



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:47 AM EDT

PDB ID : 1FIQ / pdb_00001fiq
Title : CRYSTAL STRUCTURE OF XANTHINE OXIDASE FROM BOVINE MILK
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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)	:	2.50

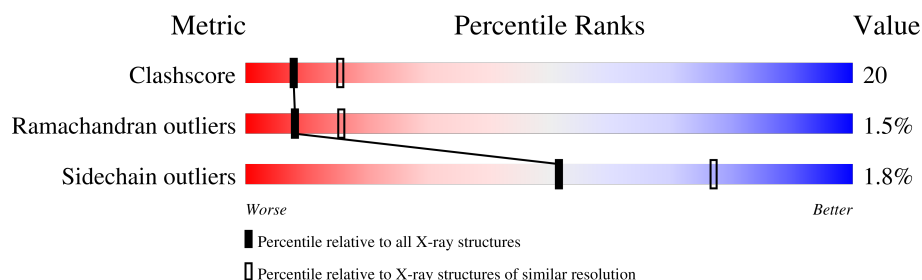
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	GOL	C	1336	-	X	X	-

2 Entry composition [i](#)

There are 9 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			

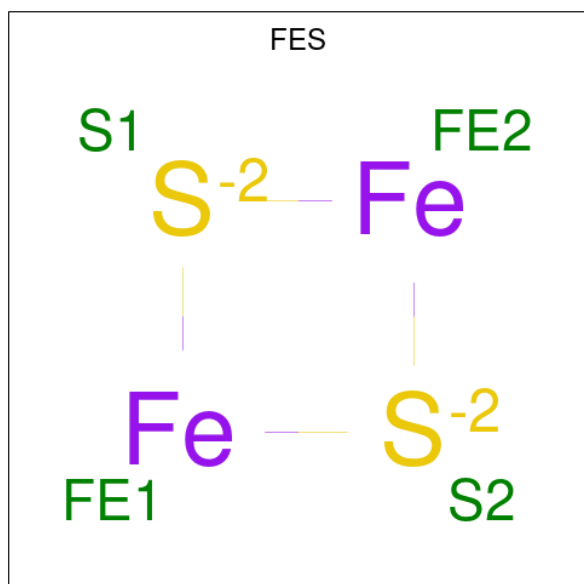
- Molecule 2 is a protein called XANTHINE OXIDASE.

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.

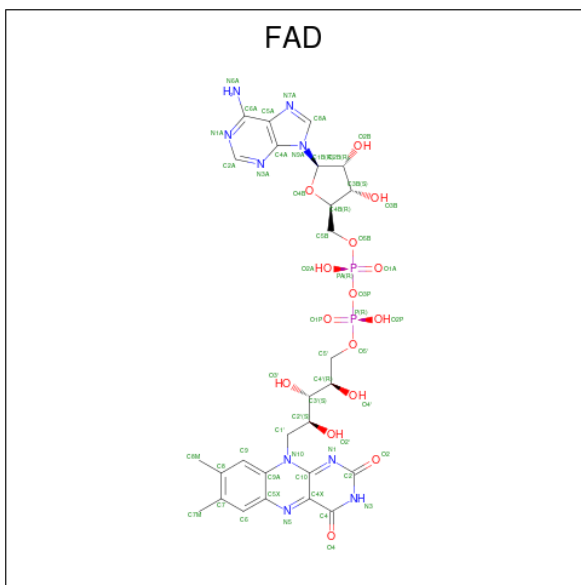
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



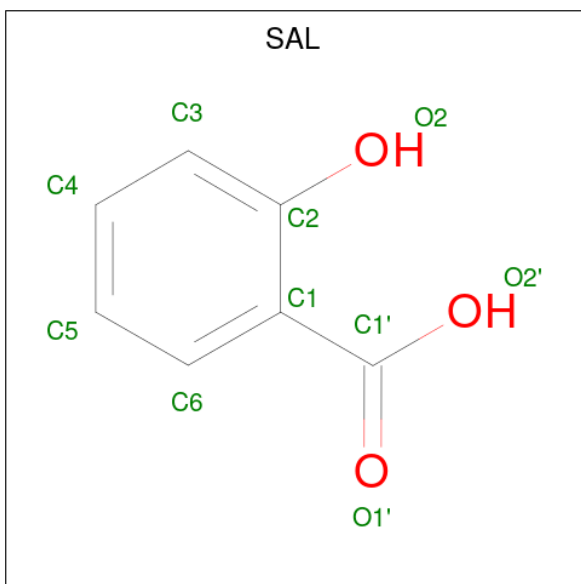
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	Fe 2	S 2	0	0
4	A	1	Total 4	Fe 2	S 2	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



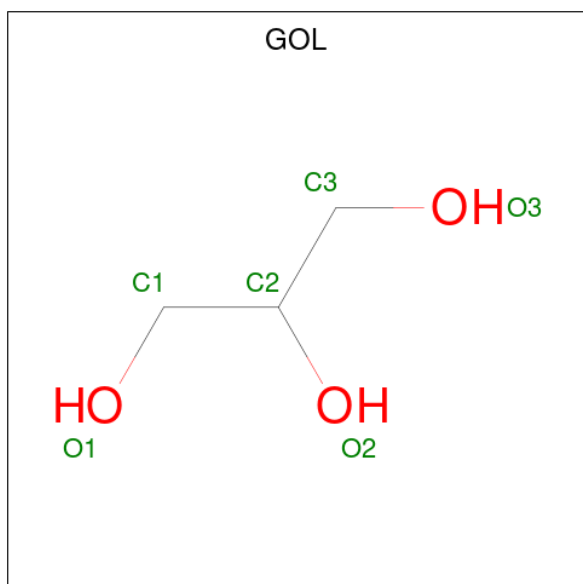
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: $C_7H_6O_3$).



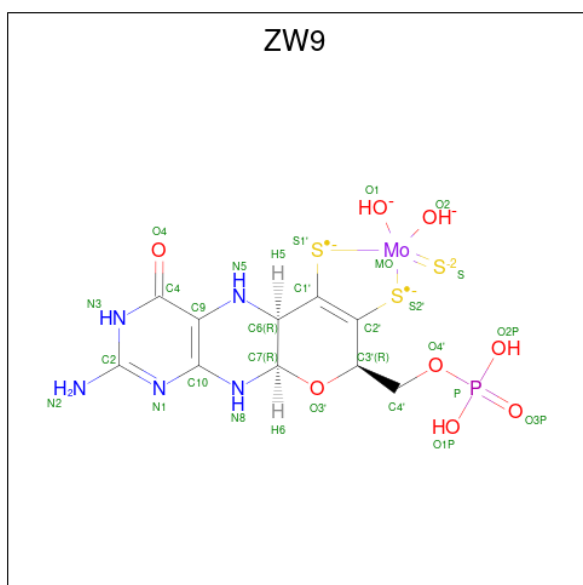
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			10	7	3		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is Molybdopterin dihydroxy-thioxo-molybdenum (CCD ID: ZW9) (formula: $C_{10}H_{14}MoN_5O_8PS_3$).



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

- Molecule 9 is water.

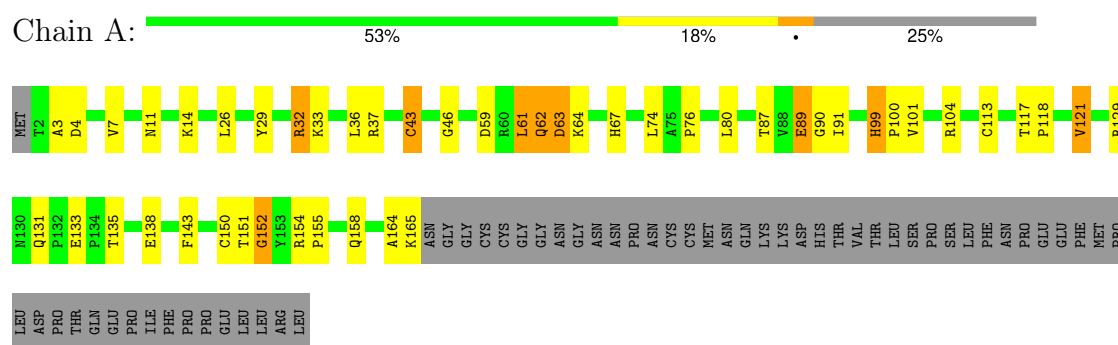
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	94	Total	O	0	0
			94	94		
9	B	119	Total	O	0	0
			119	119		
9	C	383	Total	O	0	0
			383	383		

3 Residue-property plots

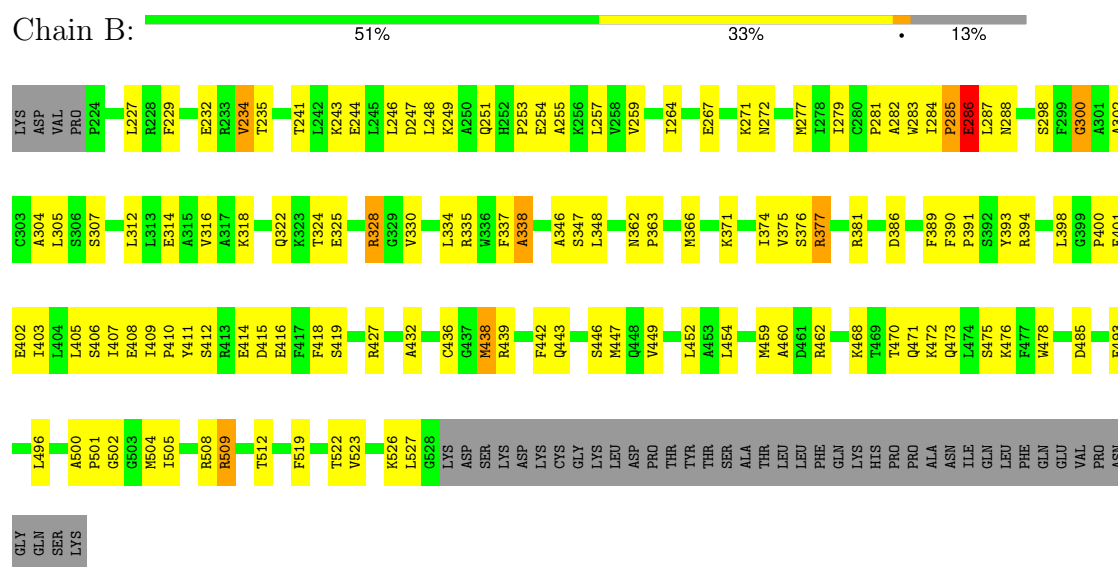
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

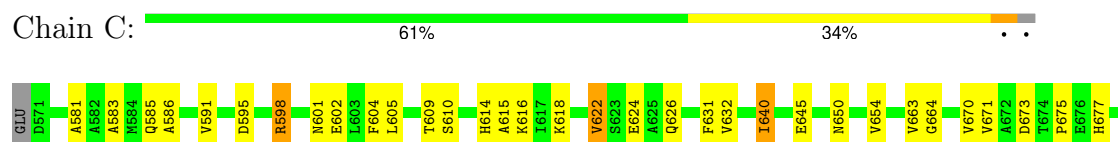
• Molecule 1: XANTHINE OXIDASE



• 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	N768
H1285	F1199	N1069	V964	S865	N769	V687
T1286	V1200	P1076	P965	G868	A769	T688
N1287	L1203	T1077	W968	I875	M770	Y689
N1288	L1208	A1078	K973	S876	Q773	D891
N1289	E1209	S1082	Q976	I877	M779	L692
T1290	H1212	T1083	D1084	N878	V782	I695
E1291	G1217	I1085	A979	R880	P783	I696
E1292	T1221	G1087	E983	H884	V784	I698
L1293	R1222	Q1088	K986	R895	N785	E699
F1294	G1223	Q1095	E990	R899	R786	E699
R1295	T1226	K1099	L998	N904	I787	D700
L1296	Y1227	E1102	P1002	S907	L788	K703
D1297	F1232	P1103	T1003	N908	M794	N704
A1300	I1235	K1105	G1006	T909	G797	N705
E1303	T1236	K1106	I1007	F911	F798	S706
A1308	E1238	N1107	S1008	R912	G799	F707
G1309	V1241	G1111	F1009	G913	E711	E711
V1310	D1246	W1116	T1010	F914	L712	L712
T1315	C1247	W1117	V1011	G915	E715	E715
LEU	P1248	M1113	P1012	G916	L719	L719
CYS	N1249	Q1122	F1013	P917	K720	K720
THR	K1250	F1132	Q1016	Q918	K721	K721
GLY	K1251	Y1133	A1017	I922	G722	G722
ALA	A1252	H1134	I1021	A923	F723	F723
PRO	I1253	T1135	D1026	E924	A726	A726
GLY	Y1254	E1143	V1031	N925	D727	D727
ASN	A1255	M1145	S1032	W926	N728	N728
CYS	G1260	H1151	H1033	M927	V729	V729
LYS	E1261	M1173	G1034	I936	V730	V730
TRP	L1266	L1174	T1036	P937	L734	L734
PRO	G1267	R1175	E1037	A938	Y735	Y735
SER	V1270	M1180	M1038	E939	I736	I736
LEU	F1271	I1274	H1043	V941	D740	D740
ARG	F1272	A1273	T1044	P941	H741	H741
VAL	I1274	M1187	K1045	F842	F742	F742
			V1047	L843	Y743	Y743
				L843	H747	H747
				L843	C748	C748
				L843	T749	T749
				L843	L752	L752
				L843	P753	P753
				L843	F850	F850
				L843	M851	M851
				L843	E757	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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SAL, FAD, ZW9, GOL, FES

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	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	6	0	3	5	0
8	C	28	0	0	0	0
9	A	94	0	0	3	0
9	B	119	0	0	1	0
9	C	383	0	0	10	2
All	All	10106	0	9447	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
9:C:1337:ZW9:S	9:C:1337:ZW9: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
2:B:241:THR:HG22	2:B:243:LYS:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	7:C:1336:GOL:O2	2.00	0.61
1:A:61:LEU:C	1:A:63:ASP:H	2.06	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	9: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
3:C:1033:HIS:CD2	3:C:1035:GLY:H	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1337:ZW9:S	9:C:1337:ZW9: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	9:C:1337:ZW9:O1P	2.09	0.53
3:C:1282:ARG:NH1	3:C:1308:ALA:O	2.42	0.53
3:C:1295:ARG:HA	9: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	9: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	9:C:1337:ZW9: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
2:B:253:PRO:HG3	2:B:401:GLU:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	9: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	9: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
2:B:452:LEU:HD23	2:B:470:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	7: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	9: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
3:C:1088:GLN:HG2	3:C:1133:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	7: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	7: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
3:C:933:THR:O	3:C:1291:LYS:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	9: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	7: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
9: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	9:C:1444:HOH:O	2.19	0.42
3:C:631:PHE:CE1	3:C:670:VAL:HG13	2.55	0.42
3:C:848:VAL:HG22	3:C:859:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	9: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
3:C:1037:GLU:HB2	3:C:1043:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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)
9:C:1509:HOH:O	9: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
9:C:1598:HOH:O	9:C:1598:HOH:O[3_556]	1.99	0.21

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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](#)

6 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	$\# Z > 2$
4	FES	A	601	1	0,4,4	-	-	-		
9	ZW9	C	1337	-	21,31,31	7.21	13 (61%)	22,52,52	4.91	16 (72%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FES	A	602	1	0,4,4	-	-	-		
5	FAD	B	606	-	58,58,58	5.08	41 (70%)	85,89,89	2.04	25 (29%)
7	GOL	C	1336	-	5,5,5	6.71	5 (100%)	5,5,5	6.04	3 (60%)
6	SAL	C	1335	-	10,10,10	1.95	4 (40%)	13,13,13	2.17	4 (30%)

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
4	FES	A	601	1	-	-	0/1/1/1
9	ZW9	C	1337	-	-	6/6/46/46	0/4/4/4
4	FES	A	602	1	-	-	0/1/1/1
5	FAD	B	606	-	-	2/34/50/50	0/6/6/6
7	GOL	C	1336	-	-	2/4/4/4	-
6	SAL	C	1335	-	-	0/4/4/4	0/1/1/1

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1337	ZW9	C7-C6	21.01	1.70	1.53
5	B	606	FAD	P-O3P	-17.11	1.41	1.59
9	C	1337	ZW9	C9-C10	16.51	1.66	1.38
5	B	606	FAD	C9A-N10	11.83	1.61	1.41
7	C	1336	GOL	C3-C2	-11.82	1.06	1.51
9	C	1337	ZW9	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
9	C	1337	ZW9	P-O4'	-7.17	1.37	1.60
5	B	606	FAD	C8-C7	6.97	1.57	1.40
9	C	1337	ZW9	C4'-C3'	-6.91	1.42	1.51
9	C	1337	ZW9	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
5	B	606	FAD	C10-N1	6.59	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1337	ZW9	P-O1P	-6.49	1.30	1.54
7	C	1336	GOL	O2-C2	-6.02	1.25	1.43
9	C	1337	ZW9	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
7	C	1336	GOL	O3-C3	-4.63	1.23	1.42
7	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
9	C	1337	ZW9	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
6	C	1335	SAL	C1-C1'	-3.03	1.43	1.49
9	C	1337	ZW9	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
9	C	1337	ZW9	C9-C4	2.83	1.50	1.41
7	C	1336	GOL	O1-C1	2.76	1.54	1.42
6	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
9	C	1337	ZW9	P-O2P	-2.53	1.45	1.54
5	B	606	FAD	C5X-N5	2.53	1.44	1.39
6	C	1335	SAL	O2'-C1'	-2.53	1.23	1.30
9	C	1337	ZW9	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
6	C	1335	SAL	C6-C1	2.32	1.43	1.39
5	B	606	FAD	C2B-C3B	2.30	1.59	1.53
5	B	606	FAD	C1'-C2'	-2.21	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606	FAD	O5B-C5B	-2.20	1.36	1.44

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1337	ZW9	C2'-C1'-S1'	13.74	127.95	120.15
7	C	1336	GOL	O3-C3-C2	10.60	158.08	110.38
9	C	1337	ZW9	C2-N1-C10	8.22	127.87	113.36
7	C	1336	GOL	O2-C2-C3	7.26	139.23	109.18
9	C	1337	ZW9	O2P-P-O4'	6.46	123.50	106.67
9	C	1337	ZW9	O4'-P-O3P	-6.14	89.85	106.44
5	B	606	FAD	C5X-C9A-N10	-6.00	112.54	117.97
9	C	1337	ZW9	C1'-C2'-S2'	-5.70	116.92	120.15
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
9	C	1337	ZW9	O4-C4-C9	-5.05	115.08	127.26
9	C	1337	ZW9	C4-C9-N5	4.74	129.19	116.27
9	C	1337	ZW9	O1P-P-O4'	4.68	118.87	106.67
9	C	1337	ZW9	O3'-C7-C6	-4.43	106.01	108.96
9	C	1337	ZW9	O4'-C4'-C3'	4.38	119.39	108.58
7	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
6	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
6	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
6	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
9	C	1337	ZW9	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
9	C	1337	ZW9	C9-C4-N3	3.24	121.03	112.13
5	B	606	FAD	N9A-C8A-N7A	3.15	118.40	113.94
9	C	1337	ZW9	O3'-C3'-C2'	2.98	113.30	109.09
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
9	C	1337	ZW9	O3'-C7-N8	-2.78	106.08	108.61
5	B	606	FAD	O3'-C3'-C2'	-2.76	102.65	108.93
9	C	1337	ZW9	N3-C2-N1	-2.68	118.42	123.32
5	B	606	FAD	C4'-C3'-C2'	-2.57	109.29	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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
6	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
9	C	1337	ZW9	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
7	C	1336	GOL	O1-C1-C2-O2
7	C	1336	GOL	C1-C2-C3-O3
9	C	1337	ZW9	C3'-C4'-O4'-P
9	C	1337	ZW9	C4'-O4'-P-O3P
9	C	1337	ZW9	C4'-O4'-P-O2P
9	C	1337	ZW9	C4'-O4'-P-O1P
9	C	1337	ZW9	C2'-C3'-C4'-O4'
5	B	606	FAD	C4'-C5'-O5'-P
9	C	1337	ZW9	O3'-C3'-C4'-O4'
5	B	606	FAD	PA-O3P-P-O2P

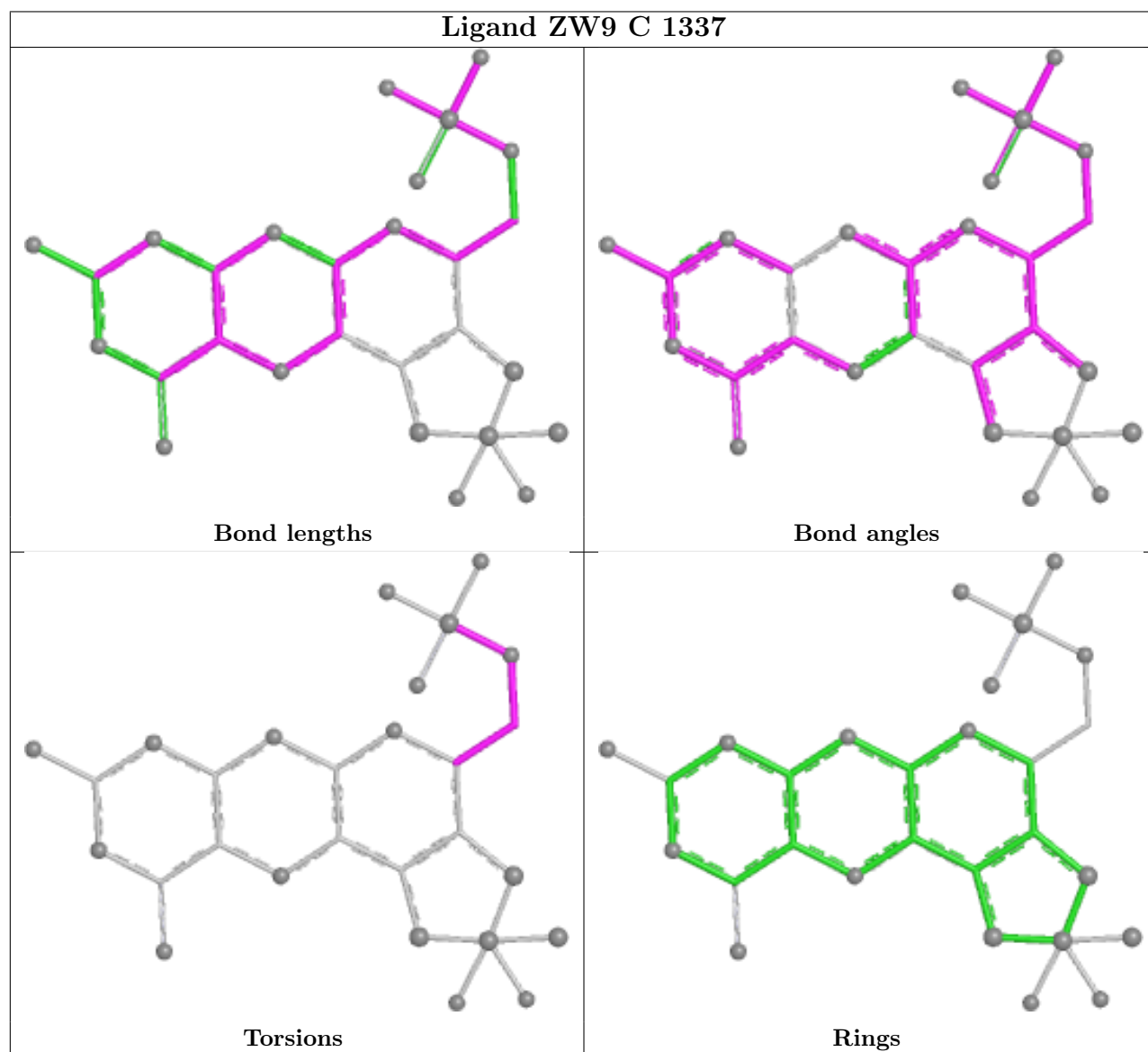
There are no ring outliers.

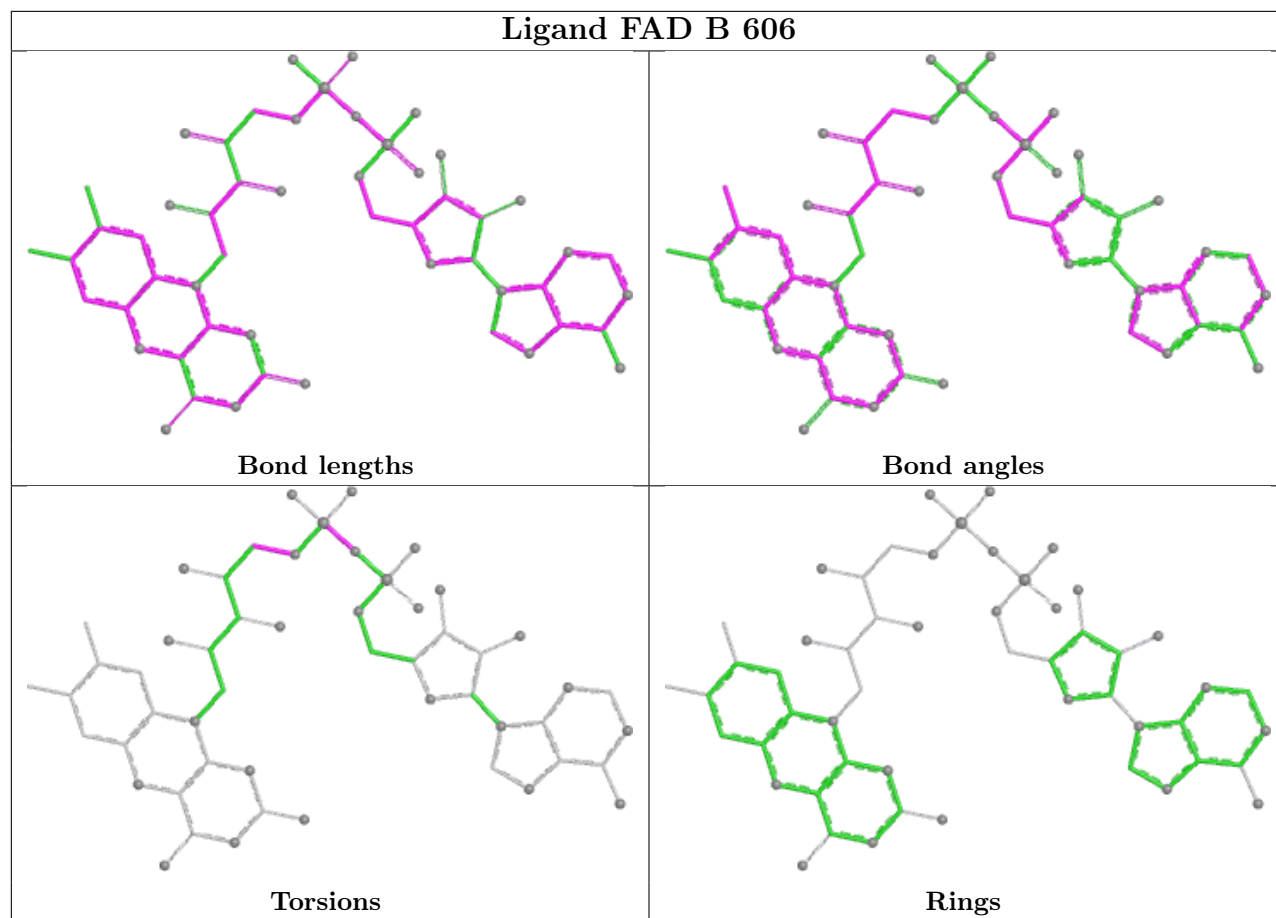
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1337	ZW9	4	0
4	A	602	FES	1	0
5	B	606	FAD	1	0
7	C	1336	GOL	5	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.