



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:52 PM UTC

PDB ID : 1FIQ / pdb_00001fiq
Title : CRYSTAL STRUCTURE OF XANTHINE OXIDASE FROM BOVINE MILK
Authors : Enroth, C.; Eger, B.T.; Okamoto, K.; Nishino, T.; Nishino, T.; Pai, E.F.
Deposited on : 2000-08-04
Resolution : 2.50 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)	:	2.49

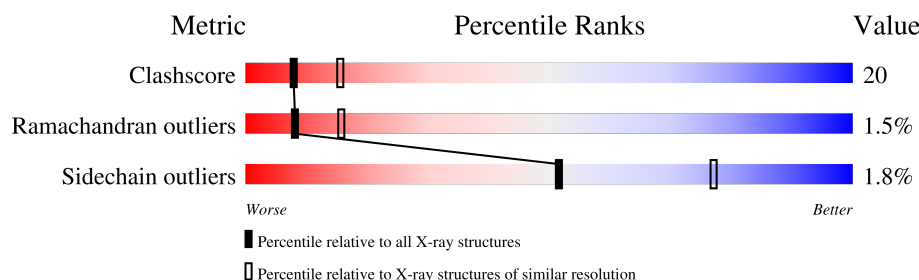
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	219	
2	B	350	
3	C	763	

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	MOS	C	1334	-	-	X	-
9	GOL	C	1336	-	X	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10106 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 OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			

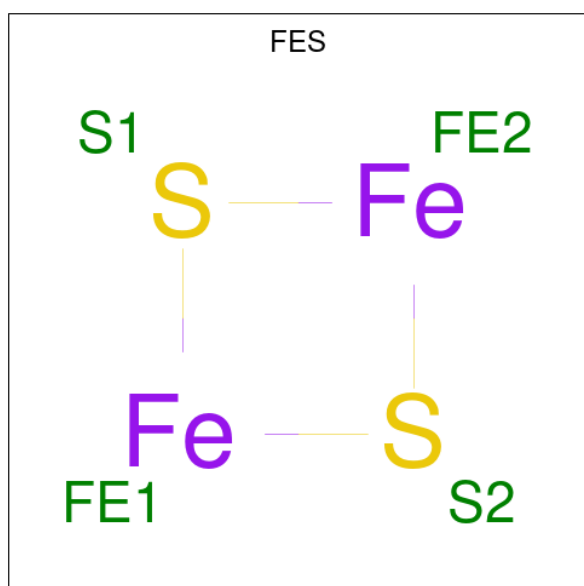
- Molecule 2 is a protein called XANTHINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			

- Molecule 3 is a protein called XANTHINE OXIDASE.

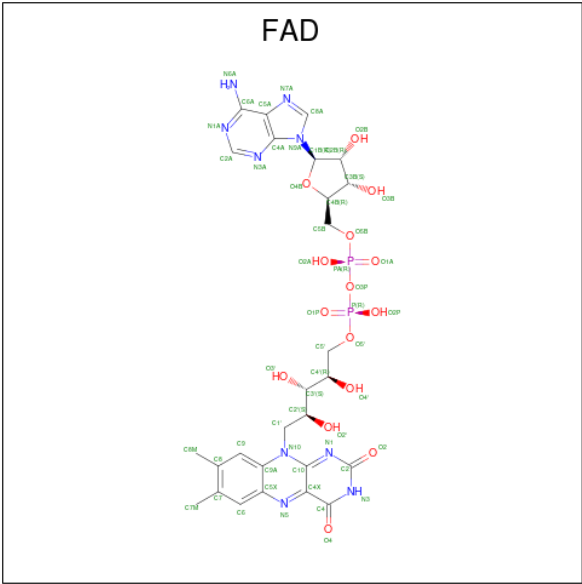
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



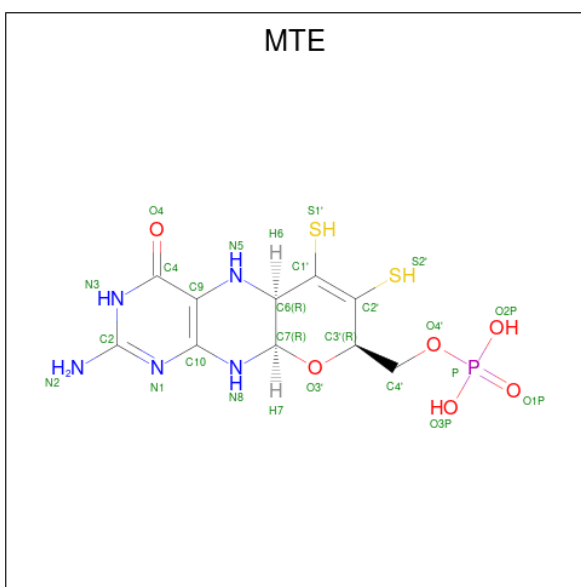
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



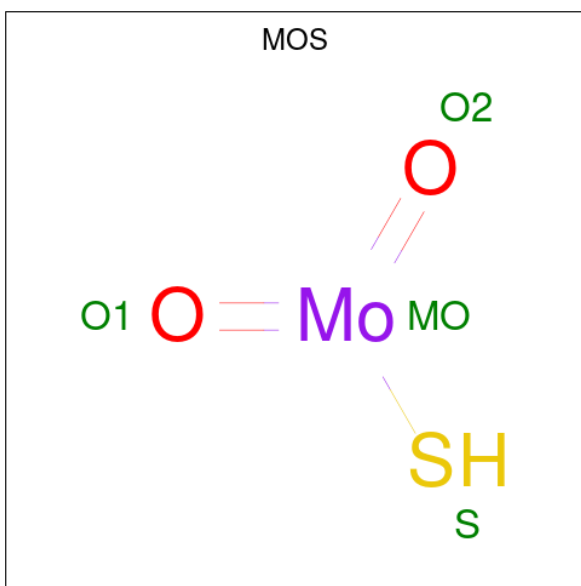
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0
			53	27	9	15	2	0

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



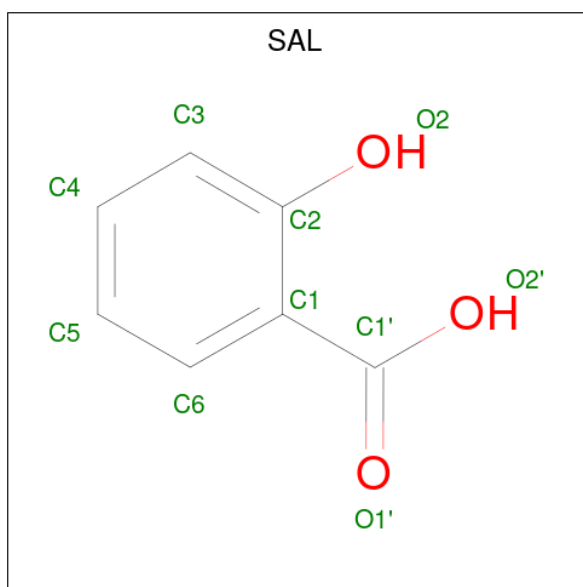
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (CCD ID: MOS) (formula: HMoO_5S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 8 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: $\text{C}_7\text{H}_6\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			10	7	3		

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



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

- Molecule 10 is water.

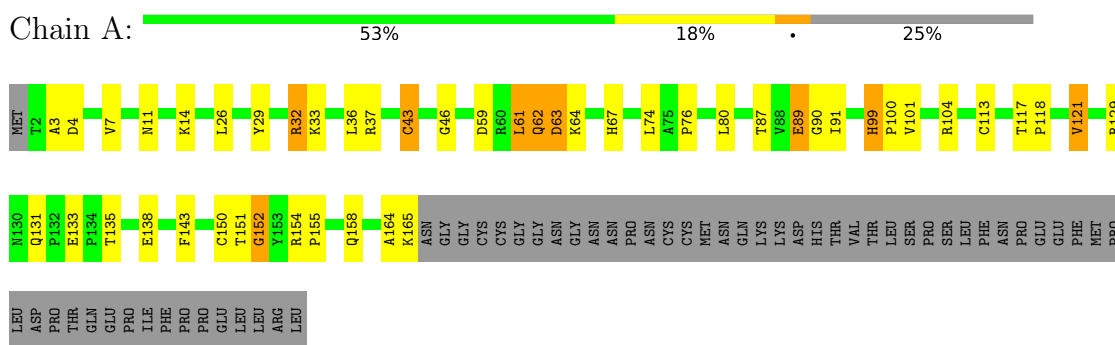
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	94	Total 94	O 94	0	0
10	B	119	Total 119	O 119	0	0
10	C	383	Total 383	O 383	0	0

3 Residue-property plots [i](#)

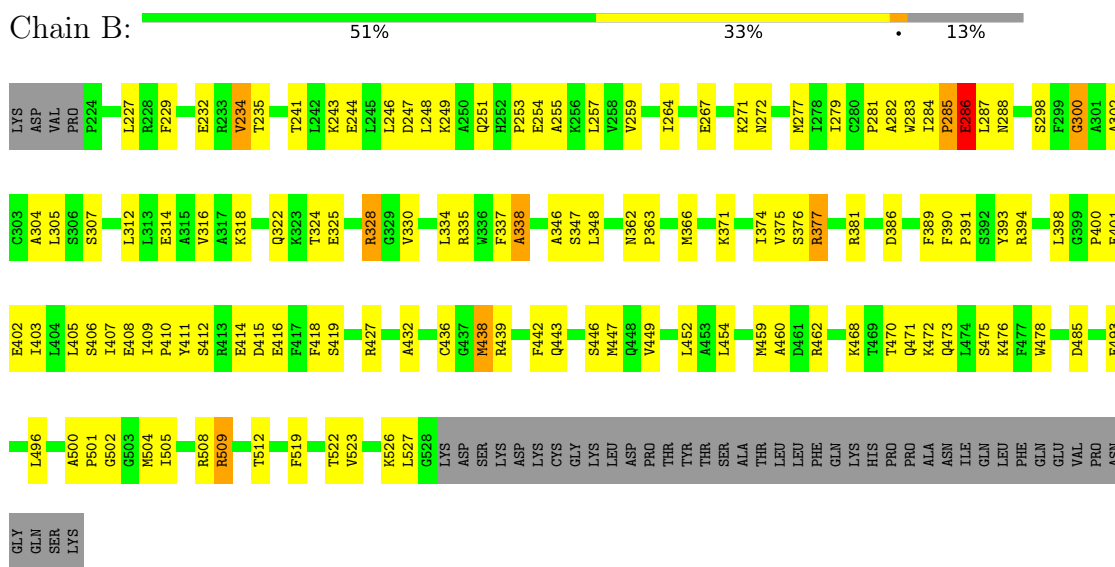
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

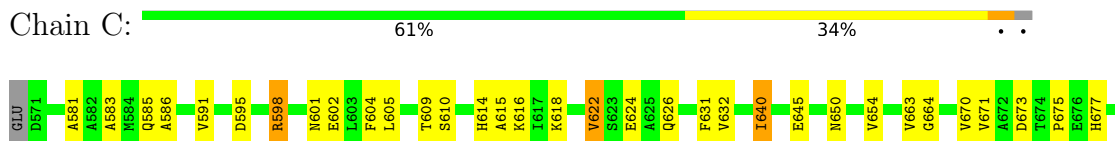
• Molecule 1: XANTHINE OXIDASE



• Molecule 2: XANTHINE OXIDASE



• Molecule 3: XANTHINE OXIDASE



I1278	D1191	Q1048	R942	T853	F763	R680
A1281	V1195	K1052	W943	I856	V764	V684
R1282	E1196	K1052	K944	I857	S765	V685
A1283	G1197	I1058	N945	A858	T766	K686
Q1284	A1198	S1059	N956	L859	Q767	K687
H1285	F1199	N1069	V964	S865	N768	V687
T1286	V1200	P1076	P965	G868	A769	T688
N1287	L1203	T1077	W968	H875	M770	T689
N1288	L1208	A1078	K973	S876	Q773	D691
N1289	E1209	S1082	Q976	I877	M779	L692
T1290	H1212	T1083	D1084	N878	V782	I695
E1291	G1217	I1085	A979	R880	P783	I696
E1292	T1221	Q1087	E983	H884	V784	I697
L1293	R1222	Q1088	K986	R895	N785	I698
F1294	G1223	Q1095	E990	R899	E699	E699
R1295	T1226	K1099	L998	N904	R786	E699
L1296	Y1227	E1102	P1002	S907	I787	D700
D1297	F1232	P1103	T1003	N908	L788	K703
A1300	I1235	K1105	G1006	T909	M794	N704
E1303	T1236	K1106	I1007	A910	G797	N705
A1308	E1238	N1107	S1008	F911	F798	S706
G1309	V1241	M1108	F1009	R912	Q799	F707
V1310	D1246	G1111	T1010	G913	R804	E711
T1315	C1247	W1116	V1011	G915	V810	L712
LEU	P1248	V1117	P1012	G916	A815	E715
CYS	N1249	M1118	F1013	P917	A816	L719
THR	K1250	Q1122	Q1016	Q918	T819	K720
GLY	K1251	F1132	A1017	I922	G820	K721
ALA	A1252	Y1133	I1021	A923	H821	K721
PRO	T1253	H1134	D1026	E924	P822	G722
GLY	Y1254	T1135	V1031	N925	V823	F723
ASN	A1255	E1143	S1032	M927	H833	A726
CYS	G1260	T1144	H1033	S928	L834	D727
LYS	E1261	M1145	G1034	E929	I835	N728
PRO	P1262	N1151	T1036	V930	T836	V729
TRP	L1264	H1151	G1035	A931	G837	V730
TRP	F1265	M1173	T1037	V932	G838	L734
LEU	G1267	L1174	M1038	T933	R839	Y735
ARG	V1270	R1175	H1043	C934	H840	I736
VAL	F1271	M1180	T1044	G935	P841	D740
	F1272	M1187	K1045	L936	F842	H741
	A1273		M1046	P937	Y743	F742
	I1274		V1047	A938	T749	Y743
				E939	L843	H747
				E940	V848	C748
				V941	P753	T749
					M851	I752
					K852	P753
						E757

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.83Å 165.40Å 154.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	97.9 (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.212 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10106	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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: MTE, FES, GOL, FAD, MOS, SAL

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	0.46	0/1277	0.97	6/1723 (0.3%)
2	B	0.38	0/2438	0.95	12/3290 (0.4%)
3	C	0.41	0/5888	0.96	26/7974 (0.3%)
All	All	0.41	0/9603	0.96	44/12987 (0.3%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	835	ILE	N-CA-C	10.37	121.10	111.45
1	A	151	THR	N-CA-C	8.30	121.90	111.69
2	B	390	PHE	CA-C-N	7.76	127.31	119.24
2	B	390	PHE	C-N-CA	7.76	127.31	119.24
3	C	743	TYR	N-CA-C	-7.49	98.73	109.96
3	C	1273	ALA	N-CA-C	-7.48	103.21	111.36
3	C	956	ASN	N-CA-C	7.34	122.19	113.23
2	B	285	PRO	N-CA-C	-7.34	99.53	111.21
2	B	286	GLU	N-CA-C	-7.26	95.34	110.80
2	B	409	ILE	CA-C-N	7.24	127.65	119.83
2	B	409	ILE	C-N-CA	7.24	127.65	119.83
3	C	1262	PRO	N-CA-C	7.12	119.39	110.70
3	C	1085	ILE	N-CA-C	6.78	116.90	110.53
1	A	152	GLY	N-CA-C	-6.76	105.74	115.27
1	A	32	ARG	N-CA-C	6.70	119.57	111.40
3	C	654	VAL	N-CA-C	-6.55	103.94	110.62
3	C	1007	ILE	N-CA-C	6.50	117.20	107.51
3	C	828	ASP	N-CA-C	-6.50	101.78	110.55
3	C	1143	GLU	N-CA-C	-6.28	98.96	109.07
1	A	99	HIS	N-CA-C	-6.05	101.73	110.08
3	C	1108	ASN	CA-C-N	5.99	125.38	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1108	ASN	C-N-CA	5.99	125.38	118.85
2	B	410	PRO	N-CA-C	5.98	120.24	111.03
3	C	1260	GLY	N-CA-C	5.78	119.64	112.64
1	A	150	CYS	N-CA-C	5.77	120.35	112.04
3	C	1198	ALA	N-CA-C	-5.68	105.00	111.14
3	C	853	THR	N-CA-C	-5.58	106.47	113.28
1	A	113	CYS	N-CA-C	-5.48	105.47	111.82
3	C	822	PRO	N-CA-C	-5.37	102.76	111.19
2	B	300	GLY	N-CA-C	-5.30	104.33	111.54
3	C	1078	ALA	N-CA-C	5.27	114.80	107.73
3	C	1011	VAL	CA-C-N	5.27	126.43	119.84
3	C	1011	VAL	C-N-CA	5.27	126.43	119.84
2	B	436	CYS	N-CA-C	5.27	117.08	109.07
2	B	234	VAL	N-CA-C	5.25	116.93	108.85
3	C	698	ILE	N-CA-C	-5.20	105.32	110.62
3	C	1026	ASP	N-CA-C	-5.12	106.63	112.92
2	B	509	ARG	N-CA-C	-5.09	105.65	111.14
3	C	1135	THR	CA-C-N	5.07	125.01	119.78
3	C	1135	THR	C-N-CA	5.07	125.01	119.78
2	B	411	TYR	N-CA-C	-5.04	103.40	110.50
3	C	640	ILE	CA-C-N	5.02	124.51	119.19
3	C	640	ILE	C-N-CA	5.02	124.51	119.19
3	C	1013	PHE	N-CA-C	5.01	119.02	113.01

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	1255	0	1265	42	0
2	B	2389	0	2459	108	0
3	C	5761	0	5685	234	1
4	A	8	0	0	1	0
5	B	53	0	31	1	0
6	C	24	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	4	0	0	3	0
8	C	10	0	4	0	0
9	C	6	0	3	5	0
10	A	94	0	0	3	0
10	B	119	0	0	1	0
10	C	383	0	0	6	2
All	All	10106	0	9457	373	3

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 20.

All (373) 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)
2:B:374:ILE:HD12	2:B:381:ARG:HH12	1.27	0.97
3:C:726:ALA:HA	3:C:851:MET:HE1	1.48	0.94
3:C:1046:MET:HE1	3:C:1087:GLY:HA2	1.52	0.89
3:C:1289:ASN:HB3	3:C:1292:GLU:HB2	1.55	0.89
2:B:438:MET:HE2	2:B:454:LEU:HD22	1.59	0.84
3:C:618:LYS:HD3	3:C:688:THR:HG21	1.58	0.84
2:B:500:ALA:HB3	2:B:505:ILE:HD11	1.59	0.83
3:C:764:VAL:HG23	3:C:766:THR:HG22	1.60	0.82
3:C:695:ILE:H	3:C:904:ASN:HD22	1.27	0.81
3:C:1180:MET:HE2	3:C:1263:PRO:HG3	1.62	0.79
3:C:833:MET:HE1	3:C:1223:GLY:N	1.97	0.79
3:C:609:THR:CG2	3:C:664:GLY:HA2	2.13	0.79
3:C:581:ALA:O	3:C:585:GLN:HG3	1.83	0.79
2:B:241:THR:CG2	2:B:243:LYS:HG2	2.14	0.78
2:B:328:ARG:HG2	2:B:328:ARG:HH11	1.49	0.78
2:B:241:THR:HB	2:B:244:GLU:HG3	1.65	0.77
7:C:1334:MOS:S	7:C:1334:MOS:MO	1.96	0.77
3:C:726:ALA:HA	3:C:851:MET:CE	2.15	0.76
2:B:286:GLU:O	2:B:287:LEU:HB2	1.84	0.75
3:C:1021:ILE:HD12	3:C:1031:VAL:HG22	1.67	0.75
3:C:1175:ARG:HG3	3:C:1238:GLU:HB3	1.68	0.73
3:C:1088:GLN:HG2	3:C:1133:TYR:CD1	2.23	0.72
3:C:848:VAL:HG21	3:C:926:TRP:HB2	1.71	0.72
3:C:1108:ASN:ND2	3:C:1111:GLY:HA3	2.06	0.70
2:B:366:MET:HE2	2:B:386:ASP:O	1.90	0.70
3:C:1249:ASN:O	3:C:1255:ALA:HA	1.93	0.69
2:B:241:THR:HG22	2:B:243:LYS:HG2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:THR:HG22	2:B:243:LYS:H	1.59	0.68
3:C:851:MET:HE3	3:C:857:VAL:HG21	1.76	0.68
3:C:1102:GLU:HB3	3:C:1103:PRO:HD3	1.75	0.67
3:C:1021:ILE:CD1	3:C:1031:VAL:HG13	2.24	0.67
2:B:285:PRO:O	2:B:286:GLU:HB2	1.95	0.67
3:C:768:ASN:ND2	3:C:1076:PRO:HB3	2.09	0.67
2:B:325:GLU:HB2	2:B:412:SER:OG	1.93	0.66
3:C:794:MET:HE3	3:C:1038:MET:HB3	1.78	0.66
3:C:622:VAL:HG23	3:C:626:GLN:HG3	1.77	0.66
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.41	0.66
3:C:979:ALA:O	3:C:983:GLU:HG3	1.96	0.65
3:C:779:MET:HG2	3:C:810:VAL:HG13	1.77	0.65
3:C:924:GLU:OE1	3:C:942:ARG:NH1	2.30	0.65
2:B:246:LEU:HB3	2:B:377:ARG:HB2	1.77	0.65
2:B:375:VAL:HG12	2:B:376:SER:N	2.11	0.65
3:C:1289:ASN:CB	3:C:1292:GLU:HB2	2.26	0.65
2:B:247:ASP:O	2:B:251:GLN:HG3	1.97	0.65
3:C:1247:CYS:N	3:C:1248:PRO:HD3	2.12	0.65
2:B:468:LYS:HB3	2:B:493:GLU:OE2	1.96	0.65
3:C:1048:GLN:HE22	3:C:1187:ASN:HB2	1.63	0.64
3:C:740:ASP:OD2	3:C:833:MET:HG2	1.97	0.64
1:A:152:GLY:HA2	3:C:1200:VAL:HG21	1.79	0.64
3:C:609:THR:HG23	3:C:664:GLY:HA2	1.79	0.64
2:B:284:ILE:HG22	2:B:285:PRO:O	1.97	0.63
3:C:1021:ILE:HD11	3:C:1031:VAL:HG13	1.80	0.63
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.16	0.63
2:B:241:THR:HG21	2:B:243:LYS:HG2	1.79	0.63
3:C:618:LYS:HD3	3:C:688:THR:CG2	2.29	0.63
3:C:833:MET:HE1	3:C:1223:GLY:CA	2.29	0.63
2:B:287:LEU:O	2:B:302:ALA:HB3	1.99	0.62
3:C:980:ARG:NH1	3:C:1175:ARG:HD3	2.14	0.62
3:C:609:THR:HG21	3:C:664:GLY:HA2	1.81	0.62
2:B:419:SER:HB2	2:B:519:PHE:CD1	2.34	0.62
3:C:695:ILE:H	3:C:904:ASN:ND2	1.97	0.62
2:B:393:TYR:CE1	2:B:394:ARG:HG2	2.33	0.62
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.80	0.62
3:C:1203:LEU:HD12	3:C:1203:LEU:O	1.99	0.62
2:B:407:ILE:HD12	2:B:407:ILE:N	2.15	0.62
3:C:880:ARG:HD2	3:C:914:PHE:HB3	1.80	0.62
3:C:747:HIS:CD2	3:C:836:THR:HG21	2.34	0.61
3:C:914:PHE:HA	9:C:1336:GOL:O2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:C	1:A:63:ASP:H	2.06	0.61
1:A:59:ASP:OD2	1:A:61:LEU:HB3	2.00	0.61
1:A:99:HIS:ND1	1:A:100:PRO:HD2	2.15	0.61
2:B:375:VAL:CG1	2:B:376:SER:N	2.64	0.61
3:C:740:ASP:CG	3:C:833:MET:HG2	2.25	0.61
3:C:1046:MET:HE1	3:C:1087:GLY:CA	2.27	0.61
2:B:286:GLU:C	2:B:288:ASN:H	2.08	0.61
3:C:752:ILE:HD12	3:C:763:PHE:HE1	1.64	0.61
3:C:986:LYS:O	3:C:990:GLU:HG3	2.01	0.61
3:C:911:PHE:O	3:C:912:ARG:C	2.44	0.61
2:B:519:PHE:O	2:B:523:VAL:HG23	2.02	0.60
3:C:757:GLU:HB3	3:C:786:ARG:HE	1.66	0.60
2:B:314:GLU:O	2:B:318:LYS:HD3	2.01	0.60
3:C:1173:ASN:O	3:C:1236:PRO:HA	2.01	0.60
1:A:32:ARG:HD3	3:C:598:ARG:NH2	2.16	0.60
2:B:504:MET:HG2	3:C:1303:GLU:OE2	2.01	0.60
3:C:964:VAL:HB	3:C:965:PRO:HD3	1.84	0.59
2:B:287:LEU:C	2:B:300:GLY:HA3	2.27	0.59
2:B:322:GLN:HG2	2:B:414:GLU:OE2	2.03	0.59
3:C:931:ALA:HA	3:C:941:VAL:HG21	1.84	0.59
2:B:285:PRO:O	2:B:286:GLU:CB	2.51	0.59
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.50	0.59
3:C:1287:ASN:ND2	3:C:1289:ASN:HB2	2.18	0.59
3:C:1278:ILE:O	3:C:1282:ARG:HG3	2.03	0.59
2:B:418:PHE:CD1	2:B:439:ARG:HB2	2.38	0.58
3:C:1088:GLN:HG3	10:C:1622:HOH:O	2.03	0.58
2:B:376:SER:HB3	2:B:402:GLU:HG2	1.86	0.57
3:C:711:GLU:N	3:C:899:ARG:NH1	2.52	0.57
3:C:868:GLY:HA3	3:C:907:SER:HA	1.85	0.57
3:C:753:PRO:HD3	3:C:816:ALA:HB1	1.85	0.57
2:B:330:VAL:O	2:B:334:LEU:HG	2.05	0.57
3:C:610:SER:O	3:C:663:VAL:O	2.22	0.57
3:C:1095:GLN:O	3:C:1099:LYS:HG2	2.05	0.57
2:B:255:ALA:HB2	2:B:277:MET:HG2	1.87	0.57
2:B:472:LYS:HG2	2:B:472:LYS:O	2.05	0.57
3:C:715:GLU:HG3	3:C:895:ARG:HB2	1.85	0.57
3:C:720:LYS:O	3:C:721:LYS:CB	2.54	0.56
3:C:703:LYS:C	3:C:704:ASN:HD22	2.14	0.56
3:C:1044:THR:O	3:C:1048:GLN:HG3	2.06	0.56
3:C:1209:GLU:HB3	3:C:1227:TYR:CZ	2.40	0.56
3:C:684:VAL:HG12	3:C:684:VAL:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1033:HIS:CD2	3:C:1035:GLY:H	2.23	0.56
7:C:1334:MOS:S	7:C:1334:MOS:O2	2.64	0.55
3:C:880:ARG:HD2	3:C:914:PHE:O	2.06	0.55
2:B:419:SER:HB2	2:B:519:PHE:HD1	1.71	0.55
1:A:152:GLY:O	3:C:1235:ILE:HG21	2.06	0.55
1:A:154:ARG:HB3	1:A:155:PRO:HD3	1.87	0.55
2:B:322:GLN:O	2:B:412:SER:HB3	2.07	0.55
3:C:829:ARG:HG3	3:C:833:MET:HE2	1.88	0.55
2:B:246:LEU:HD13	2:B:377:ARG:HA	1.88	0.55
3:C:848:VAL:HG22	3:C:859:LEU:CD1	2.37	0.55
3:C:1144:THR:O	3:C:1145:ASN:C	2.50	0.55
3:C:711:GLU:H	3:C:899:ARG:NH1	2.05	0.54
3:C:856:ILE:HD13	3:C:945:ASN:CG	2.32	0.54
2:B:376:SER:O	2:B:377:ARG:C	2.50	0.54
3:C:1058:ILE:HG13	3:C:1059:SER:N	2.23	0.54
2:B:500:ALA:HB3	2:B:505:ILE:CD1	2.34	0.54
2:B:366:MET:HE2	2:B:386:ASP:C	2.33	0.53
2:B:328:ARG:HG2	2:B:328:ARG:NH1	2.22	0.53
3:C:616:LYS:HB3	3:C:690:GLU:HB3	1.90	0.53
2:B:371:LYS:HD2	2:B:408:GLU:OE1	2.09	0.53
3:C:833:MET:HE1	3:C:1223:GLY:HA2	1.90	0.53
3:C:1082:SER:HB2	6:C:1333:MTE:O3P	2.09	0.53
3:C:1282:ARG:NH1	3:C:1308:ALA:O	2.42	0.53
3:C:1295:ARG:HA	10:C:1422:HOH:O	2.08	0.53
3:C:624:GLU:HB3	3:C:684:VAL:HG11	1.91	0.53
3:C:749:THR:HG23	3:C:764:VAL:HG12	1.91	0.53
3:C:770:MET:HE2	10:C:1702:HOH:O	2.08	0.53
2:B:284:ILE:O	2:B:286:GLU:O	2.27	0.52
2:B:406:SER:C	2:B:407:ILE:HD12	2.34	0.52
1:A:131:GLN:HE21	1:A:133:GLU:H	1.56	0.52
3:C:1143:GLU:C	3:C:1144:THR:HG23	2.34	0.52
1:A:117:THR:HB	1:A:118:PRO:HD3	1.91	0.52
3:C:601:ASN:O	3:C:821:HIS:HD2	1.93	0.52
1:A:117:THR:CG2	3:C:586:ALA:HA	2.39	0.52
2:B:381:ARG:HG3	2:B:381:ARG:HH11	1.75	0.52
3:C:934:CYS:O	3:C:936:LEU:HG	2.09	0.52
3:C:799:GLY:HA2	7:C:1334:MOS:S	2.50	0.52
2:B:257:LEU:HD23	2:B:279:ILE:HB	1.90	0.52
3:C:1003:THR:HG22	3:C:1266:LEU:HD21	1.92	0.52
3:C:1095:GLN:HB3	3:C:1099:LYS:NZ	2.25	0.51
1:A:74:LEU:O	1:A:76:PRO:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:PRO:HG3	2:B:401:GLU:HG2	1.91	0.51
3:C:645:GLU:OE2	3:C:650:ASN:HB3	2.10	0.51
3:C:604:PHE:CD2	3:C:675:PRO:HG3	2.44	0.51
1:A:61:LEU:HG	1:A:62:GLN:NE2	2.26	0.51
3:C:1017:ALA:HB1	3:C:1086:TYR:CD2	2.45	0.51
1:A:4:ASP:HB3	2:B:227:LEU:HD22	1.93	0.51
2:B:328:ARG:HH11	2:B:328:ARG:CG	2.21	0.51
3:C:1052:LYS:HD3	3:C:1254:TYR:CZ	2.46	0.51
1:A:3:ALA:HB1	10:A:687:HOH:O	2.11	0.51
3:C:605:LEU:C	3:C:605:LEU:HD23	2.36	0.51
1:A:61:LEU:C	1:A:63:ASP:N	2.68	0.51
2:B:418:PHE:HD1	2:B:439:ARG:HB2	1.76	0.51
3:C:1203:LEU:HD12	3:C:1203:LEU:C	2.36	0.50
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.93	0.50
3:C:875:HIS:CD2	3:C:879:GLU:OE2	2.64	0.50
3:C:1118:MET:O	3:C:1122:GLN:HG2	2.11	0.50
1:A:99:HIS:CE1	1:A:100:PRO:HD2	2.46	0.50
1:A:3:ALA:HB2	10:B:643:HOH:O	2.12	0.50
2:B:389:PHE:C	2:B:391:PRO:HD3	2.35	0.50
3:C:1199:PHE:CE1	3:C:1267:GLY:HA2	2.47	0.50
2:B:473:GLN:O	2:B:476:LYS:HB2	2.11	0.50
2:B:496:LEU:H	2:B:509:ARG:NH2	2.09	0.50
3:C:764:VAL:HG23	3:C:766:THR:CG2	2.36	0.50
3:C:918:GLN:O	3:C:922:ILE:HG13	2.12	0.50
3:C:632:VAL:HB	3:C:671:VAL:O	2.12	0.49
3:C:712:LEU:HD21	3:C:875:HIS:CE1	2.46	0.49
3:C:1143:GLU:O	3:C:1144:THR:HG23	2.12	0.49
1:A:37:ARG:HG2	3:C:595:ASP:HA	1.94	0.49
3:C:1016:GLN:HE21	3:C:1132:PHE:HZ	1.61	0.49
1:A:152:GLY:CA	3:C:1200:VAL:HG21	2.41	0.49
3:C:730:VAL:HG23	3:C:850:PHE:CE2	2.47	0.49
3:C:794:MET:HE1	3:C:1038:MET:HE2	1.95	0.49
3:C:1281:ALA:O	3:C:1284:GLN:HB3	2.11	0.49
2:B:267:GLU:O	2:B:271:LYS:HB3	2.13	0.49
3:C:741:HIS:CE1	3:C:838:GLY:HA2	2.48	0.49
3:C:1286:THR:CG2	3:C:1310:VAL:HB	2.43	0.49
2:B:249:LYS:NZ	2:B:400:PRO:O	2.46	0.49
3:C:1007:ILE:O	3:C:1008:SER:CB	2.60	0.49
2:B:243:LYS:HD3	2:B:243:LYS:N	2.27	0.49
3:C:1209:GLU:HB3	3:C:1227:TYR:OH	2.13	0.49
2:B:285:PRO:C	2:B:286:GLU:O	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:452:LEU:HD23	2:B:470:THR:HG22	1.95	0.48
2:B:374:ILE:HD13	2:B:398:LEU:HD23	1.95	0.48
3:C:728:ASN:HD21	3:C:852:LYS:HG2	1.77	0.48
3:C:857:VAL:O	3:C:857:VAL:HG12	2.13	0.48
3:C:696:ILE:HD13	3:C:1217:GLY:CA	2.43	0.48
2:B:375:VAL:CG1	2:B:376:SER:H	2.27	0.48
2:B:449:VAL:O	2:B:475:SER:N	2.44	0.48
1:A:91:ILE:O	1:A:99:HIS:HB2	2.14	0.48
3:C:622:VAL:HG23	3:C:622:VAL:O	2.14	0.48
2:B:257:LEU:HA	2:B:279:ILE:O	2.14	0.47
3:C:615:ALA:HA	3:C:692:LEU:HG	1.95	0.47
2:B:287:LEU:HG	2:B:405:LEU:HD12	1.97	0.47
2:B:414:GLU:O	2:B:415:ASP:HB2	2.14	0.47
5:B:606:FAD:H51A	5:B:606:FAD:H8A	1.96	0.47
3:C:1271:PHE:CE1	3:C:1300:ALA:HB2	2.48	0.47
3:C:842:PHE:CE2	3:C:865:SER:HB3	2.50	0.47
3:C:926:TRP:O	3:C:930:VAL:HG23	2.14	0.47
2:B:389:PHE:O	2:B:391:PRO:HD3	2.13	0.47
3:C:1292:GLU:O	3:C:1293:LEU:HD23	2.15	0.47
2:B:337:PHE:O	2:B:338:ALA:C	2.57	0.47
2:B:460:ALA:C	2:B:462:ARG:H	2.21	0.47
3:C:782:VAL:CG1	3:C:786:ARG:HG3	2.43	0.47
3:C:968:TRP:HZ3	3:C:1002:PRO:HD3	1.79	0.47
3:C:1270:VAL:O	3:C:1274:ILE:HG13	2.15	0.47
2:B:286:GLU:C	2:B:288:ASN:N	2.69	0.47
3:C:1284:GLN:HG3	3:C:1285:HIS:N	2.30	0.47
2:B:316:VAL:HA	2:B:324:THR:HG21	1.96	0.47
1:A:117:THR:HG22	3:C:586:ALA:HA	1.98	0.46
3:C:923:ALA:HA	3:C:926:TRP:NE1	2.30	0.46
3:C:726:ALA:CA	3:C:851:MET:HE1	2.34	0.46
3:C:909:THR:OG1	3:C:910:ALA:N	2.41	0.46
3:C:915:GLY:H	9:C:1336:GOL:HO1	1.61	0.46
1:A:154:ARG:C	1:A:154:ARG:HD2	2.41	0.46
3:C:1310:VAL:HG13	10:C:1695:HOH:O	2.16	0.46
1:A:11:ASN:OD1	1:A:90:GLY:HA3	2.15	0.46
3:C:591:VAL:HG13	3:C:595:ASP:HB2	1.97	0.46
3:C:833:MET:HE1	3:C:1222:ARG:C	2.40	0.46
3:C:1261:GLU:N	3:C:1262:PRO:CD	2.78	0.46
3:C:815:ALA:O	3:C:819:THR:HG23	2.15	0.46
3:C:1191:ASP:O	3:C:1195:VAL:HG23	2.16	0.46
3:C:699:GLU:OE2	3:C:843:LEU:HD22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1088:GLN:HG2	3:C:1133:TYR:CE1	2.50	0.46
2:B:232:GLU:OE1	3:C:677:HIS:HE1	1.99	0.46
3:C:911:PHE:C	3:C:911:PHE:CD2	2.94	0.46
3:C:1286:THR:HG22	3:C:1310:VAL:HB	1.98	0.46
3:C:720:LYS:O	3:C:721:LYS:HB2	2.15	0.45
3:C:1196:GLU:O	3:C:1200:VAL:HG23	2.16	0.45
3:C:1247:CYS:N	3:C:1248:PRO:CD	2.79	0.45
2:B:244:GLU:O	2:B:248:LEU:HG	2.17	0.45
3:C:911:PHE:HD2	3:C:912:ARG:N	2.14	0.45
3:C:782:VAL:HG13	3:C:783:PRO:HD2	1.98	0.45
3:C:839:ARG:HG3	9:C:1336:GOL:H12	1.98	0.45
3:C:911:PHE:C	3:C:911:PHE:HD2	2.24	0.45
3:C:925:ASN:O	3:C:929:GLU:HG3	2.16	0.45
2:B:246:LEU:HB3	2:B:377:ARG:CB	2.46	0.45
2:B:432:ALA:HB2	2:B:502:GLY:HA3	1.98	0.45
2:B:281:PRO:O	2:B:283:TRP:N	2.50	0.45
3:C:695:ILE:N	3:C:904:ASN:HD22	2.05	0.45
3:C:911:PHE:O	9:C:1336:GOL:H11	2.17	0.45
3:C:976:GLN:O	3:C:980:ARG:HG3	2.15	0.45
2:B:318:LYS:HD2	2:B:318:LYS:N	2.30	0.45
3:C:937:PRO:HB2	3:C:940:GLU:HB2	1.99	0.45
3:C:734:LEU:HD12	3:C:1297:ASP:OD1	2.16	0.45
1:A:29:TYR:CZ	1:A:33:LYS:HD2	2.52	0.45
2:B:259:VAL:HG11	2:B:347:SER:HB3	1.99	0.45
1:A:61:LEU:O	1:A:63:ASP:N	2.49	0.44
3:C:616:LYS:O	3:C:689:TYR:HA	2.16	0.44
1:A:101:VAL:HG12	1:A:121:VAL:HG22	2.00	0.44
2:B:427:ARG:O	2:B:427:ARG:HG2	2.16	0.44
1:A:143:PHE:HB3	3:C:1232:PHE:CE1	2.52	0.44
2:B:443:GLN:HB2	2:B:446:SER:OG	2.18	0.44
3:C:840:HIS:CE1	3:C:908:ASN:HB2	2.53	0.44
3:C:1046:MET:CE	3:C:1087:GLY:HA2	2.36	0.44
3:C:704:ASN:O	3:C:705:ASN:C	2.60	0.44
1:A:26:LEU:HD22	1:A:80:LEU:HD11	2.00	0.44
2:B:471:GLN:C	2:B:473:GLN:H	2.25	0.44
2:B:403:ILE:C	2:B:403:ILE:HD12	2.43	0.44
3:C:684:VAL:HG13	3:C:686:LYS:HZ2	1.82	0.44
3:C:821:HIS:O	3:C:823:VAL:HG23	2.18	0.44
3:C:980:ARG:NH2	3:C:998:LEU:HD11	2.33	0.44
3:C:1292:GLU:HG2	3:C:1293:LEU:N	2.33	0.44
1:A:46:GLY:HA2	4:A:602:FES:S1	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:933:THR:O	3:C:1291:LYS:HD3	2.18	0.44
2:B:393:TYR:CD1	2:B:394:ARG:HG2	2.53	0.43
3:C:614:HIS:CE1	3:C:692:LEU:HD12	2.53	0.43
3:C:1103:PRO:O	3:C:1107:LYS:HG3	2.19	0.43
1:A:67:HIS:NE2	1:A:129:ARG:NH1	2.65	0.43
3:C:749:THR:OG1	3:C:764:VAL:HG12	2.17	0.43
3:C:712:LEU:HA	10:C:1573:HOH:O	2.17	0.43
3:C:1084:ASP:OD1	3:C:1252:ALA:HB1	2.19	0.43
3:C:736:ILE:CG2	3:C:842:PHE:HB2	2.48	0.43
3:C:839:ARG:NH2	3:C:917:PRO:HG2	2.34	0.43
2:B:271:LYS:O	2:B:272:ASN:C	2.61	0.43
3:C:719:LEU:HD11	3:C:895:ARG:HD3	2.00	0.43
3:C:913:GLY:HA3	3:C:917:PRO:HG2	2.01	0.43
3:C:697:THR:H	3:C:700:ASP:HB2	1.82	0.43
3:C:840:HIS:HB2	9:C:1336:GOL:O3	2.19	0.43
3:C:1287:ASN:HD21	3:C:1289:ASN:HB2	1.81	0.43
1:A:7:VAL:HG11	1:A:14:LYS:HE3	2.01	0.43
2:B:298:SER:HA	2:B:408:GLU:HA	2.00	0.43
3:C:609:THR:HG23	3:C:664:GLY:CA	2.46	0.43
3:C:707:PHE:HB3	3:C:900:LEU:O	2.19	0.43
3:C:773:GLN:HG2	3:C:784:VAL:HG13	2.01	0.43
3:C:1175:ARG:HG3	3:C:1238:GLU:CB	2.44	0.43
3:C:1095:GLN:HB3	3:C:1099:LYS:HZ3	1.83	0.43
3:C:856:ILE:HD12	3:C:856:ILE:N	2.33	0.42
2:B:286:GLU:HB3	2:B:405:LEU:HD11	2.00	0.42
3:C:610:SER:HB3	3:C:663:VAL:O	2.18	0.42
3:C:1108:ASN:HD21	3:C:1111:GLY:HA3	1.83	0.42
10:A:687:HOH:O	2:B:229:PHE:HA	2.19	0.42
3:C:696:ILE:HD13	3:C:1217:GLY:N	2.34	0.42
3:C:680:ARG:O	3:C:684:VAL:HG23	2.19	0.42
3:C:1264:LEU:HD23	3:C:1264:LEU:C	2.44	0.42
2:B:234:VAL:HG12	2:B:235:THR:N	2.34	0.42
3:C:704:ASN:HD22	3:C:704:ASN:N	2.16	0.42
3:C:1196:GLU:HG2	3:C:1241:VAL:HG21	2.01	0.42
3:C:1246:ASP:C	3:C:1248:PRO:HD3	2.45	0.42
1:A:104:ARG:HD2	1:A:104:ARG:HA	1.69	0.42
2:B:381:ARG:HG3	2:B:381:ARG:NH1	2.34	0.42
2:B:403:ILE:HD12	2:B:403:ILE:O	2.20	0.42
2:B:508:ARG:O	2:B:512:THR:HG23	2.20	0.42
3:C:583:ALA:HB3	10:C:1444:HOH:O	2.19	0.42
3:C:631:PHE:CE1	3:C:670:VAL:HG13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:848:VAL:HG22	3:C:859:LEU:HD12	2.00	0.42
1:A:87:THR:OG1	1:A:89:GLU:HG2	2.18	0.42
3:C:602:GLU:HA	3:C:822:PRO:HG2	2.01	0.42
3:C:788:LEU:HD13	3:C:1069:ASN:HB3	2.01	0.42
1:A:62:GLN:O	1:A:63:ASP:HB3	2.19	0.41
2:B:304:ALA:O	2:B:307:SER:HB2	2.20	0.41
3:C:829:ARG:CG	3:C:833:MET:HE2	2.49	0.41
3:C:833:MET:CE	3:C:1222:ARG:C	2.93	0.41
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.85	0.41
2:B:328:ARG:NH1	2:B:328:ARG:CG	2.79	0.41
2:B:500:ALA:HA	2:B:501:PRO:HD3	1.92	0.41
3:C:840:HIS:HD2	3:C:877:ILE:HD13	1.84	0.41
3:C:1151:HIS:CE1	3:C:1251:LYS:HD2	2.55	0.41
2:B:305:LEU:HG	2:B:346:ALA:O	2.20	0.41
2:B:442:PHE:HE2	2:B:478:TRP:HB2	1.84	0.41
3:C:609:THR:CG2	3:C:610:SER:N	2.82	0.41
3:C:1143:GLU:O	3:C:1144:THR:CB	2.69	0.41
1:A:43:CYS:HA	3:C:829:ARG:HB2	2.01	0.41
1:A:158:GLN:HG3	10:A:649:HOH:O	2.20	0.41
2:B:447:MET:HE3	2:B:527:LEU:HD13	2.02	0.41
2:B:362:ASN:N	2:B:363:PRO:CD	2.83	0.41
3:C:853:THR:HG22	3:C:944:LYS:HZ2	1.85	0.41
3:C:1286:THR:HG22	3:C:1310:VAL:O	2.19	0.41
2:B:374:ILE:CD1	2:B:381:ARG:HH12	2.14	0.41
2:B:452:LEU:HD23	2:B:470:THR:HA	2.03	0.41
3:C:640:ILE:HG12	3:C:779:MET:HE1	2.03	0.41
3:C:684:VAL:CG1	3:C:686:LYS:NZ	2.83	0.41
2:B:264:ILE:HD13	2:B:267:GLU:OE2	2.20	0.41
3:C:609:THR:HG22	3:C:610:SER:O	2.21	0.41
3:C:730:VAL:HG23	3:C:850:PHE:HE2	1.85	0.41
3:C:705:ASN:HA	3:C:707:PHE:CE1	2.56	0.41
3:C:877:ILE:HG13	3:C:914:PHE:CZ	2.55	0.41
3:C:1046:MET:HE1	3:C:1086:TYR:O	2.21	0.41
3:C:1105:LYS:HG3	3:C:1116:TRP:CH2	2.55	0.41
3:C:1221:THR:HA	3:C:1226:THR:OG1	2.21	0.41
1:A:135:THR:OG1	1:A:138:GLU:HG3	2.21	0.41
3:C:624:GLU:HB2	3:C:684:VAL:HG12	2.03	0.41
3:C:850:PHE:CD2	3:C:850:PHE:N	2.88	0.41
3:C:927:MET:HE1	3:C:945:ASN:HB2	2.02	0.41
3:C:1010:THR:O	3:C:1012:PRO:HD3	2.20	0.41
3:C:1033:HIS:CE1	3:C:1046:MET:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1037:GLU:HB2	3:C:1043:HIS:CD2	2.55	0.41
3:C:736:ILE:O	3:C:736:ILE:HG23	2.20	0.41
1:A:117:THR:HG21	3:C:586:ALA:HA	2.03	0.40
1:A:164:ALA:O	1:A:165:LYS:HB2	2.20	0.40
2:B:254:GLU:OE1	2:B:254:GLU:N	2.51	0.40
2:B:459:MET:HE2	2:B:512:THR:HG21	2.03	0.40
2:B:522:THR:HG22	2:B:526:LYS:HE3	2.03	0.40
3:C:742:PHE:CZ	3:C:829:ARG:HD3	2.56	0.40
2:B:374:ILE:HD13	2:B:398:LEU:CD2	2.50	0.40
2:B:442:PHE:CE1	2:B:527:LEU:HD21	2.57	0.40
3:C:618:LYS:HB3	3:C:688:THR:HG22	2.04	0.40
3:C:853:THR:HG22	3:C:853:THR:O	2.22	0.40
2:B:416:GLU:OE1	2:B:439:ARG:NE	2.49	0.40
3:C:880:ARG:O	3:C:884:HIS:HD2	2.05	0.40
3:C:804:ARG:N	3:C:804:ARG:HD2	2.36	0.40
1:A:61:LEU:HG	1:A:62:GLN:N	2.37	0.40
2:B:271:LYS:O	2:B:271:LYS:HG3	2.22	0.40
2:B:427:ARG:HD3	3:C:1212:HIS:CG	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1509:HOH:O	10:C:1509:HOH:O[3_556]	1.82	0.38
3:C:973:LYS:NZ	3:C:973:LYS:NZ[4_556]	1.86	0.34
10:C:1598:HOH:O	10:C:1598:HOH:O[3_556]	1.99	0.21

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	162/219 (74%)	152 (94%)	5 (3%)	5 (3%)	3 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	303/350 (87%)	274 (90%)	25 (8%)	4 (1%)	9	18
3	C	743/763 (97%)	687 (92%)	47 (6%)	9 (1%)	10	20
All	All	1208/1332 (91%)	1113 (92%)	77 (6%)	18 (2%)	8	16

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	64	LYS
3	C	1008	SER
3	C	1287	ASN
2	B	282	ALA
3	C	719	LEU
3	C	721	LYS
3	C	912	ARG
3	C	1284	GLN
1	A	62	GLN
3	C	798	PHE
1	A	43	CYS
1	A	63	ASP
2	B	335	ARG
2	B	338	ALA
2	B	377	ARG
3	C	797	GLY
3	C	1253	ILE

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	137/187 (73%)	135 (98%)	2 (2%)	57	80
2	B	261/302 (86%)	255 (98%)	6 (2%)	44	72
3	C	624/639 (98%)	614 (98%)	10 (2%)	55	79
All	All	1022/1128 (91%)	1004 (98%)	18 (2%)	51	77

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	121	VAL
2	B	286	GLU
2	B	312	LEU
2	B	328	ARG
2	B	348	LEU
2	B	438	MET
2	B	485	ASP
3	C	598	ARG
3	C	622	VAL
3	C	711	GLU
3	C	723	PHE
3	C	743	TYR
3	C	939	GLU
3	C	1002	PRO
3	C	1016	GLN
3	C	1203	LEU
3	C	1208	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	82	HIS
1	A	130	ASN
1	A	131	GLN
1	A	146	ASN
2	B	226	GLN
2	B	272	ASN
2	B	273	GLN
2	B	351	ASN
2	B	423	GLN
2	B	471	GLN
2	B	473	GLN
3	C	614	HIS
3	C	626	GLN
3	C	677	HIS
3	C	683	HIS
3	C	704	ASN
3	C	728	ASN
3	C	821	HIS

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Mol	Chain	Res	Type
3	C	840	HIS
3	C	875	HIS
3	C	884	HIS
3	C	904	ASN
3	C	925	ASN
3	C	1016	GLN
3	C	1033	HIS
3	C	1048	GLN
3	C	1088	GLN
3	C	1095	GLN
3	C	1108	ASN
3	C	1287	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	MOS	C	1334	6	0,3,3	-	-	-		
4	FES	A	602	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SAL	C	1335	-	10,10,10	1.95	4 (40%)	13,13,13	2.17	4 (30%)
9	GOL	C	1336	-	5,5,5	6.71	5 (100%)	5,5,5	6.04	3 (60%)
6	MTE	C	1333	7	21,26,26	7.21	13 (61%)	19,40,40	3.98	13 (68%)
5	FAD	B	606	-	58,58,58	5.08	41 (70%)	85,89,89	2.04	25 (29%)
4	FES	A	601	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
8	SAL	C	1335	-	-	0/4/4/4	0/1/1/1
4	FES	A	602	1	-	-	0/1/1/1
9	GOL	C	1336	-	-	2/4/4/4	-
6	MTE	C	1333	7	-	6/6/34/34	0/3/3/3
5	FAD	B	606	-	-	2/34/50/50	0/6/6/6
4	FES	A	601	1	-	-	0/1/1/1

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1333	MTE	C7-C6	21.01	1.70	1.53
5	B	606	FAD	P-O3P	-17.11	1.41	1.59
6	C	1333	MTE	C9-C10	16.51	1.66	1.38
5	B	606	FAD	C9A-N10	11.83	1.61	1.41
9	C	1336	GOL	C3-C2	-11.82	1.06	1.51
6	C	1333	MTE	C6-N5	10.05	1.57	1.46
5	B	606	FAD	C4A-N3A	9.89	1.52	1.34
5	B	606	FAD	C6-C5X	8.88	1.53	1.40
5	B	606	FAD	C9A-C5X	8.65	1.55	1.41
5	B	606	FAD	C6-C7	8.44	1.51	1.39
5	B	606	FAD	C5A-C4A	7.87	1.53	1.39
5	B	606	FAD	C2A-N1A	7.78	1.47	1.33
5	B	606	FAD	C5A-C6A	7.59	1.62	1.41
6	C	1333	MTE	P-O4'	-7.17	1.37	1.60
5	B	606	FAD	C8-C7	6.97	1.57	1.40
6	C	1333	MTE	C4'-C3'	-6.91	1.42	1.51
6	C	1333	MTE	C9-N5	6.84	1.53	1.37
5	B	606	FAD	O4-C4	-6.79	1.10	1.23
5	B	606	FAD	C9-C9A	6.78	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606	FAD	C10-N1	6.59	1.46	1.33
6	C	1333	MTE	P-O3P	-6.49	1.30	1.54
9	C	1336	GOL	O2-C2	-6.02	1.25	1.43
6	C	1333	MTE	C10-N8	5.81	1.41	1.35
5	B	606	FAD	PA-O3P	5.44	1.65	1.59
5	B	606	FAD	O4B-C4B	5.34	1.56	1.45
5	B	606	FAD	C2A-N3A	4.65	1.42	1.33
5	B	606	FAD	C2-N3	4.65	1.49	1.39
9	C	1336	GOL	O3-C3	-4.63	1.23	1.42
9	C	1336	GOL	C1-C2	-4.50	1.34	1.51
5	B	606	FAD	O4B-C1B	4.43	1.52	1.42
5	B	606	FAD	C4X-N5	4.41	1.40	1.30
5	B	606	FAD	C9-C8	4.35	1.45	1.39
5	B	606	FAD	O2-C2	-4.31	1.15	1.24
6	C	1333	MTE	C2-N1	4.08	1.43	1.33
5	B	606	FAD	P-O5'	-4.05	1.43	1.59
5	B	606	FAD	PA-O2A	-3.95	1.37	1.55
5	B	606	FAD	C8A-N7A	-3.83	1.24	1.31
5	B	606	FAD	C5A-N7A	-3.77	1.32	1.39
5	B	606	FAD	C4-N3	3.38	1.45	1.38
5	B	606	FAD	P-O2P	-3.30	1.40	1.55
5	B	606	FAD	C5B-C4B	3.27	1.61	1.51
5	B	606	FAD	C4X-C10	3.19	1.53	1.44
8	C	1335	SAL	C1-C1'	-3.03	1.43	1.49
6	C	1333	MTE	O3'-C7	3.00	1.48	1.43
5	B	606	FAD	C6A-N1A	2.98	1.44	1.35
5	B	606	FAD	O4'-C4'	2.97	1.49	1.43
6	C	1333	MTE	C9-C4	2.83	1.50	1.41
9	C	1336	GOL	O1-C1	2.76	1.54	1.42
8	C	1335	SAL	C5-C6	2.75	1.43	1.38
5	B	606	FAD	C2'-C3'	2.75	1.58	1.53
5	B	606	FAD	C4A-N9A	-2.73	1.32	1.37
6	C	1333	MTE	P-O2P	-2.53	1.45	1.54
5	B	606	FAD	C5X-N5	2.53	1.44	1.39
8	C	1335	SAL	O2'-C1'	-2.53	1.23	1.30
6	C	1333	MTE	O3'-C3'	2.46	1.48	1.43
5	B	606	FAD	O5'-C5'	2.38	1.53	1.44
5	B	606	FAD	O3'-C3'	2.36	1.48	1.43
5	B	606	FAD	C3B-C4B	2.35	1.58	1.53
5	B	606	FAD	C10-N10	2.34	1.42	1.37
8	C	1335	SAL	C6-C1	2.32	1.43	1.39
5	B	606	FAD	C2B-C3B	2.30	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606	FAD	C1'-C2'	-2.21	1.49	1.52
5	B	606	FAD	O5B-C5B	-2.20	1.36	1.44

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1336	GOL	O3-C3-C2	10.60	158.08	110.38
6	C	1333	MTE	C2-N1-C10	8.22	127.87	113.36
9	C	1336	GOL	O2-C2-C3	7.26	139.23	109.18
6	C	1333	MTE	O2P-P-O4'	6.46	123.50	106.67
6	C	1333	MTE	O4'-P-O1P	-6.14	89.85	106.44
5	B	606	FAD	C5X-C9A-N10	-6.00	112.54	117.97
5	B	606	FAD	O5B-PA-O1A	-5.67	86.47	108.94
5	B	606	FAD	C9-C9A-N10	5.08	128.68	121.85
6	C	1333	MTE	O4-C4-C9	-5.05	115.08	127.26
6	C	1333	MTE	C4-C9-N5	4.74	129.19	116.27
6	C	1333	MTE	O3P-P-O4'	4.68	118.87	106.67
6	C	1333	MTE	O3'-C7-C6	-4.43	106.01	108.96
6	C	1333	MTE	O4'-C4'-C3'	4.38	119.39	108.58
9	C	1336	GOL	O1-C1-C2	4.15	129.06	110.38
5	B	606	FAD	C5X-N5-C4X	4.00	124.56	118.09
8	C	1335	SAL	O2'-C1'-O1'	-3.99	114.78	123.35
5	B	606	FAD	O5B-C5B-C4B	3.85	122.10	108.99
5	B	606	FAD	C4-C4X-N5	3.82	123.48	118.21
8	C	1335	SAL	C2-C1-C1'	3.75	123.85	120.00
5	B	606	FAD	C2A-N1A-C6A	3.63	124.69	118.73
5	B	606	FAD	C5A-C4A-N9A	-3.51	101.98	105.81
8	C	1335	SAL	C3-C2-C1	3.45	123.48	119.89
5	B	606	FAD	N3A-C4A-N9A	3.43	133.01	127.17
6	C	1333	MTE	N2-C2-N3	3.37	123.88	116.76
5	B	606	FAD	O4B-C4B-C3B	-3.33	98.53	105.15
5	B	606	FAD	O4B-C4B-C5B	-3.30	98.78	109.33
6	C	1333	MTE	C9-C4-N3	3.24	121.03	112.13
5	B	606	FAD	N9A-C8A-N7A	3.15	118.40	113.94
5	B	606	FAD	C10-N1-C2	2.94	123.21	116.85
5	B	606	FAD	C4X-C4-N3	2.79	120.35	113.25
6	C	1333	MTE	O3'-C7-N8	-2.78	106.08	108.61
5	B	606	FAD	O3'-C3'-C2'	-2.76	102.65	108.93
6	C	1333	MTE	N3-C2-N1	-2.68	118.42	123.32
5	B	606	FAD	C4'-C3'-C2'	-2.57	109.29	113.57
5	B	606	FAD	O2'-C2'-C3'	2.55	115.21	109.25
5	B	606	FAD	C9A-N10-C10	2.31	124.27	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	C4-N3-C2	-2.30	121.56	125.64
5	B	606	FAD	O5'-C5'-C4'	-2.28	103.28	109.36
8	C	1335	SAL	O2'-C1'-C1	2.27	121.73	115.28
5	B	606	FAD	C8M-C8-C7	2.26	125.39	120.76
5	B	606	FAD	C9A-C9-C8	2.20	123.64	119.22
5	B	606	FAD	O3P-PA-O1A	2.10	117.01	110.70
5	B	606	FAD	C8M-C8-C9	-2.02	116.01	119.57
6	C	1333	MTE	O4-C4-N3	2.01	123.89	120.11
5	B	606	FAD	O4'-C4'-C3'	2.00	113.93	109.25

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1333	MTE	C3'-C4'-O4'-P
6	C	1333	MTE	C4'-O4'-P-O1P
6	C	1333	MTE	C4'-O4'-P-O2P
6	C	1333	MTE	C4'-O4'-P-O3P
9	C	1336	GOL	O1-C1-C2-O2
9	C	1336	GOL	C1-C2-C3-O3
6	C	1333	MTE	C2'-C3'-C4'-O4'
5	B	606	FAD	C4'-C5'-O5'-P
6	C	1333	MTE	O3'-C3'-C4'-O4'
5	B	606	FAD	PA-O3P-P-O2P

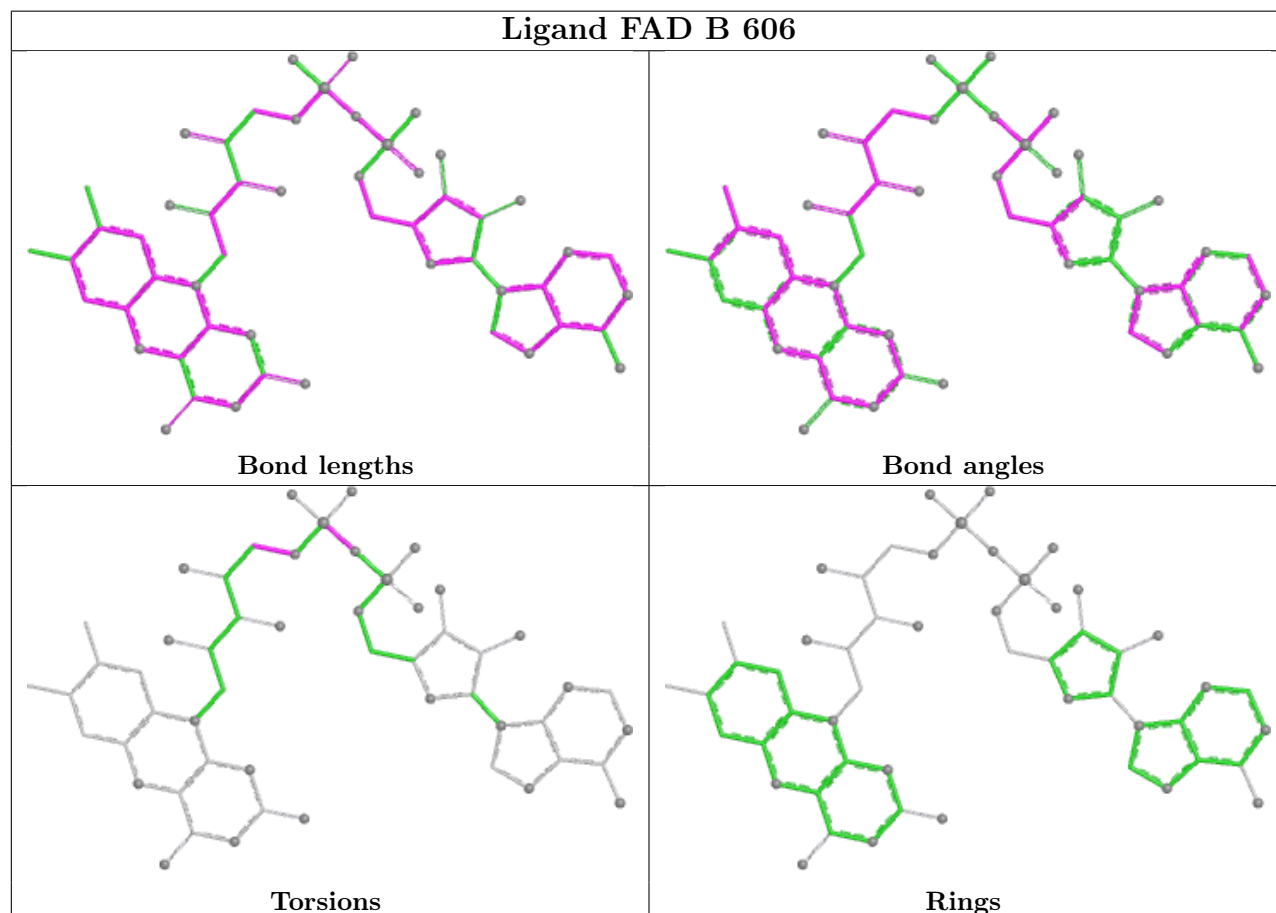
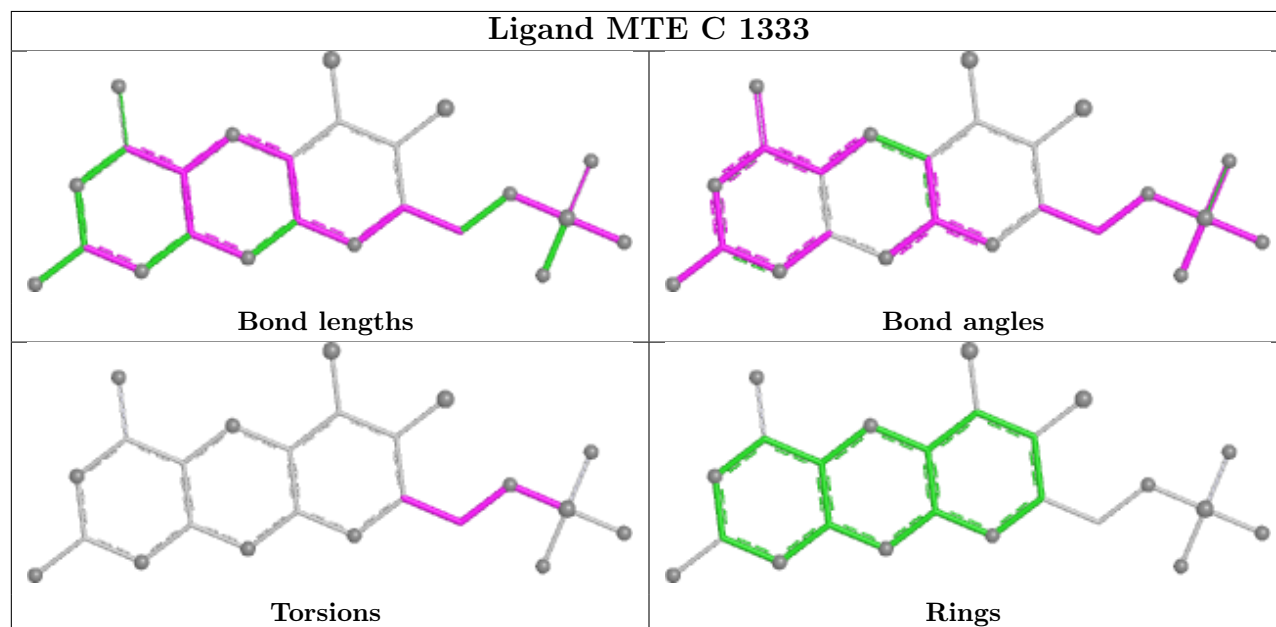
There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1334	MOS	3	0
4	A	602	FES	1	0
9	C	1336	GOL	5	0
6	C	1333	MTE	1	0
5	B	606	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.