Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2026 – 02:08 AM EDT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

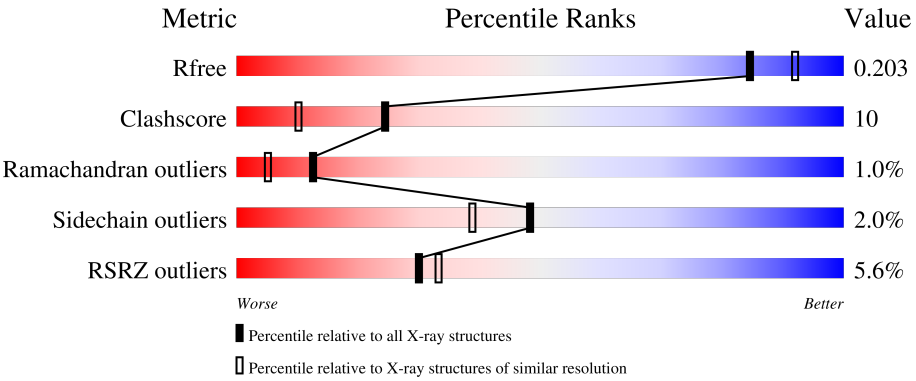
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1332	6% 77% 18%
1	B	1332	5% 77% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACY	A	1406	-	-	X	-
6	ACY	B	1406	-	-	X	-
7	GOL	A	1407	-	X	-	-
7	GOL	A	1408	-	X	-	-
7	GOL	A	1409	-	X	-	-
7	GOL	A	1410	-	X	-	-
7	GOL	B	1407	-	X	-	-
7	GOL	B	1408	-	X	-	-
7	GOL	B	1409	-	X	-	-
7	GOL	B	1410	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22481 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

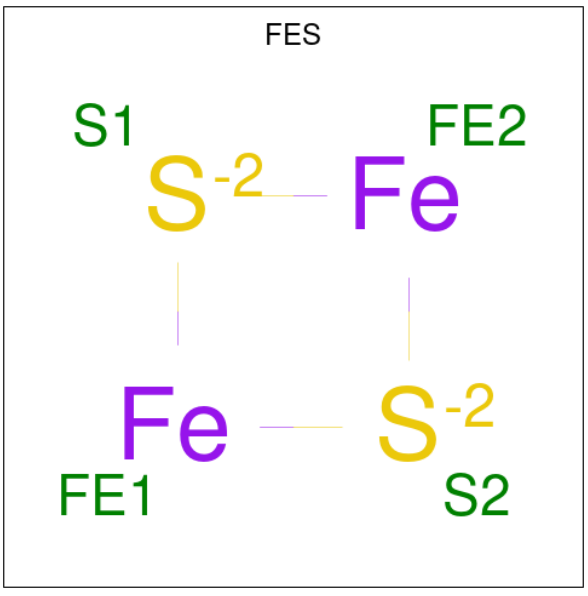
- Molecule 1 is a protein called Xanthine dehydrogenase.

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

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

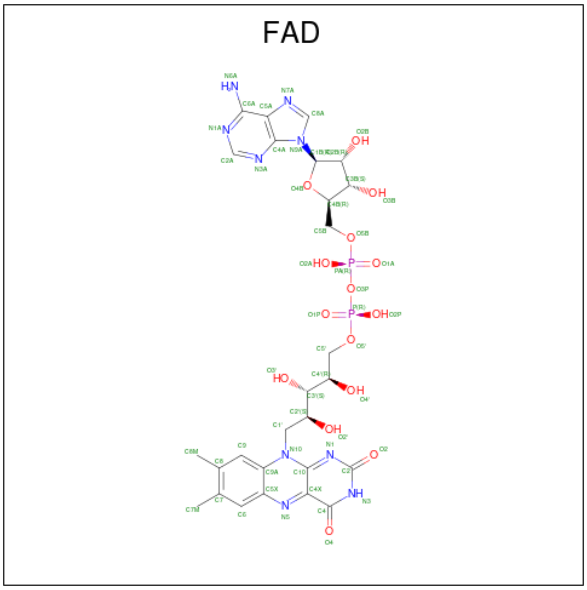
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



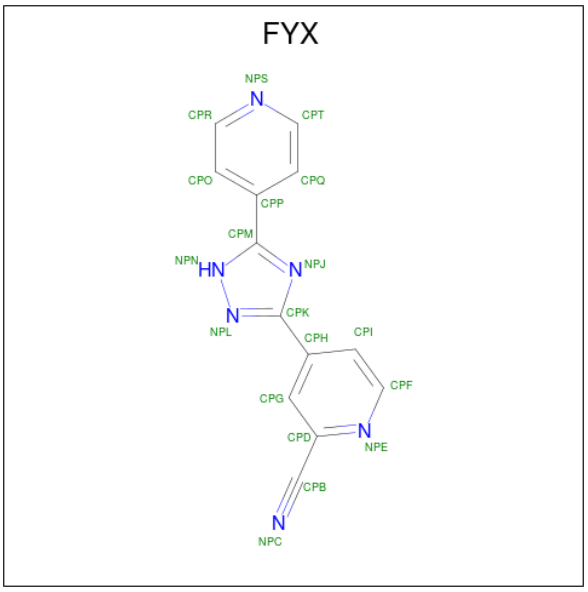
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 4 2 2	0	0
3	A	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



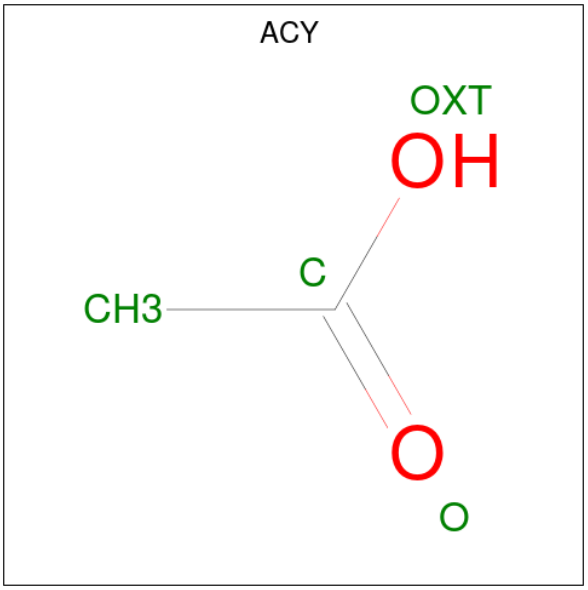
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 53 27 9 15 2	0	0
4	B	1	Total C N O P 53 27 9 15 2	0	0

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



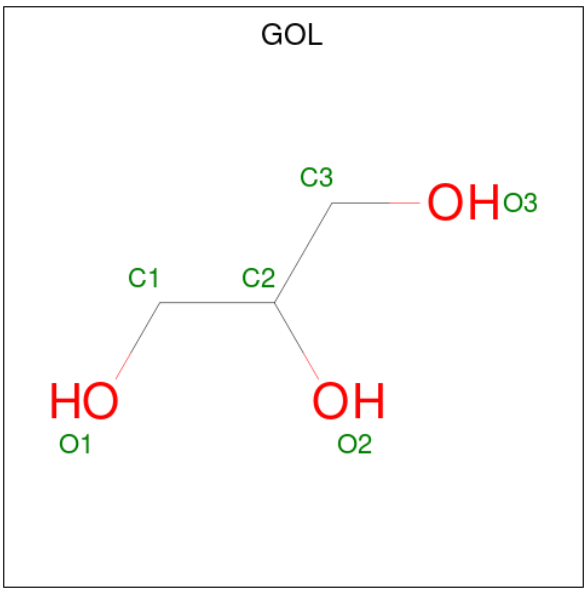
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 19 13 6	0	0
5	B	1	Total C N 19 13 6	0	0

- Molecule 6 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



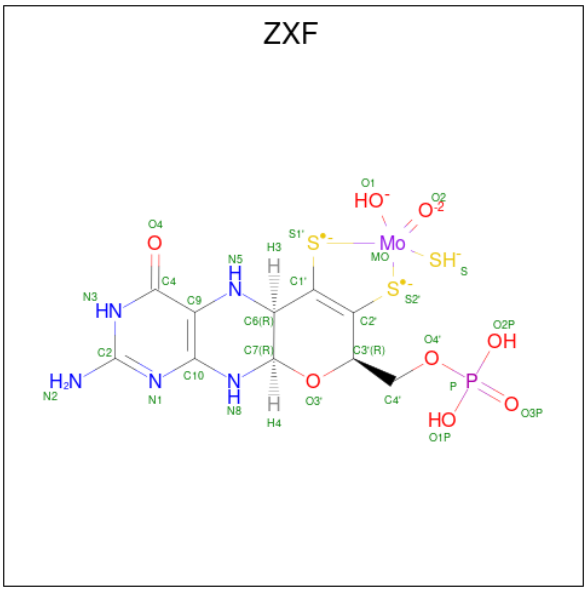
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

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



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

- Molecule 8 is Molybdopterin hydoxy-oxo-thiol-molybdenum (CCD ID: ZXF) (formula: $C_{10}H_{14}MoN_5O_8PS_3$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	A	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
8	B	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	1047	Total	O	0	0
			1047	1047		
9	B	1035	Total	O	0	0
			1035	1035		

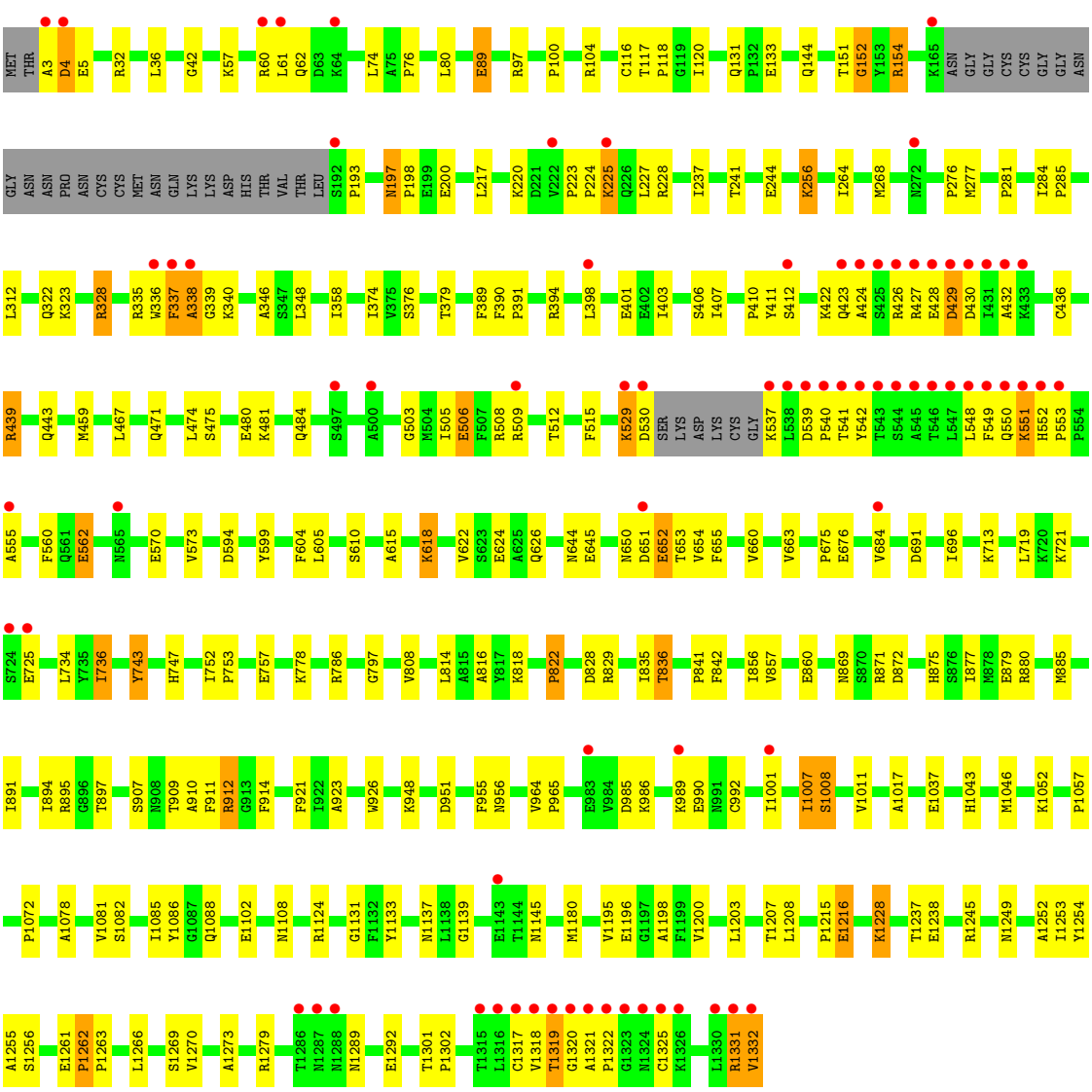
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Xanthine dehydrogenase

Chain A:

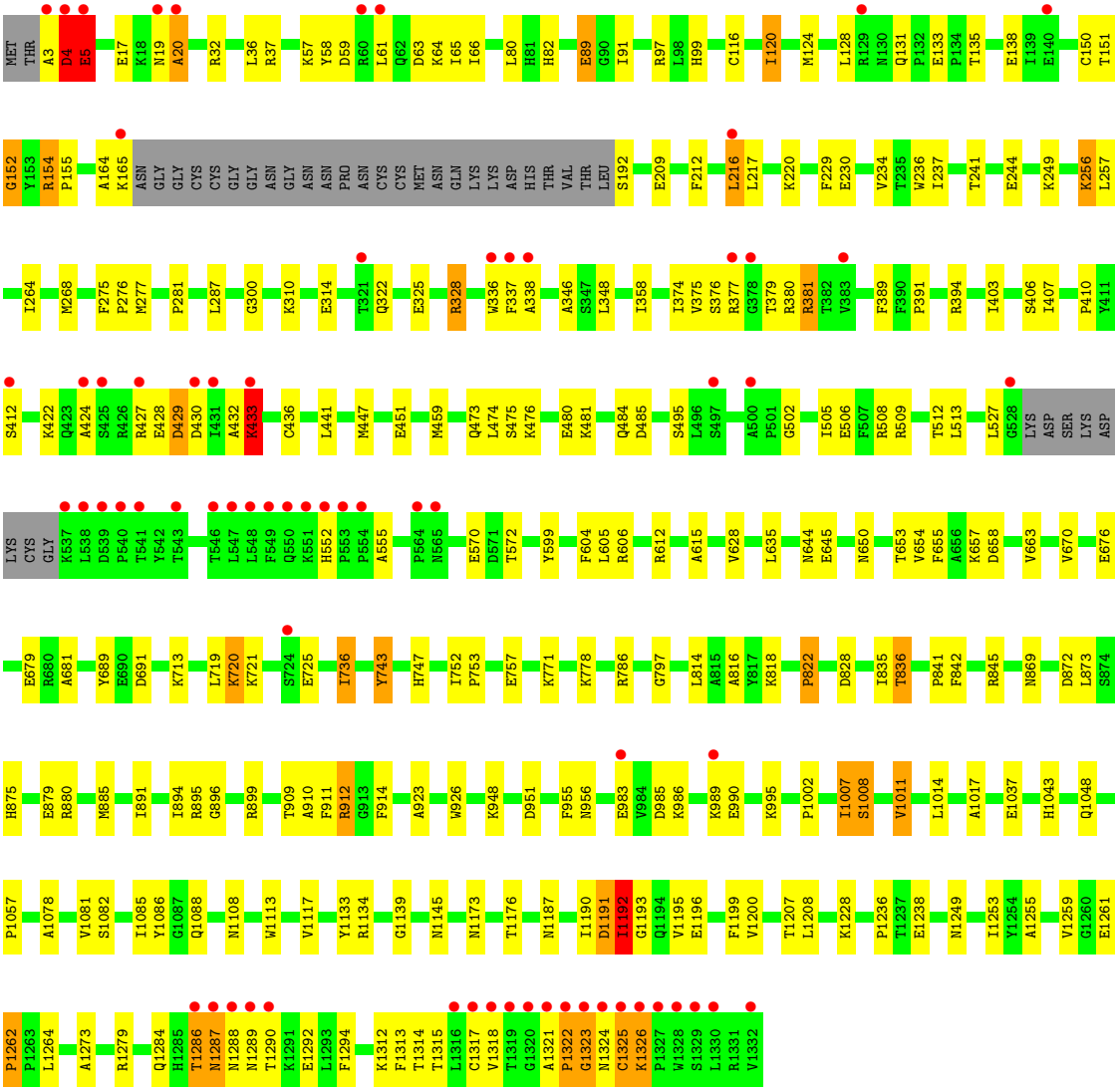




• Molecule 1: Xanthine dehydrogenase

Chain B:


5%
77%
18%


MET THR A3 D4 E5 E17 K18 N19 A20 R32 L36 R37 K57 Y58 D59 R60 L61 Q62 D63 K64 I65 I66 L80 H81 H82 E89 G90 I91 R97 L98 H99 C116 I120 M124 L128 R129 N130 Q131 P132 E133 P134 T135 E138 I139 E140 C150 T151
G152 Y153 R154 P155 A164 K165 ASN GLY GLY CYS CYS GLY GLY ASN GLY ASN ASN PRO ASN CYS CYS MET ASN GLN LYS LYS ASP HIS THR VAL THR LEU S192 E209 F212 L216 L217 K220 F229 E230 V234 T235 W236 I237 T241 E244 K249 K256 L257
I264 M268 F275 P276 M277 P281 L287 G300 K310 E314 T321 Q322 E325 R328 W336 F337 A338 A346 S347 L348 I358 I374 V375 S376 R377 G378 T379 R380 R381 T382 V383 F389 F390 P391 R394 I403 S406 I407 P410 Y411
S412 K422 Q423 A424 S425 R426 R427 E428 D429 D430 I431 A432 K433 C436 L441 M447 E451 M459 Q473 L474 S475 K476 E480 K481 Q484 D485 S495 L496 S497 A500 P501 G502 I505 E506 F507 R508 R509 T512 L513 L527 G528 LYS ASP SER LYS ASP
LYS CYS GLY K537 L538 D539 P540 T541 Y542 T543 T546 L547 L548 F549 Q550 K551 H552 P553 P554 A555 P564 N565 E570 D571 T572 Y599 F604 L605 R606 R612 A615 V628 L635 N644 E645 N650 T653 V654 F655 A656 K657 D658 V663 V670 E676
E679 R680 A681 Y689 E690 D691 K713 L719 K720 K721 S724 E725 I736 Y743 H747 I752 P753 E757 K771 K778 R786 G797 L814 A815 A816 Y817 K818 P822 D828 I835 T836 P841 F842 R845 N869 D872 L873 S874
H875 E879 R880 M885 I891 I894 R895 G896 R899 T909 A910 F911 R912 G913 F914 A923 W926 K948 D951 F955 N956 E983 Y984 D985 K986 K989 E990 K995 P1002 I1007 S1008 V1011 L1014 A1017 E1037 H1043 Q1048
P1057 A1078 V1081 S1082 I1085 Y1086 G1087 Q1088 N1108 W1113 V1117 Y1133 R1134 G1139 N1145 N1173 T1176 N1187 I1190 D1191 I1192 G1193 Q1194 V1195 E1196 F1199 V1200 T1207 L1208 K1228 P1236 T1237 E1238 N1249 I1253 Y1254 A1255 V1259 G1260 E1261
P1262 P1263 L1264 A1273 R1279 Q1284 H1285 T1286 N1287 N1288 N1289 T1290 K1291 E1292 L1293 F1294 K1312 F1313 T1314 T1315 L1316 C1317 V1318 T1319 G1320 A1321 P1322 G1323 N1324 C1325 K1326 P1327 W1328 S1329 L1330 R1331 V1332

4 Data and refinement statistics (i)

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: FYX, CA, ZXF, ACY, GOL, FAD, 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	0.34	0/10292	0.91	38/13931 (0.3%)
1	B	0.35	0/10275	0.93	36/13909 (0.3%)
All	All	0.35	0/20567	0.92	74/27840 (0.3%)

There are no bond length outliers.

All (74) bond angle outliers are listed below:

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

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

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10071	0	10071	192	0
1	B	10054	0	10053	211	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	53	0	31	3	0
4	B	53	0	31	3	0
5	A	19	0	7	0	0
5	B	19	0	7	0	0
6	A	4	0	3	3	0
6	B	4	0	3	4	0
7	A	24	0	16	5	0
7	B	24	0	15	3	0
8	A	28	0	0	3	0
8	B	28	0	0	3	0
9	A	1047	0	0	15	0
9	B	1035	0	0	14	0
All	All	22481	0	20237	403	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 (403) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LYS:NZ	9:A:1501:HOH:O	1.60	1.26
1:A:1088:GLN:NE2	7:A:1410:GOL:O3	1.86	1.08
1:A:3:ALA:HB1	1:A:228:ARG:H	1.17	1.06
1:B:1286:THR:HG22	1:B:1287:ASN:H	1.28	0.98
1:B:229:PHE:HA	9:B:1501:HOH:O	1.65	0.95
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.35	0.89
1:A:3:ALA:HB1	1:A:228:ARG:N	1.91	0.83
1:A:736:ILE:CG2	1:A:842:PHE:HB2	2.08	0.83
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.43	0.82
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.46	0.81
1:B:1289:ASN:HB3	1:B:1292:GLU:HB2	1.60	0.81
1:B:131:GLN:HE21	1:B:133:GLU:H	1.25	0.81
1:B:249:LYS:HD3	1:B:257:LEU:HD11	1.62	0.81
1:A:422:LYS:HE3	1:A:432:ALA:HB2	1.63	0.80
1:B:736:ILE:CG2	1:B:842:PHE:HB2	2.10	0.80
1:B:433:LYS:HE3	1:B:433:LYS:HA	1.64	0.80
1:A:719:LEU:HD11	1:A:895:ARG:HB2	1.65	0.79
1:A:1088:GLN:HE22	7:A:1410:GOL:C3	1.95	0.79
1:B:1253:ILE:HD12	7:B:1410:GOL:H12	1.63	0.78
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.17	0.78
1:B:17:GLU:HG3	1:B:20:ALA:HB2	1.66	0.78
1:B:1321:ALA:HB1	1:B:1322:PRO:HD2	1.64	0.78
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.49	0.77
1:B:509:ARG:O	1:B:513:LEU:HD13	1.84	0.77
1:A:594:ASP:OD1	7:A:1408:GOL:O3	2.01	0.76
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	1.84	0.76
1:B:57:LYS:HZ3	1:B:66:ILE:HD11	1.50	0.76
1:B:3:ALA:HB3	1:B:19:ASN:C	2.11	0.75
1:B:19:ASN:O	1:B:20:ALA:HB3	1.85	0.75
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.86	0.75
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.50	0.75
1:B:1088:GLN:HG2	1:B:1133:TYR:CD1	2.22	0.75
1:B:57:LYS:NZ	1:B:66:ILE:HD11	2.02	0.74
1:A:264:ILE:HG22	1:A:268:MET:HE2	1.69	0.74
1:A:509:ARG:NH1	1:A:1317:CYS:HB2	2.05	0.72
1:A:131:GLN:HE21	1:A:133:GLU:H	1.36	0.71
1:A:358:ILE:HD11	9:A:2471:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ALA:N	1:B:19:ASN:HA	2.05	0.70
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	1.87	0.70
1:A:736:ILE:O	1:A:736:ILE:HG23	1.91	0.69
1:A:719:LEU:HD11	1:A:895:ARG:CB	2.23	0.69
1:B:1286:THR:HG22	1:B:1287:ASN:N	2.05	0.68
1:A:1180:MET:HE1	1:A:1266:LEU:HD12	1.76	0.67
1:A:736:ILE:HG21	1:A:842:PHE:HB2	1.76	0.66
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.77	0.66
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.59	0.66
1:B:36:LEU:HD22	1:B:89:GLU:HG3	1.75	0.66
1:A:914:PHE:HA	6:A:1406:ACY:H1	1.77	0.66
1:A:505:ILE:O	1:A:509:ARG:HG3	1.96	0.65
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.61	0.65
1:A:1289:ASN:HD22	1:A:1292:GLU:HB2	1.59	0.65
1:B:555:ALA:HB3	1:B:1238:GLU:HG3	1.79	0.65
1:A:573:VAL:HG21	1:A:1052:LYS:HD2	1.76	0.65
1:B:495:SER:HA	1:B:509:ARG:NH1	2.12	0.65
1:A:506:GLU:HG2	1:A:1319:THR:HB	1.77	0.64
8:B:1411:ZXF:O2	8:B:1411:ZXF:MO	1.68	0.64
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.79	0.64
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.79	0.64
1:B:17:GLU:CG	1:B:20:ALA:HB2	2.28	0.64
1:B:32:ARG:HH12	1:B:676:GLU:CD	2.06	0.64
8:A:1411:ZXF:O2	8:A:1411:ZXF:MO	1.70	0.63
1:B:19:ASN:O	1:B:20:ALA:CB	2.45	0.63
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.63	0.63
1:A:541:THR:CG2	1:A:992:CYS:HB2	2.29	0.63
1:B:911:PHE:H	6:B:1406:ACY:H3	1.64	0.63
1:A:336:TRP:HB3	1:A:427:ARG:O	1.99	0.63
1:A:335:ARG:NH2	1:A:549:PHE:HB3	2.14	0.62
1:A:684:VAL:HG12	1:A:684:VAL:O	2.00	0.62
1:B:375:VAL:HG22	1:B:380:ARG:HG3	1.81	0.62
1:B:986:LYS:HA	1:B:989:LYS:NZ	2.14	0.62
1:A:217:LEU:O	1:A:220:LYS:HG2	2.00	0.62
1:A:474:LEU:O	1:A:475:SER:HB2	2.00	0.62
1:B:995:LYS:HZ1	1:B:1284:GLN:HE21	1.45	0.62
1:A:509:ARG:HG2	9:A:1504:HOH:O	1.99	0.62
1:B:422:LYS:HE3	1:B:432:ALA:HB2	1.82	0.61
1:B:736:ILE:HG21	1:B:842:PHE:HB2	1.82	0.61
1:A:1008:SER:HA	1:A:1081:VAL:HG11	1.83	0.61
1:B:495:SER:HA	1:B:509:ARG:HH12	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ILE:HD11	4:A:1404:FAD:H3B	1.82	0.61
1:B:1286:THR:CG2	1:B:1287:ASN:H	2.08	0.61
1:B:914:PHE:HA	6:B:1406:ACY:H2	1.82	0.61
1:B:911:PHE:N	6:B:1406:ACY:H3	2.15	0.61
1:A:4:ASP:HB3	9:A:1738:HOH:O	2.00	0.60
1:B:325:GLU:HB2	1:B:412:SER:OG	2.01	0.60
1:B:3:ALA:HB3	1:B:20:ALA:N	2.15	0.60
1:A:376:SER:HB3	1:A:379:THR:OG1	2.01	0.60
1:B:736:ILE:HG23	1:B:736:ILE:O	2.02	0.60
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.84	0.60
1:A:3:ALA:HA	1:A:227:LEU:HD22	1.84	0.60
1:B:61:LEU:O	1:B:61:LEU:HD23	2.02	0.59
1:A:97:ARG:NH1	1:A:97:ARG:HB2	2.17	0.59
1:A:338:ALA:HA	1:A:429:ASP:OD1	2.01	0.59
1:B:721:LYS:O	1:B:725:GLU:HG3	2.02	0.59
1:B:1008:SER:HA	1:B:1081:VAL:HG11	1.83	0.59
1:B:336:TRP:HB3	1:B:427:ARG:O	2.02	0.59
1:B:241:THR:OG1	1:B:244:GLU:HG3	2.03	0.59
1:B:1286:THR:HG22	1:B:1287:ASN:ND2	2.17	0.59
1:B:512:THR:OG1	1:B:513:LEU:HD12	2.03	0.59
1:B:328:ARG:HG2	9:B:2133:HOH:O	2.03	0.59
1:A:346:ALA:HB1	4:A:1404:FAD:H4'	1.84	0.58
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.84	0.58
1:B:474:LEU:O	1:B:475:SER:HB2	2.03	0.58
1:A:1321:ALA:HB1	1:A:1325:CYS:HB2	1.85	0.58
1:B:720:LYS:HB2	1:B:720:LYS:NZ	2.20	0.57
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.40	0.57
1:A:237:ILE:HD12	1:A:277:MET:HE3	1.87	0.56
1:A:736:ILE:HG23	1:A:842:PHE:H	1.69	0.56
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.06	0.56
1:A:32:ARG:HH12	1:A:676:GLU:CD	2.14	0.56
1:A:818:LYS:HE2	9:A:1953:HOH:O	2.04	0.56
1:B:381:ARG:CG	1:B:381:ARG:HH11	2.19	0.56
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.06	0.55
1:B:948:LYS:HG2	1:B:951:ASP:OD2	2.06	0.55
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.07	0.55
1:A:555:ALA:HB3	1:A:1238:GLU:HG3	1.88	0.55
1:B:4:ASP:CB	9:B:1501:HOH:O	2.54	0.55
1:B:909:THR:O	6:B:1406:ACY:H1	2.06	0.54
1:A:154:ARG:HD2	9:A:1858:HOH:O	2.07	0.54
1:B:1207:THR:OG1	1:B:1208:LEU:HD13	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ALA:HA	1:A:227:LEU:CD2	2.38	0.54
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.71	0.54
1:A:406:SER:C	1:A:407:ILE:HD12	2.32	0.54
1:A:430:ASP:HB2	1:A:1228:LYS:HE2	1.90	0.54
1:B:986:LYS:HA	1:B:989:LYS:HZ1	1.72	0.54
1:A:340:LYS:HE3	9:A:1719:HOH:O	2.08	0.53
1:A:407:ILE:HD12	1:A:407:ILE:N	2.23	0.53
1:A:885:MET:HE2	1:A:894:ILE:HD11	1.90	0.53
1:A:948:LYS:HG2	1:A:951:ASP:OD2	2.07	0.53
1:A:1203:LEU:HD13	1:A:1270:VAL:HG21	1.91	0.53
1:B:635:LEU:HD21	1:B:818:LYS:HG2	1.90	0.53
1:A:877:ILE:HD13	6:A:1406:ACY:H3	1.89	0.53
1:A:1001:ILE:CG1	1:A:1269:SER:HB3	2.39	0.53
1:B:875:HIS:O	1:B:879:GLU:HG3	2.09	0.53
1:A:1289:ASN:ND2	1:A:1292:GLU:HB2	2.22	0.52
1:B:612:ARG:NH1	1:B:689:TYR:HB2	2.23	0.52
1:B:1007:ILE:O	1:B:1008:SER:CB	2.57	0.52
1:B:604:PHE:HD2	7:B:1408:GOL:H11	1.74	0.52
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.43	0.52
1:B:256:LYS:HG3	1:B:275:PHE:CD2	2.44	0.52
1:A:1180:MET:HE3	1:A:1195:VAL:HG13	1.92	0.52
1:B:513:LEU:HD12	1:B:513:LEU:N	2.24	0.52
1:B:736:ILE:HG23	1:B:842:PHE:H	1.73	0.52
1:B:753:PRO:HD3	1:B:816:ALA:HB1	1.92	0.52
1:A:552:HIS:HB3	1:A:1237:THR:HG21	1.92	0.52
1:B:1007:ILE:O	1:B:1008:SER:HB3	2.08	0.52
1:B:5:GLU:HG3	9:B:2470:HOH:O	2.09	0.52
1:A:604:PHE:CD2	1:A:675:PRO:HG3	2.44	0.51
1:A:911:PHE:O	1:A:912:ARG:C	2.52	0.51
1:B:4:ASP:O	1:B:19:ASN:O	2.28	0.51
1:A:439:ARG:HH11	1:A:439:ARG:HB3	1.75	0.51
1:A:736:ILE:HG22	1:A:842:PHE:HB2	1.89	0.51
1:A:394:ARG:HD2	9:A:1944:HOH:O	2.09	0.51
1:A:719:LEU:HD13	1:A:860:GLU:OE2	2.10	0.51
1:B:3:ALA:C	9:B:1501:HOH:O	2.54	0.51
1:A:1082:SER:HB2	8:A:1411:ZXF:O1P	2.10	0.51
1:B:374:ILE:HB	1:B:381:ARG:HD3	1.91	0.51
1:A:1331:ARG:O	1:A:1332:VAL:HG12	2.11	0.51
1:A:622:VAL:O	1:A:626:GLN:HG3	2.10	0.51
1:A:624:GLU:HB2	1:A:684:VAL:HG12	1.91	0.51
1:B:381:ARG:HH11	1:B:381:ARG:HG2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:THR:HG22	1:A:992:CYS:HB2	1.92	0.51
1:A:552:HIS:CG	1:A:553:PRO:HD2	2.46	0.51
1:A:875:HIS:O	1:A:879:GLU:HG3	2.10	0.50
1:A:1301:THR:HB	1:A:1302:PRO:HD2	1.93	0.50
1:B:310:LYS:O	1:B:314:GLU:HG3	2.10	0.50
1:B:1326:LYS:O	1:B:1326:LYS:HG3	2.11	0.50
1:A:506:GLU:CD	1:A:506:GLU:H	2.18	0.50
1:A:42:GLY:O	1:A:829:ARG:HD2	2.12	0.50
1:A:1007:ILE:O	1:A:1008:SER:CB	2.59	0.50
1:B:131:GLN:HE21	1:B:133:GLU:N	2.04	0.50
1:B:911:PHE:O	1:B:912:ARG:C	2.55	0.50
1:B:1314:THR:O	1:B:1318:VAL:HG13	2.11	0.50
1:A:323:LYS:HE2	1:A:411:TYR:HB3	1.92	0.50
1:A:358:ILE:HD11	9:A:1812:HOH:O	2.11	0.50
1:B:403:ILE:C	1:B:403:ILE:HD12	2.37	0.50
1:B:407:ILE:HD12	1:B:407:ILE:N	2.26	0.50
1:B:358:ILE:HD11	9:B:2278:HOH:O	2.12	0.50
1:B:338:ALA:HA	1:B:429:ASP:OD1	2.12	0.50
1:A:374:ILE:HD13	1:A:398:LEU:CD2	2.41	0.50
1:B:1289:ASN:CB	1:B:1292:GLU:HB2	2.37	0.50
1:A:1001:ILE:HG12	1:A:1269:SER:HB3	1.93	0.50
1:B:82:HIS:HA	1:B:216:LEU:HD21	1.94	0.50
1:B:424:ALA:HB1	1:B:430:ASP:OD2	2.12	0.50
1:B:3:ALA:O	1:B:19:ASN:O	2.30	0.49
1:A:509:ARG:HH11	1:A:1317:CYS:HB2	1.77	0.49
1:A:1319:THR:O	1:A:1319:THR:HG23	2.12	0.49
1:B:1191:ASP:O	1:B:1195:VAL:HG23	2.13	0.49
1:A:508:ARG:O	1:A:512:THR:HG23	2.13	0.49
1:A:1007:ILE:O	1:A:1008:SER:HB3	2.12	0.49
1:B:192:SER:HB3	9:B:2223:HOH:O	2.13	0.49
1:B:508:ARG:O	1:B:512:THR:HG23	2.13	0.49
1:A:1052:LYS:HD3	1:A:1254:TYR:CZ	2.48	0.49
1:B:719:LEU:HD11	1:B:895:ARG:CB	2.42	0.49
1:B:64:LYS:HG2	1:B:65:ILE:N	2.28	0.49
1:B:1287:ASN:O	1:B:1288:ASN:HB2	2.12	0.49
1:B:1324:ASN:O	1:B:1326:LYS:N	2.46	0.48
1:B:1287:ASN:H	1:B:1287:ASN:HD22	1.62	0.48
1:A:428:GLU:O	1:A:429:ASP:C	2.56	0.48
1:A:459:MET:HE2	1:A:512:THR:HG21	1.96	0.48
1:B:757:GLU:HB3	1:B:786:ARG:HE	1.78	0.48
1:A:337:PHE:C	1:A:337:PHE:CD2	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:ARG:CZ	1:B:679:GLU:HG3	2.43	0.48
1:B:394:ARG:HD2	9:B:1556:HOH:O	2.13	0.48
1:A:985:ASP:O	1:A:989:LYS:HG3	2.13	0.48
1:A:1207:THR:O	1:A:1208:LEU:HD12	2.14	0.48
1:B:1011:VAL:HG23	1:B:1011:VAL:O	2.13	0.48
1:A:986:LYS:HA	1:A:989:LYS:NZ	2.29	0.48
1:A:467:LEU:O	1:A:471:GLN:HG2	2.13	0.47
1:B:61:LEU:HD23	1:B:61:LEU:C	2.39	0.47
1:B:281:PRO:HB2	1:B:287:LEU:CD1	2.43	0.47
1:B:1078:ALA:HB1	8:B:1411:ZXF:O1	2.14	0.47
1:B:217:LEU:O	1:B:220:LYS:HG2	2.14	0.47
1:A:116:CYS:O	1:A:120:ILE:HG13	2.14	0.47
1:A:1052:LYS:HE2	9:A:2248:HOH:O	2.14	0.47
1:B:124:MET:HE3	1:B:128:LEU:HG	1.95	0.47
1:B:509:ARG:O	1:B:513:LEU:CD1	2.58	0.47
1:A:736:ILE:CG2	1:A:736:ILE:O	2.61	0.47
1:A:964:VAL:HB	1:A:965:PRO:HD3	1.95	0.47
1:B:154:ARG:HD2	9:B:1968:HOH:O	2.15	0.47
1:B:1088:GLN:HG2	1:B:1133:TYR:CE1	2.48	0.47
1:A:225:LYS:C	1:A:225:LYS:HD3	2.40	0.47
1:A:503:GLY:C	1:A:505:ILE:HD12	2.40	0.47
1:A:856:ILE:HD12	1:A:856:ILE:N	2.29	0.47
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.30	0.47
1:B:1264:LEU:C	1:B:1264:LEU:HD23	2.40	0.47
1:A:144:GLN:HB2	1:A:339:GLY:HA2	1.97	0.47
1:B:3:ALA:HB1	1:B:20:ALA:O	2.15	0.47
1:B:379:THR:HG22	1:B:380:ARG:N	2.30	0.47
1:A:555:ALA:O	1:A:1238:GLU:HA	2.15	0.46
1:A:1252:ALA:HB3	1:A:1256:SER:O	2.15	0.46
1:B:216:LEU:HD13	1:B:216:LEU:O	2.15	0.46
1:B:152:GLY:HA2	1:B:1200:VAL:HG21	1.97	0.46
1:B:212:PHE:CZ	1:B:216:LEU:HD12	2.50	0.46
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.78	0.46
1:B:1315:THR:HG22	1:B:1315:THR:O	2.14	0.46
1:A:548:LEU:HD12	1:A:548:LEU:N	2.30	0.46
1:A:549:PHE:CD1	1:A:549:PHE:C	2.93	0.46
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.98	0.46
1:B:480:GLU:O	1:B:484:GLN:HG3	2.16	0.46
1:B:337:PHE:C	1:B:337:PHE:CD2	2.94	0.46
1:B:513:LEU:HD22	1:B:1317:CYS:SG	2.56	0.46
1:B:1082:SER:HB2	8:B:1411:ZXF:O1P	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLU:N	1:B:412:SER:OG	2.48	0.46
1:B:389:PHE:O	1:B:391:PRO:HD3	2.16	0.46
1:B:1287:ASN:O	1:B:1288:ASN:CB	2.64	0.46
1:A:322:GLN:O	1:A:412:SER:HB3	2.16	0.46
1:A:752:ILE:CD1	1:A:822:PRO:HB3	2.45	0.46
1:B:264:ILE:HD11	4:B:1404:FAD:H3B	1.96	0.46
1:A:424:ALA:HB1	1:A:430:ASP:OD2	2.15	0.46
1:A:615:ALA:HB2	1:A:691:ASP:HA	1.97	0.46
1:A:721:LYS:HD2	1:A:721:LYS:C	2.41	0.46
1:A:570:GLU:CD	1:A:1057:PRO:HG3	2.40	0.46
1:B:459:MET:HE2	1:B:512:THR:HG21	1.98	0.46
1:B:713:LYS:HD2	1:B:895:ARG:NH1	2.30	0.46
1:A:225:LYS:HB2	1:A:225:LYS:NZ	2.30	0.45
1:A:1124:ARG:HD2	1:B:1134:ARG:HG3	1.98	0.45
1:B:1325:CYS:O	1:B:1326:LYS:HB3	2.15	0.45
1:A:651:ASP:CG	1:A:871:ARG:HH11	2.24	0.45
1:B:506:GLU:HG3	9:B:2113:HOH:O	2.16	0.45
1:A:529:LYS:O	1:A:530:ASP:HB2	2.16	0.45
1:A:1215:PRO:HD2	1:A:1216:GLU:OE2	2.17	0.45
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.31	0.45
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.45
1:B:135:THR:OG1	1:B:138:GLU:HG3	2.16	0.45
1:B:375:VAL:HG12	1:B:376:SER:N	2.31	0.45
1:A:540:PRO:C	1:A:542:TYR:H	2.25	0.45
1:B:381:ARG:CG	1:B:381:ARG:NH1	2.79	0.45
1:B:1207:THR:O	1:B:1208:LEU:HD12	2.17	0.45
1:A:480:GLU:O	1:A:484:GLN:HG3	2.16	0.45
1:A:599:TYR:HA	1:B:599:TYR:HA	1.97	0.45
1:A:605:LEU:HD23	1:A:605:LEU:C	2.41	0.45
1:A:877:ILE:CD1	6:A:1406:ACY:H3	2.47	0.45
1:B:473:GLN:O	1:B:476:LYS:HB2	2.17	0.45
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.81	0.45
1:A:117:THR:HB	1:A:118:PRO:HD3	1.98	0.45
1:A:650:ASN:ND2	1:A:778:LYS:HE3	2.25	0.45
1:A:907:SER:N	7:A:1407:GOL:O3	2.38	0.45
1:B:376:SER:OG	1:B:379:THR:HB	2.17	0.45
1:A:423:GLN:HB2	1:A:515:PHE:HZ	1.82	0.44
1:A:1001:ILE:HD11	1:A:1269:SER:HB3	1.98	0.44
1:B:3:ALA:HB3	1:B:19:ASN:CA	2.47	0.44
1:B:97:ARG:NH1	1:B:97:ARG:HB2	2.32	0.44
1:B:376:SER:O	1:B:377:ARG:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:VAL:HG21	1:B:681:ALA:HA	1.99	0.44
1:B:1279:ARG:HD3	9:B:1527:HOH:O	2.17	0.44
1:A:276:PRO:HG2	9:A:2426:HOH:O	2.17	0.44
1:B:4:ASP:HB3	9:B:1501:HOH:O	2.16	0.44
1:B:37:ARG:HG2	9:B:2106:HOH:O	2.17	0.44
1:B:116:CYS:O	1:B:120:ILE:HG13	2.17	0.44
1:B:257:LEU:O	4:B:1404:FAD:H2B	2.16	0.44
1:B:909:THR:OG1	1:B:910:ALA:N	2.49	0.44
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.49	0.44
1:A:509:ARG:HH12	1:A:1317:CYS:HA	1.82	0.44
1:B:986:LYS:O	1:B:990:GLU:HG3	2.18	0.44
1:A:337:PHE:C	1:A:337:PHE:HD2	2.26	0.44
1:B:605:LEU:C	1:B:605:LEU:HD23	2.43	0.44
1:A:358:ILE:HD12	1:A:358:ILE:C	2.41	0.44
1:A:734:LEU:HD21	1:A:921:PHE:CE2	2.53	0.44
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.17	0.44
1:B:572:THR:OG1	1:B:1048:GLN:HG2	2.18	0.44
1:A:725:GLU:HG3	1:A:857:VAL:HG11	2.00	0.44
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.82	0.44
1:A:152:GLY:HA2	1:A:1200:VAL:HG21	2.00	0.44
1:B:237:ILE:HD11	1:B:277:MET:HE2	2.00	0.44
1:B:322:GLN:O	1:B:412:SER:HB2	2.18	0.44
1:A:1017:ALA:HB1	1:A:1086:TYR:CD2	2.53	0.43
1:A:60:ARG:HG2	1:A:60:ARG:HH11	1.82	0.43
1:A:713:LYS:HD3	1:A:897:THR:HG22	2.00	0.43
1:A:1198:ALA:HB3	1:A:1263:PRO:HB2	2.00	0.43
1:B:164:ALA:O	1:B:165:LYS:HB3	2.17	0.43
1:B:406:SER:C	1:B:407:ILE:HD12	2.43	0.43
1:B:91:ILE:O	1:B:99:HIS:HB2	2.18	0.43
1:B:428:GLU:O	1:B:429:ASP:C	2.61	0.43
1:A:74:LEU:O	1:A:76:PRO:HD3	2.19	0.43
1:A:403:ILE:C	1:A:403:ILE:HD12	2.43	0.43
1:A:509:ARG:HH12	1:A:1317:CYS:CA	2.31	0.43
1:A:651:ASP:OD2	1:A:871:ARG:NH1	2.51	0.43
1:A:1207:THR:OG1	1:A:1208:LEU:HD13	2.18	0.43
1:A:1245:ARG:HG2	9:A:1516:HOH:O	2.18	0.43
1:B:375:VAL:CG1	1:B:376:SER:N	2.82	0.43
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.53	0.43
1:A:549:PHE:HE1	1:A:551:LYS:HG2	1.84	0.43
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.32	0.43
1:B:670:VAL:HG11	1:B:681:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:ILE:CD1	1:B:822:PRO:HB3	2.48	0.43
1:B:985:ASP:O	1:B:989:LYS:HG3	2.18	0.43
1:A:624:GLU:HB3	1:A:684:VAL:HG11	2.00	0.43
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.54	0.43
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.88	0.43
1:A:618:LYS:HE3	1:A:618:LYS:HA	2.01	0.43
1:B:264:ILE:O	1:B:268:MET:HG2	2.19	0.43
1:B:1113:TRP:O	1:B:1117:VAL:HG23	2.18	0.43
1:B:346:ALA:HB1	4:B:1404:FAD:H4'	2.01	0.42
1:B:872:ASP:CG	1:B:873:LEU:H	2.25	0.42
1:A:1078:ALA:HB1	8:A:1411:ZXF:O1	2.19	0.42
1:B:1187:ASN:CG	1:B:1190:ILE:HG13	2.44	0.42
1:B:1192:ILE:HA	1:B:1195:VAL:HB	2.01	0.42
1:A:97:ARG:HB2	1:A:97:ARG:CZ	2.50	0.42
1:B:555:ALA:O	1:B:1238:GLU:HA	2.20	0.42
1:B:1279:ARG:HG2	1:B:1294:PHE:HE2	1.84	0.42
1:A:909:THR:OG1	1:A:910:ALA:N	2.49	0.42
1:B:644:ASN:O	1:B:653:THR:HA	2.20	0.42
1:B:1011:VAL:CG2	1:B:1014:LEU:HD12	2.50	0.42
1:B:1312:LYS:HE3	1:B:1313:PHE:CZ	2.54	0.42
1:B:1176:THR:HG21	1:B:1199:PHE:CZ	2.55	0.42
1:B:505:ILE:HG22	1:B:506:GLU:N	2.34	0.42
1:B:899:ARG:HD2	1:B:899:ARG:HA	1.85	0.42
1:A:610:SER:HB2	1:A:660:VAL:HG11	2.01	0.42
1:A:1253:ILE:HD12	7:A:1410:GOL:H12	2.01	0.42
1:B:154:ARG:N	1:B:155:PRO:HD2	2.34	0.42
1:B:1259:VAL:HG22	1:B:1259:VAL:O	2.19	0.42
1:B:377:ARG:NH1	1:B:377:ARG:HG2	2.35	0.42
1:B:447:MET:HG2	1:B:527:LEU:HD13	2.02	0.42
1:B:1323:GLY:O	1:B:1324:ASN:C	2.63	0.42
1:A:197:ASN:O	1:A:200:GLU:HG2	2.20	0.42
1:B:657:LYS:O	1:B:658:ASP:HB2	2.18	0.42
1:B:880:ARG:HD2	1:B:914:PHE:O	2.20	0.42
1:B:1173:ASN:O	1:B:1236:PRO:HA	2.20	0.42
1:B:1253:ILE:HD12	7:B:1410:GOL:C1	2.42	0.42
1:A:540:PRO:O	1:A:541:THR:HB	2.18	0.42
1:A:651:ASP:OD1	1:A:871:ARG:HG3	2.20	0.42
1:A:1279:ARG:HD2	9:A:1550:HOH:O	2.20	0.41
1:B:58:TYR:CD2	1:B:220:LYS:HB2	2.54	0.41
1:A:100:PRO:O	1:A:104:ARG:HG3	2.20	0.41
1:A:428:GLU:N	1:A:428:GLU:CD	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:MET:HA	1:A:1046:MET:HE2	2.03	0.41
1:A:3:ALA:O	1:A:4:ASP:C	2.63	0.41
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.55	0.41
1:B:1287:ASN:H	1:B:1287:ASN:ND2	2.17	0.41
1:A:736:ILE:HG22	1:A:842:PHE:CB	2.50	0.41
1:B:655:PHE:CE1	1:B:814:LEU:HD23	2.56	0.41
1:B:885:MET:HE2	1:B:894:ILE:HD11	2.01	0.41
1:A:193:PRO:HG2	1:A:560:PHE:CE1	2.55	0.41
1:B:615:ALA:HB2	1:B:691:ASP:HA	2.02	0.41
1:B:1289:ASN:O	1:B:1290:THR:HB	2.21	0.41
1:B:3:ALA:HB1	1:B:230:GLU:O	2.20	0.41
1:B:358:ILE:C	1:B:358:ILE:HD12	2.46	0.41
1:B:481:LYS:HE2	1:B:485:ASP:OD1	2.21	0.41
1:A:193:PRO:HB3	1:A:562:GLU:HG2	2.01	0.41
1:A:505:ILE:HD12	1:A:505:ILE:N	2.36	0.41
1:A:857:VAL:HG12	1:A:857:VAL:O	2.20	0.41
1:A:256:LYS:HE3	4:A:1404:FAD:O3B	2.21	0.41
1:A:401:GLU:HB2	9:A:1746:HOH:O	2.21	0.41
1:A:426:ARG:NH2	1:A:429:ASP:O	2.52	0.41
1:A:644:ASN:O	1:A:653:THR:HA	2.21	0.41
1:A:808:VAL:HG23	9:A:1801:HOH:O	2.21	0.41
1:B:3:ALA:CB	1:B:230:GLU:O	2.69	0.41
1:B:509:ARG:HH11	1:B:509:ARG:HG2	1.86	0.41
1:B:885:MET:SD	1:B:896:GLY:HA3	2.61	0.41
1:A:284:ILE:HA	1:A:285:PRO:HD2	1.89	0.41
1:A:60:ARG:HG2	1:A:60:ARG:NH1	2.36	0.40
1:A:509:ARG:NH1	1:A:1317:CYS:CB	2.80	0.40
1:B:59:ASP:O	1:B:63:ASP:N	2.53	0.40
1:B:229:PHE:HB2	1:B:236:TRP:HB3	2.03	0.40
1:B:570:GLU:CD	1:B:1057:PRO:HG3	2.47	0.40
1:A:389:PHE:O	1:A:391:PRO:HD3	2.21	0.40
1:B:502:GLY:HA3	9:B:2269:HOH:O	2.20	0.40
1:A:197:ASN:HA	1:A:198:PRO:HD3	1.92	0.40
1:B:513:LEU:N	1:B:513:LEU:CD1	2.84	0.40
1:A:986:LYS:O	1:A:990:GLU:HG3	2.21	0.40
1:A:1216:GLU:CD	1:A:1216:GLU:H	2.28	0.40
1:B:275:PHE:HA	1:B:276:PRO:HD2	1.93	0.40
1:B:771:LYS:HA	1:B:771:LYS:HD3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1292/1332 (97%)	1235 (96%)	43 (3%)	14 (1%)	11	4
1	B	1290/1332 (97%)	1235 (96%)	42 (3%)	13 (1%)	12	5
All	All	2582/2664 (97%)	2470 (96%)	85 (3%)	27 (1%)	12	5

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	1008	SER
1	A	1322	PRO
1	B	4	ASP
1	B	5	GLU
1	B	1008	SER
1	B	1287	ASN
1	A	429	ASP
1	A	1319	THR
1	B	1139	GLY
1	A	61	LEU
1	A	338	ALA
1	A	539	ASP
1	A	912	ARG
1	A	1318	VAL
1	B	20	ALA
1	B	429	ASP
1	B	912	ARG
1	A	529	LYS
1	B	1322	PRO
1	B	1325	CYS
1	B	1326	LYS
1	A	797	GLY
1	A	1139	GLY
1	B	797	GLY

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Mol	Chain	Res	Type
1	A	1320	GLY
1	B	1323	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1100/1128 (98%)	1075 (98%)	25 (2%)	44	33
1	B	1098/1128 (97%)	1080 (98%)	18 (2%)	55	46
All	All	2198/2256 (97%)	2155 (98%)	43 (2%)	48	39

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

Mol	Chain	Res	Type
1	A	57	LYS
1	A	89	GLU
1	A	154	ARG
1	A	225	LYS
1	A	256	LYS
1	A	281	PRO
1	A	312	LEU
1	A	328	ARG
1	A	337	PHE
1	A	348	LEU
1	A	439	ARG
1	A	481	LYS
1	A	506	GLU
1	A	537	LYS
1	A	550	GLN
1	A	551	LYS
1	A	562	GLU
1	A	618	LYS
1	A	652	GLU
1	A	736	ILE
1	A	743	TYR

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

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

Mol	Chain	Res	Type
1	A	131	GLN
1	A	251	GLN
1	A	351	ASN
1	A	550	GLN
1	A	567	GLN
1	A	650	ASN
1	A	705	ASN
1	A	976	GLN
1	A	1088	GLN
1	A	1145	ASN
1	A	1148	ASN
1	A	1284	GLN
1	A	1289	ASN
1	B	62	GLN
1	B	131	GLN
1	B	144	GLN

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Mol	Chain	Res	Type
1	B	146	ASN
1	B	226	GLN
1	B	272	ASN
1	B	333	GLN
1	B	351	ASN
1	B	473	GLN
1	B	552	HIS
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	991	ASN
1	B	1145	ASN
1	B	1212	HIS
1	B	1220	HIS
1	B	1284	GLN
1	B	1287	ASN
1	B	1324	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	$\#\|Z\|>2$
7	GOL	B	1408	-	5,5,5	5.25	4 (80%)	5,5,5	6.77	3 (60%)
7	GOL	A	1410	-	5,5,5	5.25	4 (80%)	5,5,5	6.77	3 (60%)
4	FAD	A	1404	-	58,58,58	1.76	16 (27%)	85,89,89	2.15	29 (34%)
7	GOL	B	1410	-	5,5,5	5.25	4 (80%)	5,5,5	6.77	3 (60%)
6	ACY	A	1406	-	3,3,3	1.21	0	3,3,3	1.68	1 (33%)
3	FES	A	1402	1	0,4,4	-	-	-		
7	GOL	A	1409	-	5,5,5	5.24	4 (80%)	5,5,5	6.77	3 (60%)
6	ACY	B	1406	-	3,3,3	1.16	0	3,3,3	1.71	1 (33%)
3	FES	B	1402	1	0,4,4	-	-	-		
5	FYX	B	1405	8	21,21,21	2.56	10 (47%)	27,28,28	2.97	14 (51%)
8	ZXF	B	1411	5	24,31,31	5.52	12 (50%)	22,52,52	4.38	12 (54%)
5	FYX	A	1405	8	21,21,21	2.59	11 (52%)	27,28,28	2.99	13 (48%)
4	FAD	B	1404	-	58,58,58	1.73	15 (25%)	85,89,89	2.27	28 (32%)
8	ZXF	A	1411	5	24,31,31	5.52	11 (45%)	22,52,52	4.46	13 (59%)
7	GOL	B	1409	-	5,5,5	5.25	4 (80%)	5,5,5	6.77	3 (60%)
7	GOL	B	1407	-	5,5,5	5.25	4 (80%)	5,5,5	6.77	3 (60%)
3	FES	A	1403	1	0,4,4	-	-	-		
3	FES	B	1403	1	0,4,4	-	-	-		
7	GOL	A	1407	-	5,5,5	5.24	4 (80%)	5,5,5	6.77	3 (60%)
7	GOL	A	1408	-	5,5,5	5.24	4 (80%)	5,5,5	6.77	3 (60%)

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	1402	1	-	-	0/1/1/1
5	FYX	A	1405	8	-	0/8/10/10	0/3/3/3
7	GOL	B	1408	-	-	2/4/4/4	-
7	GOL	A	1409	-	-	2/4/4/4	-
7	GOL	A	1410	-	-	2/4/4/4	-
7	GOL	B	1410	-	-	2/4/4/4	-
4	FAD	A	1404	-	-	1/34/50/50	0/6/6/6
4	FAD	B	1404	-	-	2/34/50/50	0/6/6/6
3	FES	B	1403	1	-	-	0/1/1/1
8	ZXF	A	1411	5	-	3/6/46/46	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	1407	-	-	2/4/4/4	-
3	FES	B	1402	1	-	-	0/1/1/1
5	FYX	B	1405	8	-	0/8/10/10	0/3/3/3
7	GOL	A	1408	-	-	2/4/4/4	-
7	GOL	B	1409	-	-	2/4/4/4	-
3	FES	A	1403	1	-	-	0/1/1/1
7	GOL	B	1407	-	-	2/4/4/4	-
8	ZXF	B	1411	5	-	3/6/46/46	0/4/4/4

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1411	ZXF	C7-C6	19.33	1.69	1.53
8	A	1411	ZXF	C7-C6	18.98	1.68	1.53
8	A	1411	ZXF	C9-C10	13.54	1.61	1.38
8	B	1411	ZXF	C9-C10	13.49	1.61	1.38
7	B	1409	GOL	C3-C2	-9.90	1.14	1.51
7	B	1407	GOL	C3-C2	-9.89	1.14	1.51
7	B	1408	GOL	C3-C2	-9.89	1.14	1.51
7	A	1410	GOL	C3-C2	-9.89	1.14	1.51
7	B	1410	GOL	C3-C2	-9.88	1.14	1.51
7	A	1407	GOL	C3-C2	-9.88	1.14	1.51
7	A	1409	GOL	C3-C2	-9.88	1.14	1.51
7	A	1408	GOL	C3-C2	-9.88	1.14	1.51
8	A	1411	ZXF	C9-N5	7.57	1.55	1.37
8	B	1411	ZXF	P-O4'	-6.74	1.39	1.60
8	A	1411	ZXF	P-O4'	-6.55	1.39	1.60
8	B	1411	ZXF	C9-N5	5.39	1.50	1.37
4	A	1404	FAD	C10-N1	5.10	1.43	1.33
8	B	1411	ZXF	P-O1P	-4.98	1.36	1.54
8	A	1411	ZXF	P-O1P	-4.98	1.36	1.54
4	B	1404	FAD	C10-N1	4.82	1.43	1.33
5	A	1405	FYX	NPN-NPL	-4.48	1.27	1.36
5	B	1405	FYX	CPH-CPK	-4.47	1.40	1.47
5	B	1405	FYX	NPN-NPL	-4.41	1.27	1.36
8	B	1411	ZXF	C6-N5	4.40	1.51	1.46
5	A	1405	FYX	CPH-CPK	-4.29	1.40	1.47
5	B	1405	FYX	CPP-CPM	-4.09	1.39	1.47
8	A	1411	ZXF	O4-C4	4.04	1.31	1.23
5	B	1405	FYX	CPB-NPC	3.99	1.23	1.14
5	A	1405	FYX	CPP-CPM	-3.95	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1408	GOL	C1-C2	-3.90	1.36	1.51
7	A	1409	GOL	C1-C2	-3.89	1.37	1.51
7	B	1407	GOL	C1-C2	-3.89	1.37	1.51
7	A	1410	GOL	C1-C2	-3.88	1.37	1.51
7	A	1408	GOL	C1-C2	-3.88	1.37	1.51
7	B	1409	GOL	C1-C2	-3.88	1.37	1.51
7	A	1407	GOL	C1-C2	-3.87	1.37	1.51
5	A	1405	FYX	CPB-NPC	3.87	1.23	1.14
7	B	1410	GOL	C1-C2	-3.87	1.37	1.51
5	A	1405	FYX	CPK-NPL	3.85	1.38	1.32
8	B	1411	ZXF	O4-C4	3.74	1.30	1.23
5	B	1405	FYX	CPK-NPL	3.65	1.37	1.32
4	B	1404	FAD	C4X-N5	3.58	1.38	1.30
4	A	1404	FAD	C4X-N5	3.55	1.38	1.30
7	B	1407	GOL	O2-C2	-3.54	1.33	1.43
7	A	1409	GOL	O2-C2	-3.54	1.33	1.43
7	B	1409	GOL	O2-C2	-3.54	1.33	1.43
7	B	1410	GOL	O2-C2	-3.54	1.33	1.43
7	A	1410	GOL	O2-C2	-3.53	1.33	1.43
7	A	1407	GOL	O2-C2	-3.53	1.33	1.43
7	B	1408	GOL	O2-C2	-3.52	1.33	1.43
7	A	1408	GOL	O2-C2	-3.51	1.33	1.43
7	A	1410	GOL	O1-C1	3.51	1.57	1.42
7	B	1410	GOL	O1-C1	3.50	1.57	1.42
7	A	1407	GOL	O1-C1	3.50	1.57	1.42
7	A	1408	GOL	O1-C1	3.50	1.57	1.42
7	B	1408	GOL	O1-C1	3.49	1.57	1.42
7	B	1407	GOL	O1-C1	3.49	1.57	1.42
7	B	1409	GOL	O1-C1	3.49	1.57	1.42
7	A	1409	GOL	O1-C1	3.47	1.57	1.42
4	A	1404	FAD	C10-N10	3.38	1.44	1.37
4	B	1404	FAD	C5A-N7A	-3.20	1.33	1.39
4	B	1404	FAD	C10-N10	3.20	1.44	1.37
8	A	1411	ZXF	C10-N8	3.16	1.38	1.35
8	B	1411	ZXF	C10-N8	3.13	1.38	1.35
4	A	1404	FAD	C5A-N7A	-3.10	1.33	1.39
4	A	1404	FAD	C9-C9A	3.04	1.44	1.39
4	B	1404	FAD	C6-C7	2.99	1.43	1.39
4	B	1404	FAD	C9A-C5X	2.94	1.45	1.41
5	A	1405	FYX	CPM-NPJ	2.91	1.38	1.33
4	B	1404	FAD	C4A-N3A	2.88	1.39	1.34
4	A	1404	FAD	C6-C7	2.88	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1404	FAD	C9A-C5X	2.86	1.45	1.41
4	B	1404	FAD	C9-C9A	2.86	1.44	1.39
5	B	1405	FYX	CPM-NPJ	2.85	1.38	1.33
5	A	1405	FYX	CPQ-CPP	2.80	1.43	1.39
8	B	1411	ZXF	C2-N1	2.79	1.39	1.33
4	A	1404	FAD	P-O1P	2.73	1.60	1.50
8	B	1411	ZXF	O4'-C4'	-2.71	1.34	1.44
5	B	1405	FYX	CPQ-CPP	2.69	1.43	1.39
4	A	1404	FAD	C4A-N3A	2.65	1.39	1.34
4	B	1404	FAD	C9A-N10	2.65	1.45	1.41
8	A	1411	ZXF	C2-N1	2.65	1.39	1.33
4	A	1404	FAD	C9A-N10	2.62	1.45	1.41
4	B	1404	FAD	PA-O1A	2.62	1.59	1.50
5	A	1405	FYX	CPG-CPH	2.58	1.43	1.39
4	B	1404	FAD	P-O1P	2.57	1.59	1.50
4	A	1404	FAD	PA-O1A	2.57	1.59	1.50
8	A	1411	ZXF	MO-S1'	2.56	2.43	2.39
5	B	1405	FYX	CPG-CPH	2.53	1.43	1.39
4	B	1404	FAD	C6-C5X	2.40	1.43	1.40
5	A	1405	FYX	CPG-CPD	2.36	1.41	1.39
4	A	1404	FAD	C6-C5X	2.35	1.43	1.40
4	A	1404	FAD	C1'-C2'	2.35	1.55	1.52
4	A	1404	FAD	C4-N3	2.34	1.43	1.38
5	B	1405	FYX	CPM-NPN	2.29	1.38	1.34
5	A	1405	FYX	CPM-NPN	2.29	1.38	1.34
8	B	1411	ZXF	P-O2P	-2.28	1.46	1.54
4	B	1404	FAD	C4-N3	2.26	1.43	1.38
8	A	1411	ZXF	P-O2P	-2.25	1.46	1.54
5	A	1405	FYX	CPO-CPP	2.24	1.42	1.39
4	B	1404	FAD	C1'-C2'	2.21	1.55	1.52
8	A	1411	ZXF	O4'-C4'	-2.18	1.36	1.44
5	B	1405	FYX	CPG-CPD	2.16	1.41	1.39
4	B	1404	FAD	C8M-C8	2.10	1.54	1.51
8	B	1411	ZXF	C4'-C3'	-2.07	1.49	1.51
4	A	1404	FAD	C8M-C8	2.03	1.54	1.51
4	A	1404	FAD	C8-C7	2.00	1.45	1.40

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1410	GOL	O3-C3-C2	13.82	172.58	110.38
7	A	1408	GOL	O3-C3-C2	13.81	172.56	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1407	GOL	O3-C3-C2	13.81	172.55	110.38
7	A	1410	GOL	O3-C3-C2	13.81	172.54	110.38
7	B	1407	GOL	O3-C3-C2	13.81	172.54	110.38
7	B	1409	GOL	O3-C3-C2	13.81	172.54	110.38
7	B	1408	GOL	O3-C3-C2	13.80	172.50	110.38
7	A	1409	GOL	O3-C3-C2	13.80	172.49	110.38
8	B	1411	ZXF	C2'-C1'-S1'	13.27	127.68	120.15
8	A	1411	ZXF	C2'-C1'-S1'	13.06	127.56	120.15
8	A	1411	ZXF	C1'-C2'-S2'	-8.54	115.31	120.15
8	B	1411	ZXF	C1'-C2'-S2'	-7.90	115.67	120.15
8	A	1411	ZXF	C2-N1-C10	7.86	127.24	113.36
8	B	1411	ZXF	C2-N1-C10	7.85	127.22	113.36
5	A	1405	FYX	NPL-CPK-NPJ	-6.82	104.46	114.17
4	A	1404	FAD	N3A-C2A-N1A	-6.81	118.28	128.58
5	B	1405	FYX	NPL-CPK-NPJ	-6.78	104.52	114.17
4	B	1404	FAD	N3A-C2A-N1A	-6.66	118.50	128.58
5	A	1405	FYX	CPF-NPE-CPD	6.24	124.94	116.51
5	B	1405	FYX	CPF-NPE-CPD	6.23	124.93	116.51
4	B	1404	FAD	C2B-C1B-N9A	5.90	127.97	113.30
4	A	1404	FAD	C5'-C4'-C3'	-5.44	101.95	112.22
8	B	1411	ZXF	O4-C4-C9	-5.43	114.16	127.26
4	B	1404	FAD	O4'-C4'-C3'	5.35	121.77	109.25
7	B	1409	GOL	O2-C2-C3	5.31	131.16	109.18
7	A	1410	GOL	O2-C2-C3	5.30	131.14	109.18
7	B	1410	GOL	O2-C2-C3	5.30	131.11	109.18
7	B	1407	GOL	O2-C2-C3	5.30	131.10	109.18
7	A	1409	GOL	O2-C2-C3	5.29	131.10	109.18
7	B	1408	GOL	O2-C2-C3	5.29	131.10	109.18
7	A	1407	GOL	O2-C2-C3	5.29	131.09	109.18
8	A	1411	ZXF	O4-C4-C9	-5.29	114.50	127.26
7	A	1408	GOL	O2-C2-C3	5.28	131.06	109.18
4	B	1404	FAD	C5'-C4'-C3'	-5.18	102.45	112.22
5	A	1405	FYX	CPI-CPF-NPE	-4.90	117.97	123.97
5	B	1405	FYX	CPI-CPF-NPE	-4.85	118.03	123.97
4	A	1404	FAD	C2B-C1B-N9A	4.74	125.09	113.30
4	B	1404	FAD	O2B-C2B-C3B	4.53	126.35	111.82
8	A	1411	ZXF	O3'-C7-N8	-4.51	104.51	108.61
4	A	1404	FAD	O4'-C4'-C3'	4.51	119.80	109.25
8	B	1411	ZXF	O3'-C7-N8	-4.46	104.56	108.61
4	B	1404	FAD	O2'-C2'-C3'	4.44	119.65	109.25
4	B	1404	FAD	C5A-C4A-N3A	-4.36	120.71	126.72
4	A	1404	FAD	C5A-C4A-N3A	-4.36	120.72	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1405	FYX	CPK-NPL-NPN	4.35	110.99	102.97
5	B	1405	FYX	CPK-NPL-NPN	4.32	110.92	102.97
5	A	1405	FYX	CPM-NPJ-CPK	4.27	109.29	103.35
5	A	1405	FYX	CPT-NPS-CPR	4.14	126.32	116.86
5	B	1405	FYX	CPT-NPS-CPR	4.10	126.24	116.86
4	A	1404	FAD	O3'-C3'-C4'	4.06	118.16	108.93
4	A	1404	FAD	C2A-N3A-C4A	4.05	121.72	111.83
5	B	1405	FYX	CPM-NPJ-CPK	4.04	108.98	103.35
4	B	1404	FAD	C2A-N3A-C4A	3.98	121.55	111.83
4	B	1404	FAD	O5'-C5'-C4'	-3.97	98.78	109.36
8	A	1411	ZXF	C4-C9-N5	3.92	126.96	116.27
4	A	1404	FAD	O2'-C2'-C3'	3.73	117.97	109.25
4	B	1404	FAD	C5X-N5-C4X	3.57	123.87	118.09
8	A	1411	ZXF	O3'-C7-C6	-3.51	106.62	108.96
8	A	1411	ZXF	N2-C2-N3	3.51	124.16	116.76
4	B	1404	FAD	C9A-C5X-N5	-3.49	118.75	122.45
8	B	1411	ZXF	N2-C2-N3	3.46	124.07	116.76
4	A	1404	FAD	C5X-N5-C4X	3.46	123.68	118.09
8	B	1411	ZXF	C4-C9-N5	3.43	125.62	116.27
4	A	1404	FAD	C9A-C5X-N5	-3.36	118.89	122.45
5	A	1405	FYX	CPO-CPR-NPS	-3.30	117.97	123.60
5	B	1405	FYX	CPO-CPR-NPS	-3.27	118.03	123.60
8	B	1411	ZXF	C9-C4-N3	3.19	120.89	112.13
5	A	1405	FYX	NPN-CPM-NPJ	-3.18	104.55	110.32
8	B	1411	ZXF	O3'-C3'-C2'	3.18	113.57	109.09
8	A	1411	ZXF	C9-C4-N3	3.14	120.76	112.13
4	B	1404	FAD	O3'-C3'-C4'	3.13	116.05	108.93
5	B	1405	FYX	NPN-CPM-NPJ	-3.12	104.67	110.32
5	A	1405	FYX	CPH-CPK-NPL	3.11	128.13	122.57
4	A	1404	FAD	N3A-C4A-N9A	3.07	132.40	127.17
8	A	1411	ZXF	C7-C6-N5	3.06	110.87	107.87
4	B	1404	FAD	N3A-C4A-N9A	3.04	132.34	127.17
4	B	1404	FAD	C1'-N10-C9A	3.02	126.50	120.63
5	B	1405	FYX	CPG-CPD-NPE	-3.00	119.55	123.57
5	A	1405	FYX	CPG-CPD-NPE	-2.98	119.56	123.57
5	A	1405	FYX	CPQ-CPT-NPS	-2.92	118.61	123.60
5	B	1405	FYX	CPH-CPK-NPL	2.86	127.68	122.57
5	B	1405	FYX	CPQ-CPT-NPS	-2.86	118.73	123.60
8	B	1411	ZXF	O3'-C7-C6	-2.79	107.10	108.96
5	B	1405	FYX	CPH-CPK-NPJ	2.79	127.80	122.92
4	B	1404	FAD	C4-C4X-N5	2.76	122.02	118.21
4	A	1404	FAD	C4-C4X-N5	2.76	122.02	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1408	GOL	O1-C1-C2	2.74	122.70	110.38
4	A	1404	FAD	C10-C4X-N5	-2.73	119.22	124.81
4	B	1404	FAD	C10-C4X-N5	-2.73	119.22	124.81
4	A	1404	FAD	C4X-C4-N3	2.73	120.21	113.25
7	B	1409	GOL	O1-C1-C2	2.73	122.68	110.38
7	A	1409	GOL	O1-C1-C2	2.73	122.67	110.38
7	A	1410	GOL	O1-C1-C2	2.73	122.66	110.38
7	B	1407	GOL	O1-C1-C2	2.73	122.65	110.38
7	B	1410	GOL	O1-C1-C2	2.72	122.64	110.38
4	B	1404	FAD	C4X-C4-N3	2.72	120.17	113.25
7	A	1407	GOL	O1-C1-C2	2.72	122.60	110.38
7	A	1408	GOL	O1-C1-C2	2.71	122.58	110.38
4	A	1404	FAD	C1'-N10-C9A	2.70	125.88	120.63
4	A	1404	FAD	C4-N3-C2	-2.67	120.89	125.64
4	B	1404	FAD	C4-N3-C2	-2.67	120.90	125.64
4	A	1404	FAD	O2B-C2B-C3B	2.66	120.36	111.82
8	B	1411	ZXF	O4-C4-N3	2.57	124.95	120.11
5	A	1405	FYX	CPH-CPK-NPJ	2.56	127.40	122.92
4	B	1404	FAD	C4A-C5A-N7A	-2.52	107.70	110.58
4	A	1404	FAD	O3B-C3B-C4B	-2.52	103.84	111.08
4	B	1404	FAD	C5A-N7A-C8A	2.51	107.40	103.45
4	B	1404	FAD	C2A-N1A-C6A	2.49	122.82	118.73
4	A	1404	FAD	C4A-C5A-N7A	-2.46	107.77	110.58
8	A	1411	ZXF	O4-C4-N3	2.46	124.74	120.11
4	A	1404	FAD	C5A-N7A-C8A	2.44	107.28	103.45
4	A	1404	FAD	C2A-N1A-C6A	2.44	122.73	118.73
4	B	1404	FAD	O3B-C3B-C4B	-2.42	104.12	111.08
4	A	1404	FAD	O5B-PA-O1A	2.42	118.51	108.94
4	A	1404	FAD	C8M-C8-C9	-2.39	115.36	119.57
4	A	1404	FAD	O4B-C1B-N9A	-2.38	103.51	108.09
4	B	1404	FAD	C4'-C3'-C2'	-2.35	109.66	113.57
8	A	1411	ZXF	O3'-C3'-C2'	2.32	112.37	109.09
4	B	1404	FAD	C8M-C8-C9	-2.32	115.49	119.57
6	B	1406	ACY	O-C-CH3	-2.31	113.06	122.53
5	B	1405	FYX	CPQ-CPP-CPO	2.29	121.48	118.57
4	A	1404	FAD	C3B-C2B-C1B	2.27	105.75	101.46
6	A	1406	ACY	O-C-CH3	-2.26	113.25	122.53
4	A	1404	FAD	O5'-P-O1P	2.15	117.45	108.94
5	B	1405	FYX	CPP-CPM-NPJ	2.14	128.22	124.96
5	A	1405	FYX	CPQ-CPP-CPO	2.13	121.28	118.57
4	B	1404	FAD	C4X-C10-N10	2.13	119.53	116.48
8	A	1411	ZXF	N3-C2-N1	-2.13	119.42	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1404	FAD	N9A-C8A-N7A	-2.12	110.93	113.94
4	A	1404	FAD	C7M-C7-C6	-2.11	115.86	119.57
8	B	1411	ZXF	N3-C2-N1	-2.10	119.48	123.32
4	A	1404	FAD	C4X-C10-N10	2.09	119.47	116.48
4	B	1404	FAD	C10-N1-C2	2.08	121.35	116.85
4	A	1404	FAD	C8M-C8-C7	2.05	124.94	120.76
4	B	1404	FAD	O2A-PA-O5B	2.02	116.72	107.57

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1411	ZXF	C4'-O4'-P-O1P
8	B	1411	ZXF	C4'-O4'-P-O2P
8	B	1411	ZXF	C4'-O4'-P-O1P
7	A	1407	GOL	O2-C2-C3-O3
7	A	1408	GOL	O2-C2-C3-O3
7	A	1409	GOL	O2-C2-C3-O3
7	A	1410	GOL	O2-C2-C3-O3
7	B	1407	GOL	O2-C2-C3-O3
7	B	1408	GOL	O2-C2-C3-O3
7	B	1409	GOL	O2-C2-C3-O3
7	B	1410	GOL	O2-C2-C3-O3
7	A	1407	GOL	O1-C1-C2-O2
7	A	1408	GOL	O1-C1-C2-O2
7	A	1409	GOL	O1-C1-C2-O2
7	A	1410	GOL	O1-C1-C2-O2
7	B	1407	GOL	O1-C1-C2-O2
7	B	1408	GOL	O1-C1-C2-O2
7	B	1409	GOL	O1-C1-C2-O2
7	B	1410	GOL	O1-C1-C2-O2
8	A	1411	ZXF	C3'-C4'-O4'-P
8	B	1411	ZXF	C3'-C4'-O4'-P
8	A	1411	ZXF	C4'-O4'-P-O2P
4	B	1404	FAD	O2'-C2'-C3'-C4'
4	B	1404	FAD	C5'-O5'-P-O1P
4	A	1404	FAD	C4'-C5'-O5'-P

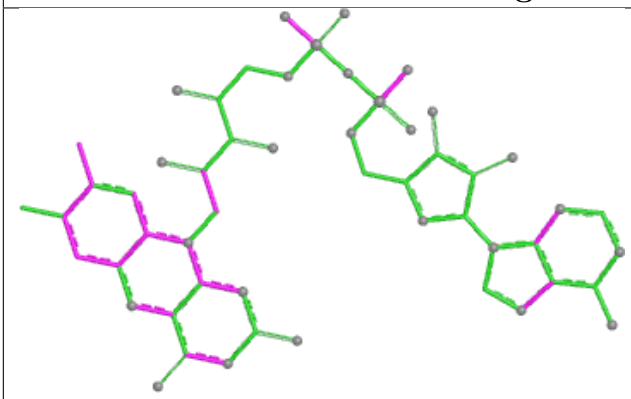
There are no ring outliers.

11 monomers are involved in 27 short contacts:

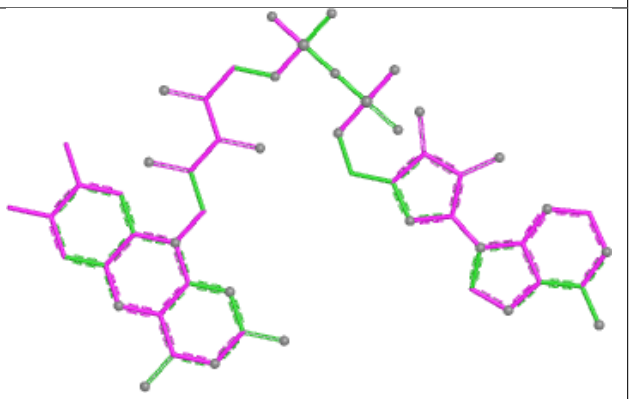
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1408	GOL	1	0
7	A	1410	GOL	3	0
4	A	1404	FAD	3	0
7	B	1410	GOL	2	0
6	A	1406	ACY	3	0
6	B	1406	ACY	4	0
8	B	1411	ZXF	3	0
4	B	1404	FAD	3	0
8	A	1411	ZXF	3	0
7	A	1407	GOL	1	0
7	A	1408	GOL	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

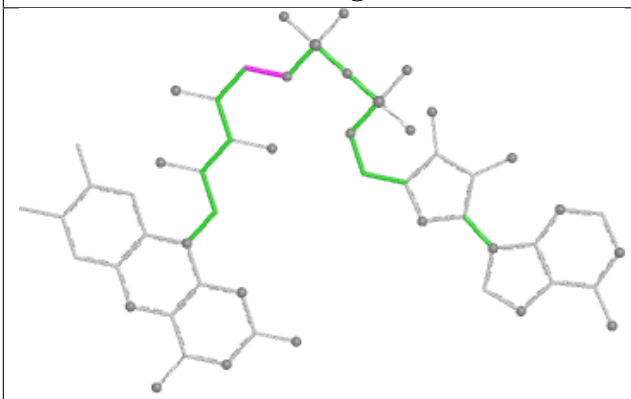
Ligand FAD A 1404



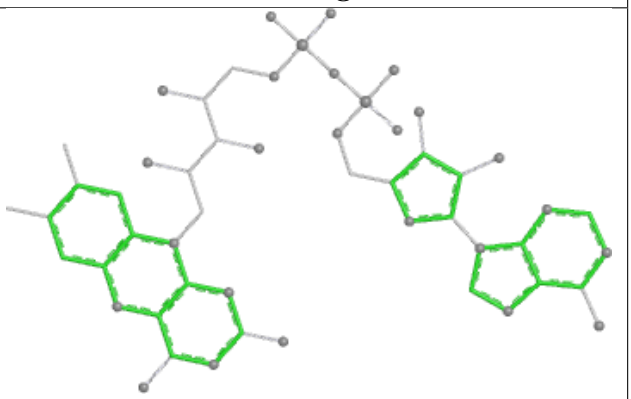
Bond lengths



Bond angles

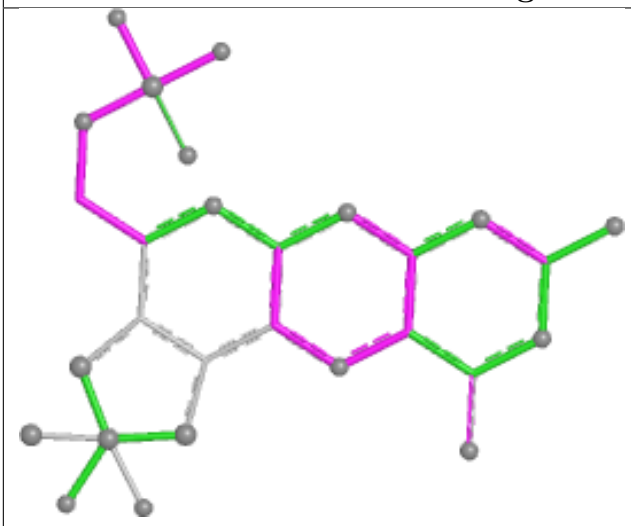


Torsions

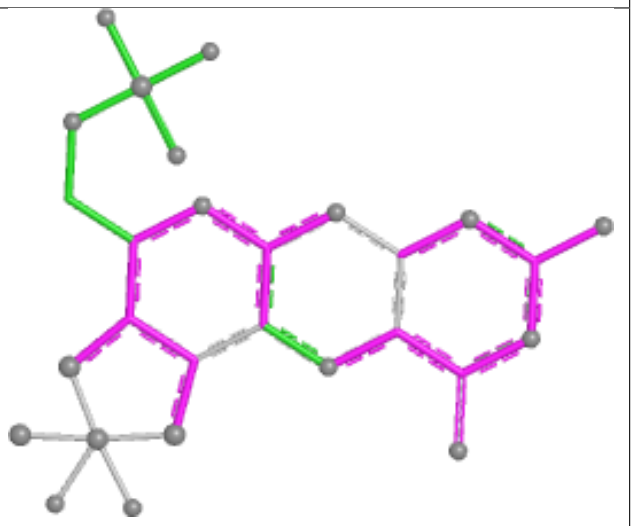


Rings

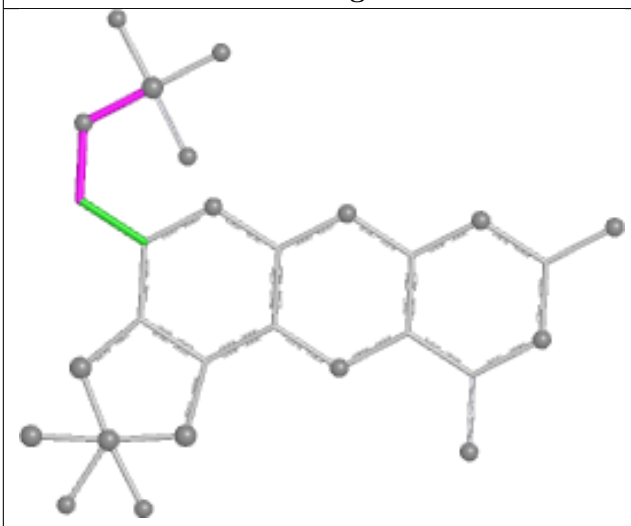
Ligand ZXF B 1411



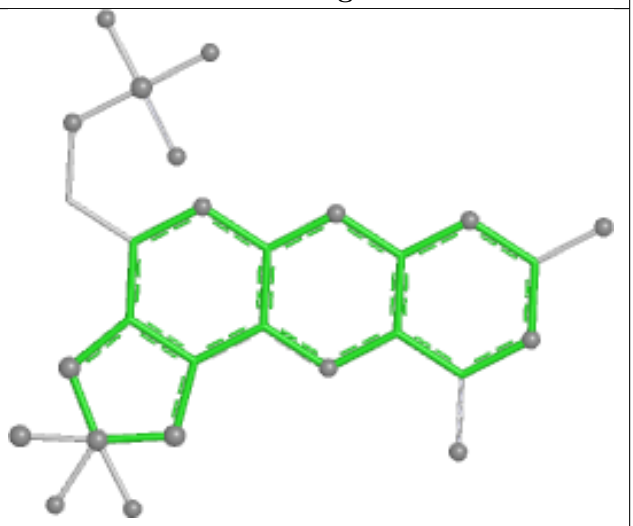
Bond lengths



Bond angles

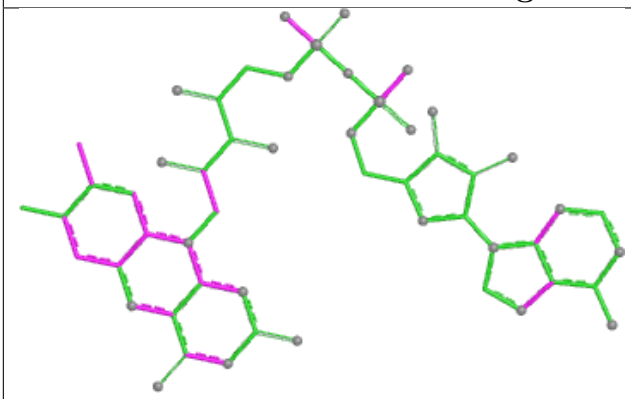


Torsions

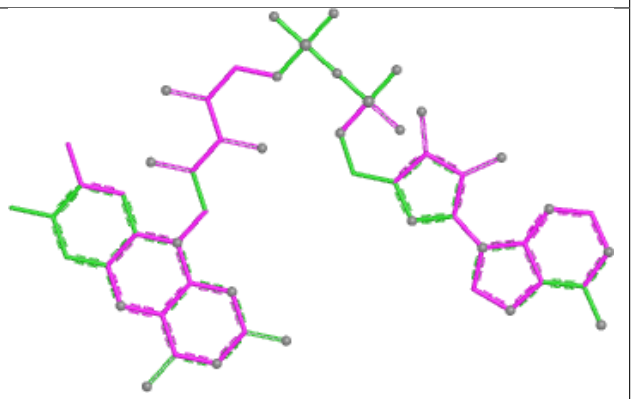


Rings

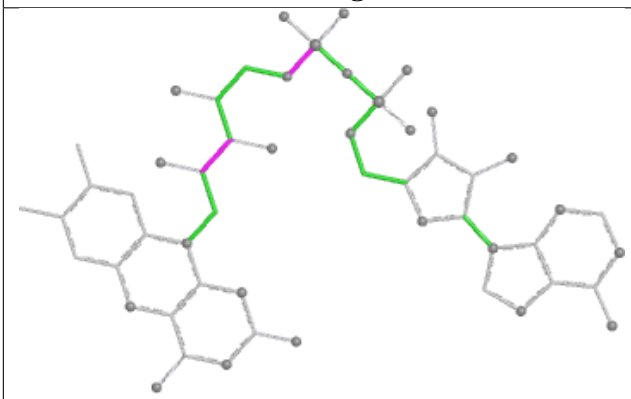
Ligand FAD B 1404



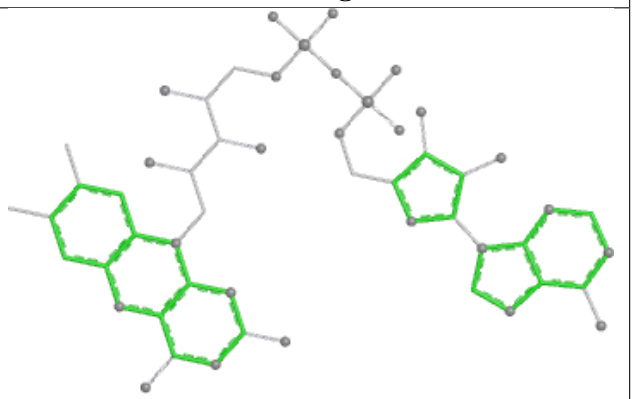
Bond lengths



Bond angles

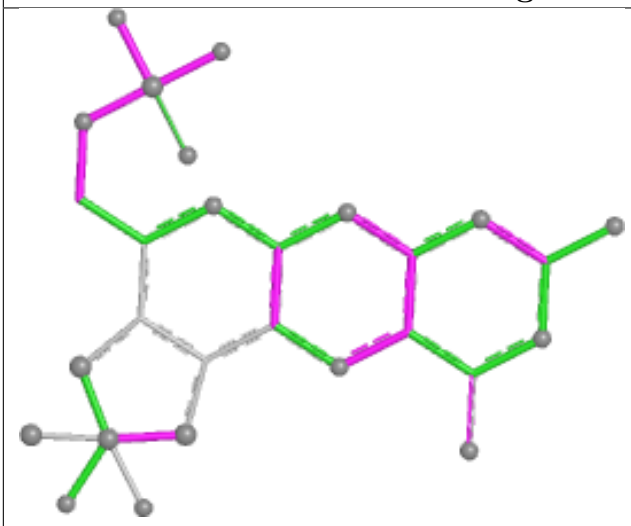


Torsions

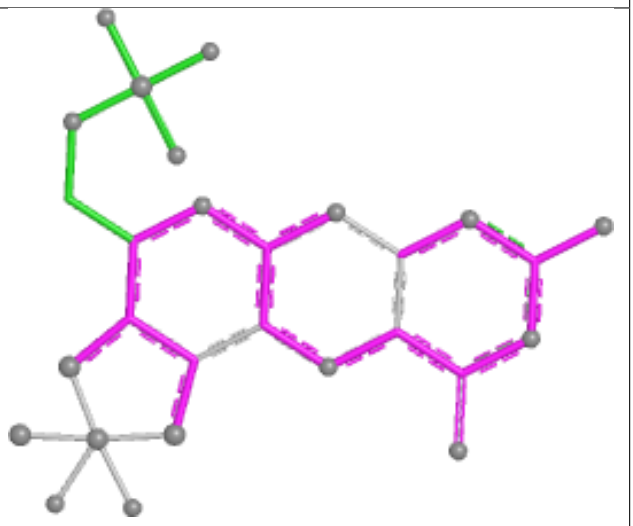


Rings

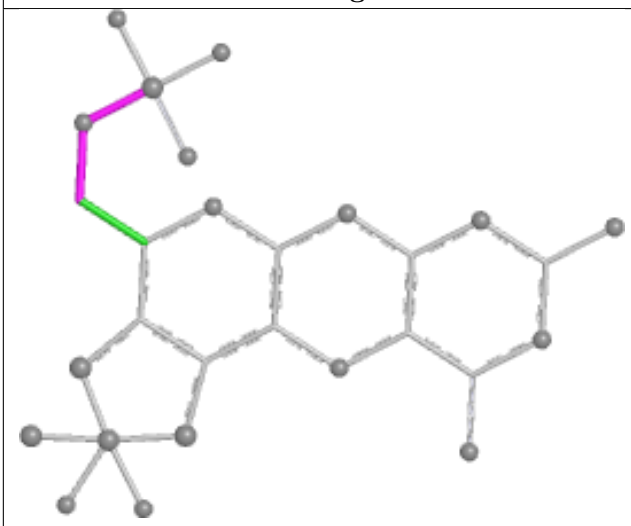
Ligand ZXF A 1411



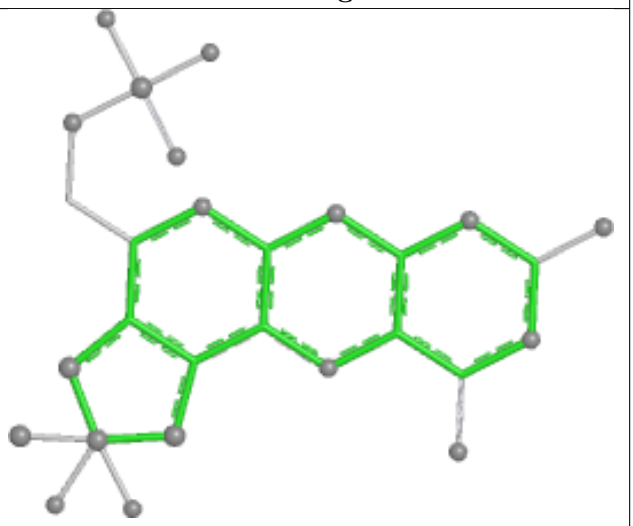
Bond lengths



Bond angles



Torsions



Rings

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1298/1332 (97%)	0.01	76 (5%)	28	31	9, 18, 39, 61	0
1	B	1296/1332 (97%)	0.02	69 (5%)	32	36	9, 19, 38, 61	0
All	All	2594/2664 (97%)	0.02	145 (5%)	30	33	9, 18, 39, 61	0

All (145) RSRZ outliers are listed below:

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

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

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

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

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

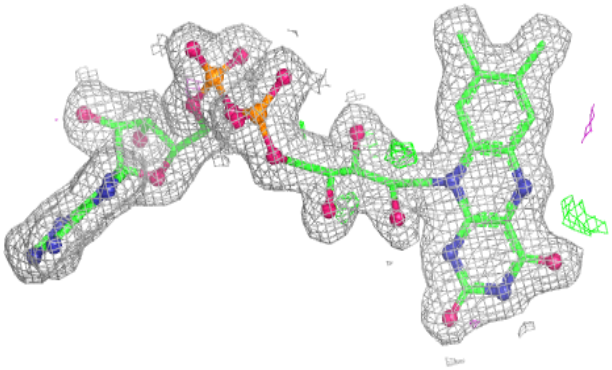
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

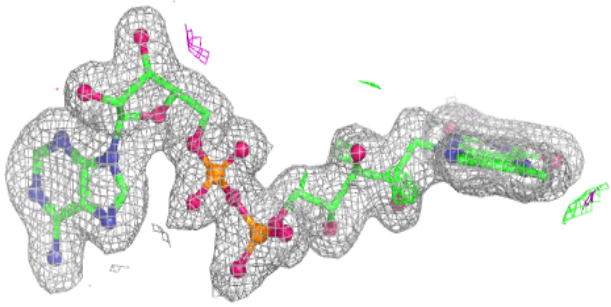
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	A	1410	6/6	0.65	0.22	40,42,43,45	0
7	GOL	B	1410	6/6	0.66	0.24	42,43,45,46	0
7	GOL	B	1408	6/6	0.71	0.23	34,38,41,42	0
7	GOL	B	1409	6/6	0.81	0.16	31,35,37,40	0
7	GOL	A	1407	6/6	0.81	0.16	23,29,30,36	0
7	GOL	A	1408	6/6	0.82	0.17	29,34,35,37	0
7	GOL	A	1409	6/6	0.82	0.15	29,34,38,41	0
7	GOL	B	1407	6/6	0.85	0.12	24,29,31,31	0
5	FYX	B	1405	19/19	0.93	0.08	14,18,24,27	0
5	FYX	A	1405	19/19	0.94	0.07	15,18,27,27	0
6	ACY	A	1406	4/4	0.96	0.05	4,9,13,13	0
6	ACY	B	1406	4/4	0.96	0.05	7,13,13,16	0
4	FAD	A	1404	53/53	0.97	0.06	12,16,20,24	0
4	FAD	B	1404	53/53	0.97	0.06	12,17,21,23	0
3	FES	B	1403	4/4	0.99	0.03	11,12,12,12	0
2	CA	A	1401	1/1	0.99	0.03	12,12,12,12	0
3	FES	A	1402	4/4	0.99	0.03	11,11,11,11	0
3	FES	A	1403	4/4	0.99	0.02	11,11,12,12	0
3	FES	B	1402	4/4	0.99	0.02	11,11,12,12	0
8	ZXF	A	1411	28/28	0.99	0.05	8,12,16,17	0
8	ZXF	B	1411	28/28	0.99	0.05	9,12,15,16	0
2	CA	B	1401	1/1	1.00	0.02	16,16,16,16	0

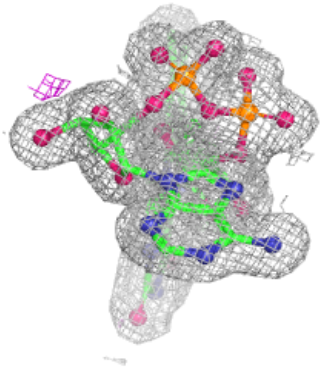
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD A 1404:

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

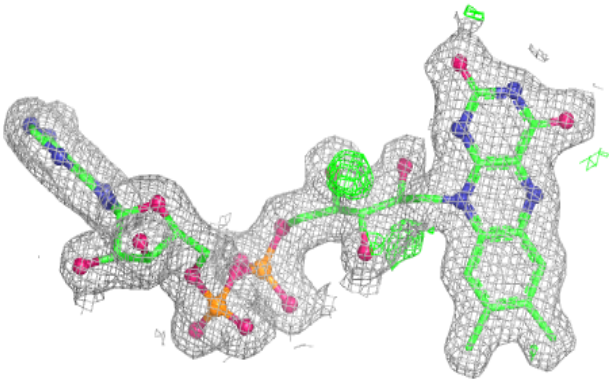


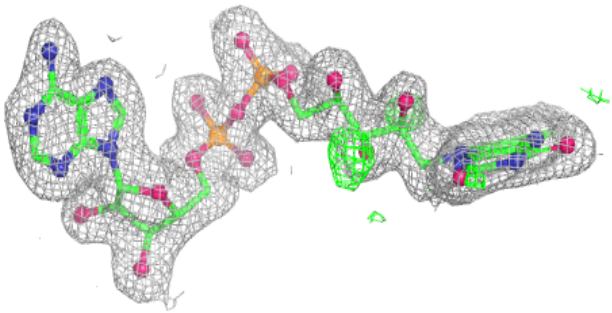


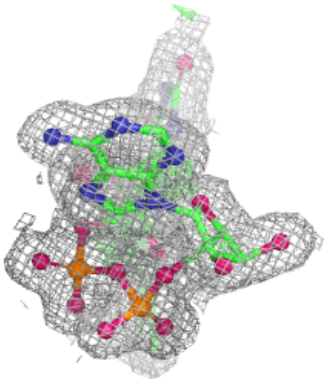


Electron density around FAD B 1404:

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

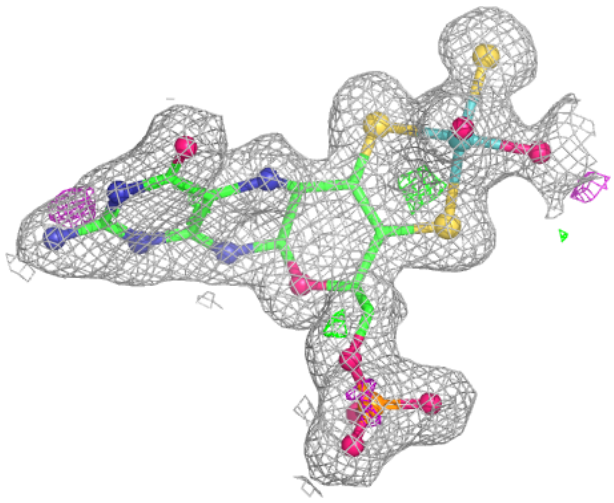


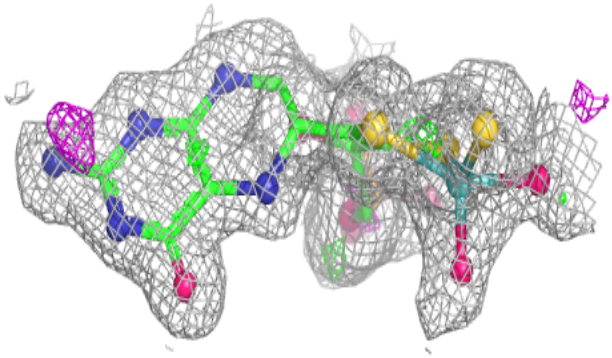


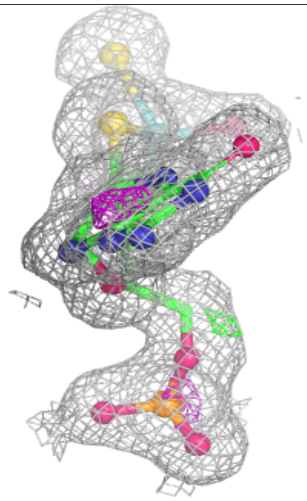


Electron density around ZXF A 1411:

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

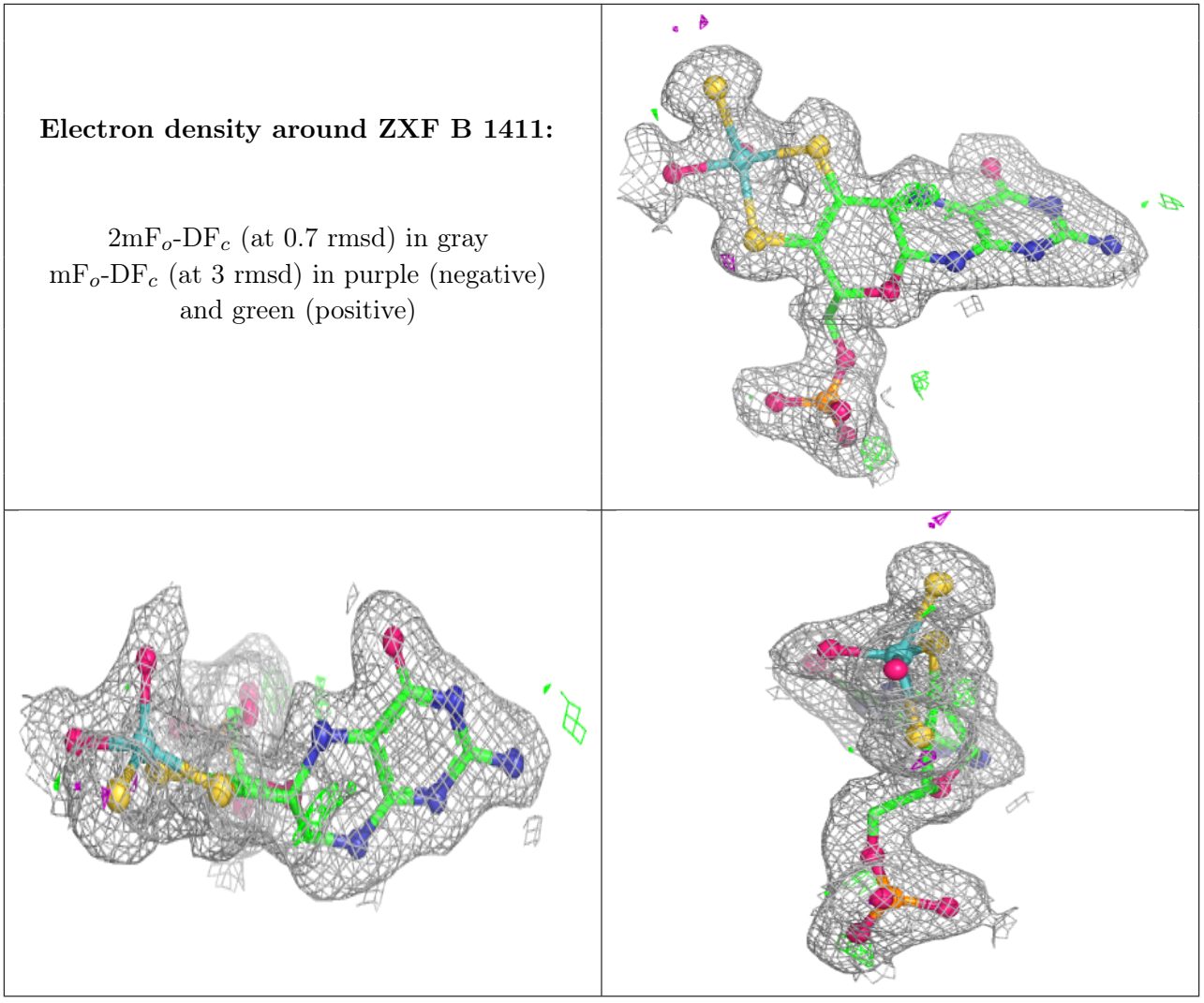






Electron density around ZXF B 1411:

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



6.5 Other polymers (i)

There are no such residues in this entry.