.44
5	B	4006	FAD	C2A-N3A	4.12	1.41	1.33
5	B	4006	FAD	C1'-C2'	4.11	1.58	1.52
5	A	3006	FAD	C4-N3	4.10	1.46	1.38
5	B	4006	FAD	C9-C8	4.09	1.45	1.39
5	B	4006	FAD	C8A-N7A	-4.08	1.23	1.31
5	A	3006	FAD	C10-N10	4.07	1.46	1.37
5	A	3006	FAD	C4X-N5	4.04	1.39	1.30
5	A	3006	FAD	O4B-C1B	3.99	1.51	1.42
6	B	4007	GOL	O1-C1	3.94	1.59	1.42
8	B	4020	ZW9	O3'-C3'	3.94	1.51	1.43
5	A	3006	FAD	C4X-C10	3.88	1.55	1.44
6	B	4007	GOL	C1-C2	-3.86	1.37	1.51
5	A	3006	FAD	PA-O3P	3.82	1.63	1.59
8	A	4010	ZW9	C2-N1	3.75	1.42	1.33
8	A	4010	ZW9	O4-C4	3.70	1.30	1.23
5	B	4006	FAD	C4-N3	3.69	1.45	1.38
5	A	3006	FAD	C10-N1	3.65	1.40	1.33
5	A	3006	FAD	C6-C5X	3.58	1.45	1.40
5	B	4006	FAD	O2B-C2B	-3.58	1.34	1.43
5	A	3006	FAD	PA-O2A	-3.49	1.39	1.55
5	B	4006	FAD	O2'-C2'	3.32	1.50	1.43
5	B	4006	FAD	PA-O2A	-3.32	1.40	1.55
8	B	4020	ZW9	C2-N1	3.31	1.41	1.33
8	A	4010	ZW9	O3'-C3'	3.27	1.49	1.43
5	B	4006	FAD	C2-N3	3.23	1.46	1.39
5	A	3006	FAD	C8A-N7A	-3.23	1.25	1.31
4	A	3005	SAL	C5-C6	3.18	1.44	1.38
5	A	3006	FAD	PA-O5B	-3.11	1.47	1.59
5	B	4006	FAD	O3'-C3'	3.08	1.50	1.43
5	A	3006	FAD	C6A-N1A	3.05	1.44	1.35
4	A	3005	SAL	C1-C1'	-3.04	1.43	1.49
4	B	4005	SAL	C1-C1'	-3.03	1.43	1.49
4	B	4005	SAL	C5-C6	3.02	1.44	1.38
5	B	4006	FAD	C2'-C3'	-2.96	1.48	1.53
5	B	4006	FAD	C5B-C4B	2.93	1.60	1.51
8	A	4010	ZW9	P-O2P	-2.89	1.44	1.54
5	B	4006	FAD	C10-N1	2.85	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4006	FAD	C10-N10	2.78	1.43	1.37
8	A	4010	ZW9	C4-N3	2.75	1.44	1.38
6	B	4008	GOL	O3-C3	-2.75	1.30	1.42
5	A	3006	FAD	O4-C4	-2.75	1.18	1.23
5	B	4006	FAD	C6A-N1A	2.66	1.43	1.35
5	A	3006	FAD	C5X-N5	2.58	1.44	1.39
4	B	4005	SAL	O2'-C1'	-2.54	1.23	1.30
4	B	4005	SAL	C6-C1	2.51	1.43	1.39
4	A	3005	SAL	O2'-C1'	-2.47	1.23	1.30
5	A	3006	FAD	C2'-C3'	-2.42	1.49	1.53
6	A	3008	GOL	O3-C3	-2.40	1.32	1.42
5	A	3006	FAD	O2'-C2'	2.35	1.48	1.43
4	A	3005	SAL	C6-C1	2.34	1.43	1.39
4	A	3005	SAL	C3-C2	2.31	1.43	1.39
8	A	4010	ZW9	C9-C4	2.30	1.48	1.41
5	B	4006	FAD	P-O2P	-2.29	1.44	1.55
5	A	3006	FAD	C8A-N9A	2.25	1.41	1.37
4	B	4005	SAL	C3-C2	2.21	1.43	1.39
8	A	4010	ZW9	C10-N1	2.20	1.39	1.36
5	A	3006	FAD	C4A-N9A	-2.14	1.33	1.37
5	B	4006	FAD	C8A-N9A	2.14	1.41	1.37
6	A	3008	GOL	C1-C2	-2.13	1.43	1.51
8	B	4020	ZW9	O3'-C7	2.09	1.46	1.43
5	A	3006	FAD	P-O5'	-2.05	1.51	1.59
5	B	4006	FAD	C6A-N6A	-2.04	1.29	1.34
8	B	4020	ZW9	P-O2P	-2.03	1.47	1.54
6	A	3007	GOL	O1-C1	2.02	1.50	1.42
5	A	3006	FAD	C7M-C7	-2.01	1.47	1.51

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	4020	ZW9	C2'-C1'-S1'	13.75	127.95	120.15
6	A	3007	GOL	O3-C3-C2	12.39	166.16	110.38
6	B	4008	GOL	O3-C3-C2	12.21	165.33	110.38
6	B	4007	GOL	O3-C3-C2	12.14	165.04	110.38
6	A	3008	GOL	O3-C3-C2	11.58	162.50	110.38
8	A	4010	ZW9	C2'-C1'-S1'	11.22	126.52	120.15
8	A	4010	ZW9	C2-N1-C10	7.61	126.78	113.36
8	B	4020	ZW9	C2-N1-C10	7.34	126.32	113.36
6	A	3008	GOL	O2-C2-C3	6.81	137.36	109.18
8	A	4010	ZW9	C1'-C2'-S2'	-6.76	116.31	120.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	4006	FAD	C5'-C4'-C3'	-6.73	99.52	112.22
6	B	4008	GOL	O2-C2-C3	6.54	136.26	109.18
5	A	3006	FAD	C5'-C4'-C3'	-6.40	100.14	112.22
8	B	4020	ZW9	O4-C4-C9	-6.11	112.53	127.26
8	A	4010	ZW9	O4'-C4'-C3'	5.90	123.13	108.58
6	B	4007	GOL	O2-C2-C3	5.89	133.55	109.18
6	A	3007	GOL	O2-C2-C3	5.80	133.20	109.18
5	B	4006	FAD	O5B-PA-O1A	-5.75	86.14	108.94
8	A	4010	ZW9	O4-C4-C9	-5.39	114.26	127.26
5	A	3006	FAD	O5B-PA-O1A	-5.33	87.81	108.94
8	B	4020	ZW9	C1'-C2'-S2'	-5.31	117.14	120.15
5	A	3006	FAD	C5X-C9A-N10	-4.94	113.50	117.97
5	B	4006	FAD	C5X-C9A-N10	-4.94	113.50	117.97
6	A	3008	GOL	O1-C1-C2	4.89	132.38	110.38
8	B	4020	ZW9	O3'-C7-C6	-4.82	105.75	108.96
8	B	4020	ZW9	O4'-C4'-C3'	4.71	120.20	108.58
8	A	4010	ZW9	O1P-P-O4'	4.64	118.76	106.67
6	B	4008	GOL	O1-C1-C2	4.62	131.18	110.38
5	A	3006	FAD	O4B-C4B-C5B	-4.49	94.96	109.33
8	A	4010	ZW9	C4-C9-N5	4.41	128.29	116.27
5	B	4006	FAD	C4'-C3'-C2'	-4.33	106.36	113.57
5	B	4006	FAD	C9-C9A-N10	4.17	127.47	121.85
4	A	3005	SAL	O2'-C1'-O1'	-4.16	114.40	123.35
8	B	4020	ZW9	C4-C9-N5	4.16	127.62	116.27
5	A	3006	FAD	C4-C4X-N5	4.10	123.86	118.21
4	B	4005	SAL	O2'-C1'-O1'	-4.09	114.55	123.35
5	B	4006	FAD	C4-C4X-N5	3.97	123.70	118.21
6	B	4007	GOL	O1-C1-C2	3.93	128.07	110.38
5	A	3006	FAD	C9-C9A-N10	3.85	127.03	121.85
4	B	4005	SAL	C2-C1-C1'	3.82	123.92	120.00
5	A	3006	FAD	O3'-C3'-C2'	-3.75	100.41	108.93
8	A	4010	ZW9	N2-C2-N3	3.75	124.67	116.76
5	B	4006	FAD	O4B-C4B-C5B	-3.74	97.36	109.33
6	A	3007	GOL	O1-C1-C2	3.73	127.17	110.38
5	A	3006	FAD	N3A-C2A-N1A	-3.59	123.14	128.58
8	B	4020	ZW9	N2-C2-N3	3.59	124.34	116.76
5	B	4006	FAD	N3A-C4A-N9A	3.58	133.26	127.17
8	A	4010	ZW9	O3'-C7-C6	-3.54	106.60	108.96
5	A	3006	FAD	C2A-N1A-C6A	3.50	124.47	118.73
5	B	4006	FAD	O3'-C3'-C2'	-3.48	101.01	108.93
5	A	3006	FAD	N3A-C4A-N9A	3.45	133.04	127.17
8	A	4010	ZW9	O3'-C3'-C2'	3.44	113.95	109.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4005	SAL	C3-C2-C1	3.41	123.44	119.89
4	A	3005	SAL	C2-C1-C1'	3.39	123.48	120.00
4	A	3005	SAL	C3-C2-C1	3.38	123.41	119.89
8	A	4010	ZW9	O3'-C7-N8	-3.34	105.58	108.61
8	B	4020	ZW9	O4-C4-N3	3.30	126.33	120.11
5	A	3006	FAD	O5B-C5B-C4B	3.29	120.21	108.99
8	B	4020	ZW9	C9-C4-N3	3.28	121.15	112.13
5	B	4006	FAD	C5A-C4A-N9A	-3.28	102.24	105.81
8	A	4010	ZW9	C9-C4-N3	3.23	121.00	112.13
5	A	3006	FAD	C5X-N5-C4X	3.23	123.31	118.09
8	B	4020	ZW9	O3'-C7-N8	-3.20	105.70	108.61
5	B	4006	FAD	C10-N1-C2	3.17	123.72	116.85
5	A	3006	FAD	C10-N1-C2	3.16	123.69	116.85
5	B	4006	FAD	C5X-N5-C4X	3.12	123.14	118.09
5	A	3006	FAD	C8M-C8-C9	-3.10	114.11	119.57
5	B	4006	FAD	C8M-C8-C9	-3.08	114.15	119.57
5	B	4006	FAD	C8M-C8-C7	3.06	127.00	120.76
5	A	3006	FAD	C5A-C4A-N9A	-2.98	102.56	105.81
5	A	3006	FAD	C4'-C3'-C2'	-2.91	108.72	113.57
5	B	4006	FAD	C2A-N1A-C6A	2.89	123.48	118.73
5	B	4006	FAD	O4B-C4B-C3B	-2.88	99.43	105.15
8	B	4020	ZW9	O3'-C3'-C2'	2.87	113.14	109.09
5	B	4006	FAD	O2P-P-O5'	2.80	120.25	107.57
5	A	3006	FAD	C8M-C8-C7	2.77	126.43	120.76
5	A	3006	FAD	O2P-P-O5'	2.72	119.89	107.57
8	A	4010	ZW9	N3-C2-N1	-2.69	118.41	123.32
4	A	3005	SAL	O2'-C1'-C1	2.57	122.59	115.28
5	B	4006	FAD	O5B-C5B-C4B	2.57	117.73	108.99
8	B	4020	ZW9	O1P-P-O4'	2.55	113.32	106.67
5	A	3006	FAD	O4B-C4B-C3B	-2.50	100.20	105.15
6	A	3007	GOL	O2-C2-C1	2.48	119.45	109.18
8	A	4010	ZW9	O4-C4-N3	2.46	124.74	120.11
5	A	3006	FAD	O2A-PA-O3P	2.45	113.89	107.27
4	B	4005	SAL	O2'-C1'-C1	2.42	122.16	115.28
5	B	4006	FAD	O2A-PA-O5B	2.42	118.52	107.57
5	A	3006	FAD	O2A-PA-O5B	2.37	118.29	107.57
5	B	4006	FAD	N3A-C2A-N1A	-2.36	125.01	128.58
5	B	4006	FAD	O3P-PA-O1A	2.32	117.69	110.70
5	B	4006	FAD	O2A-PA-O3P	2.32	113.55	107.27
8	B	4020	ZW9	N3-C2-N1	-2.11	119.46	123.32
6	B	4007	GOL	O2-C2-C1	2.09	117.83	109.18
5	A	3006	FAD	C4X-C4-N3	2.07	118.53	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3006	FAD	C4-N3-C2	-2.06	121.98	125.64
5	B	4006	FAD	C9A-N10-C10	2.03	123.85	120.75

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	3006	FAD	C2'
5	A	3006	FAD	C3'
5	B	4006	FAD	C2'
5	B	4006	FAD	C3'

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	3007	GOL	C1-C2-C3-O3
6	A	3008	GOL	O1-C1-C2-C3
6	A	3008	GOL	C1-C2-C3-O3
6	B	4007	GOL	C1-C2-C3-O3
6	B	4008	GOL	O1-C1-C2-C3
6	B	4008	GOL	C1-C2-C3-O3
8	A	4010	ZW9	C3'-C4'-O4'-P
8	B	4020	ZW9	C3'-C4'-O4'-P
6	B	4007	GOL	O1-C1-C2-O2
5	A	3006	FAD	O3'-C3'-C4'-C5'
6	A	3007	GOL	O1-C1-C2-O2
5	B	4006	FAD	O3'-C3'-C4'-C5'
5	A	3006	FAD	O3'-C3'-C4'-O4'
5	B	4006	FAD	O3'-C3'-C4'-O4'
5	B	4006	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

9 monomers are involved in 30 short contacts:

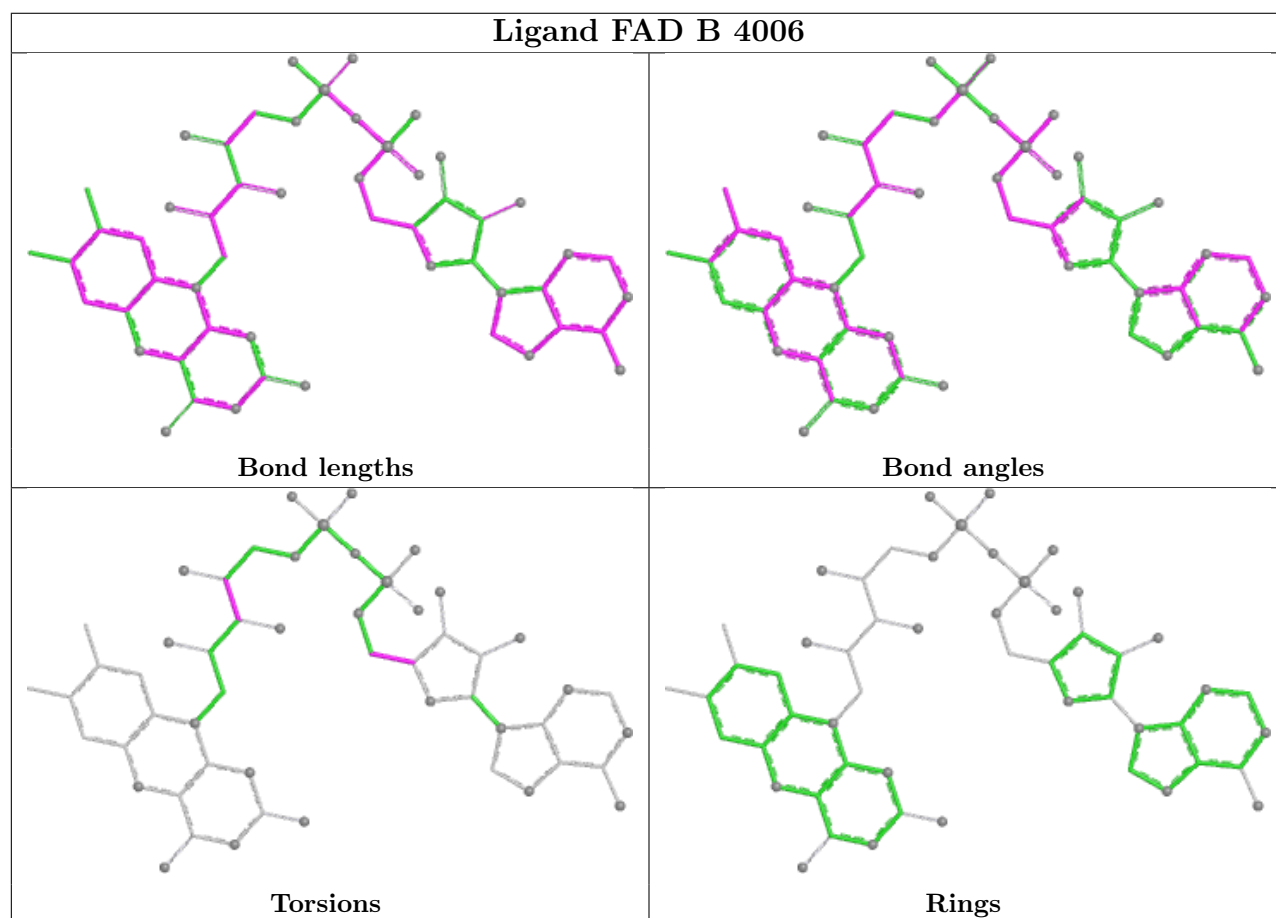
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	4007	GOL	7	0
5	B	4006	FAD	2	0
8	B	4020	ZW9	4	0
6	B	4008	GOL	4	0
8	A	4010	ZW9	3	0
5	A	3006	FAD	2	0
4	B	4005	SAL	1	0

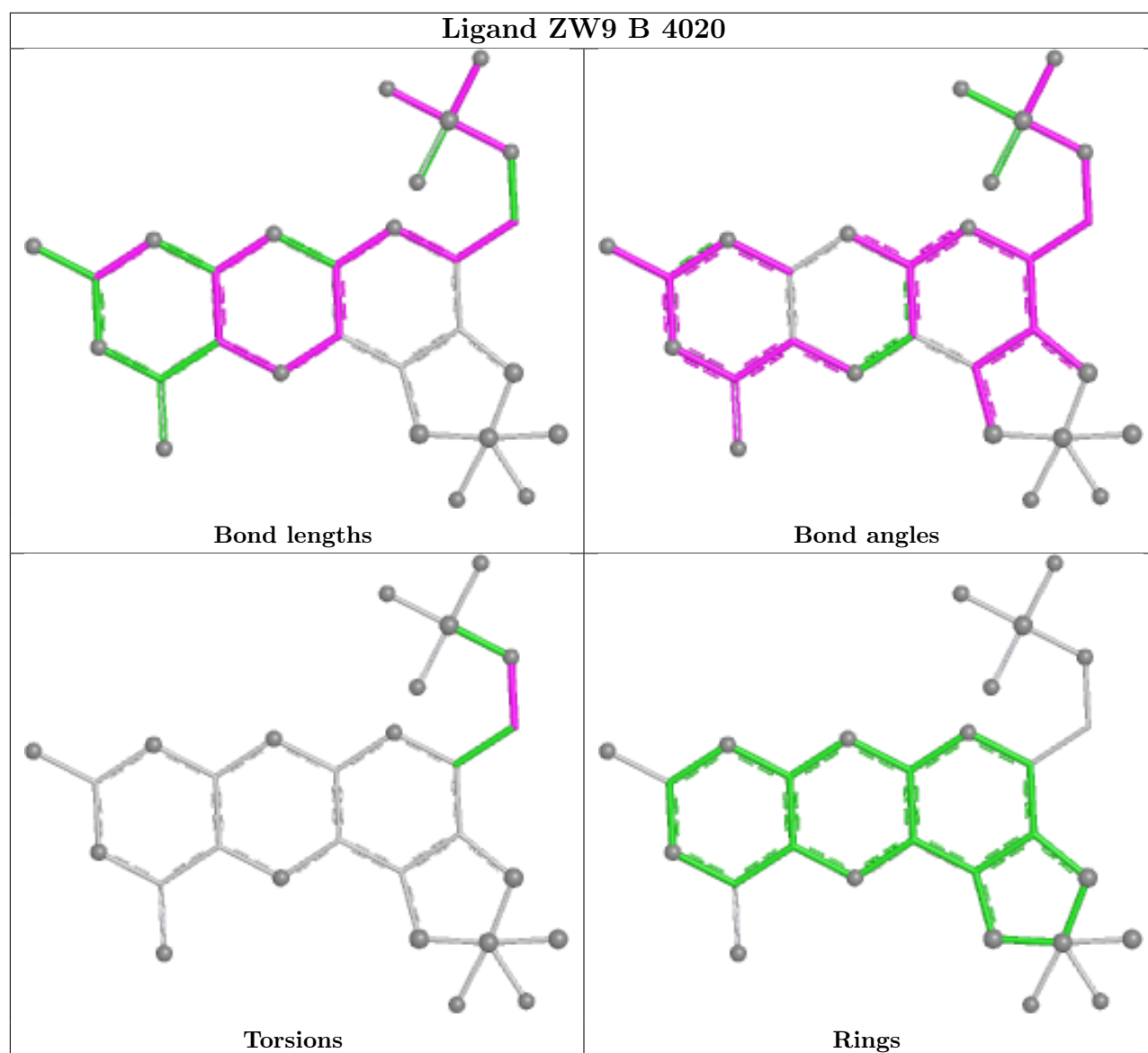
Continued on next page...

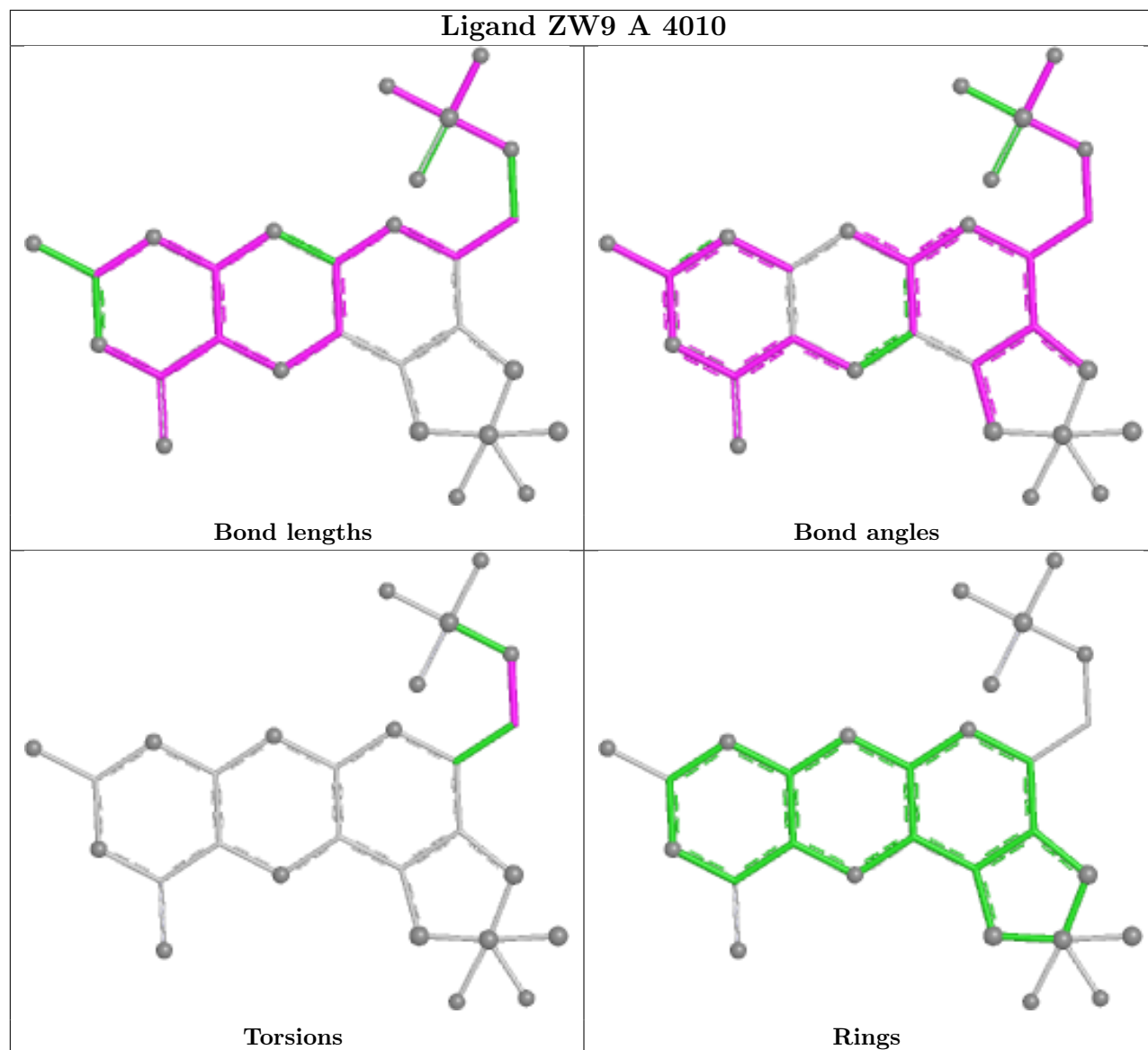
Continued from previous page...

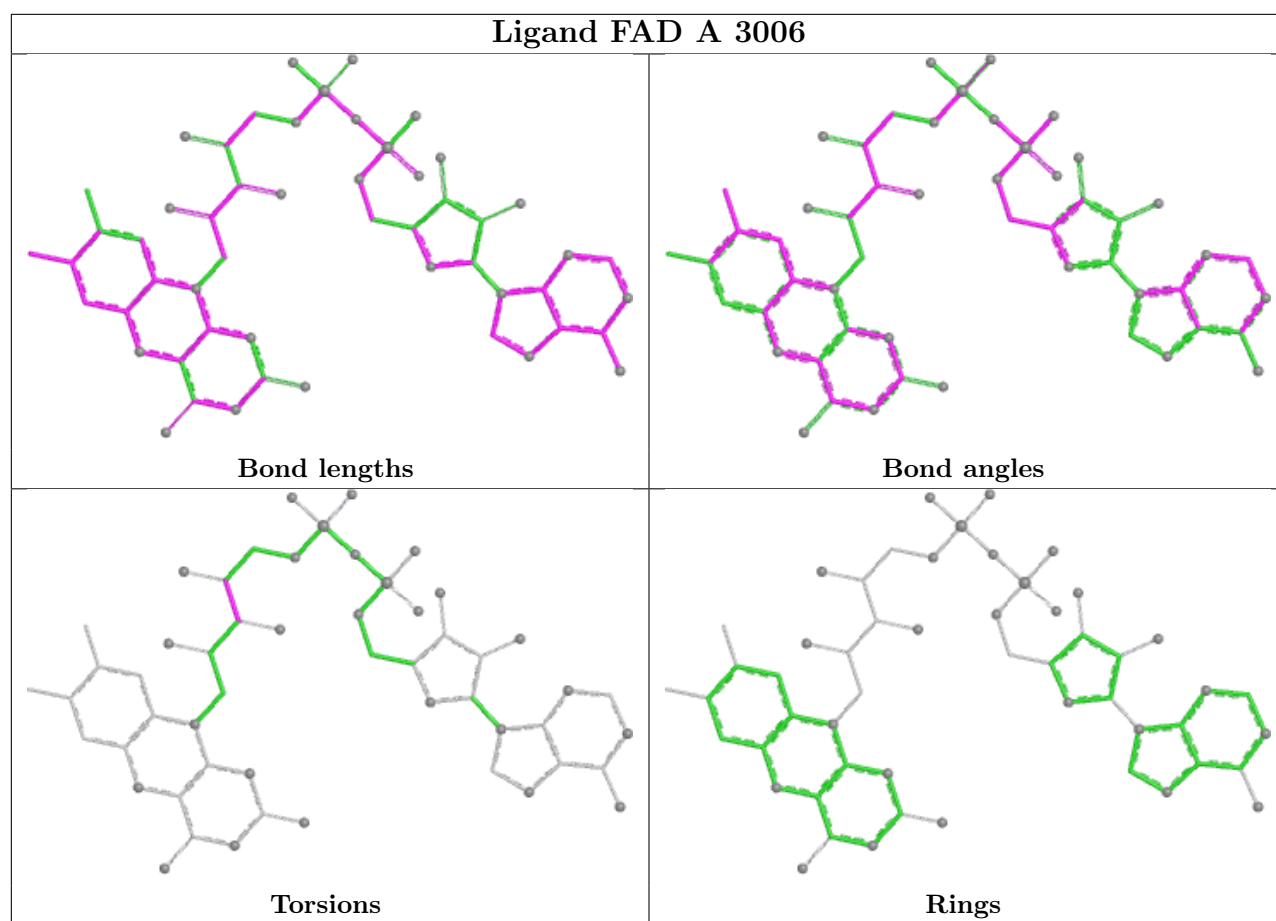
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	3007	GOL	4	0
6	A	3008	GOL	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.