Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:24 AM GMT

PDB ID	:	3AMZ
Title	:	Bovine Xanthine Oxidoreductase urate bound form
Authors	:	Okamoto, K.; Eger, B.T.; Pai, E.F.; Nishino, T.
Deposited on	:	2010-08-27
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

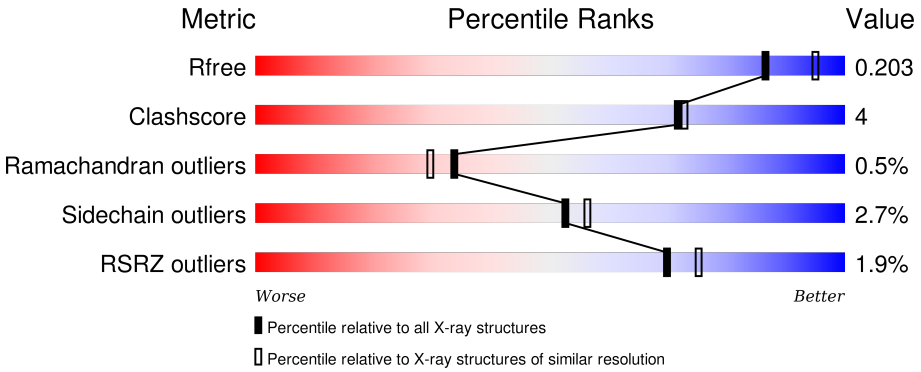
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	2% 86% 9%
1	B	1332	2% 87% 9%

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
10	URC	B	1338	-	-	-	X
7	GOL	A	1335	-	-	-	X
7	GOL	B	1335	-	-	-	X
9	MOS	A	1338	-	-	X	-

2 Entry composition

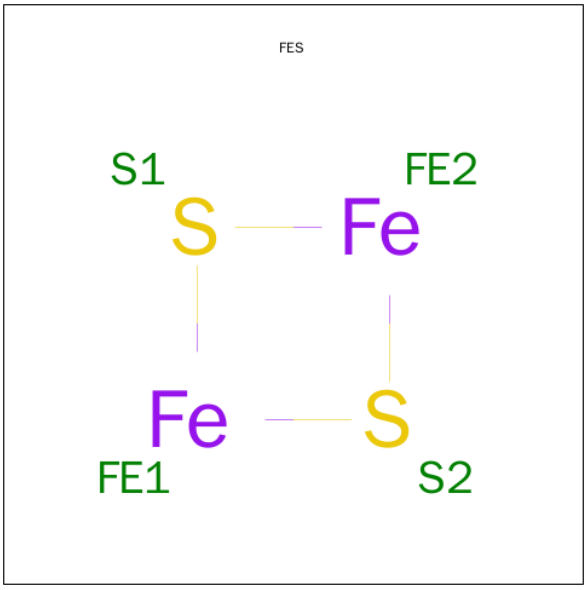
There are 11 unique types of molecules in this entry. The entry contains 22382 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1291	Total	C	N	O	S	0	0	0
			10024	6374	1718	1872	60			
1	B	1289	Total	C	N	O	S	0	0	0
			10013	6368	1716	1869	60			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

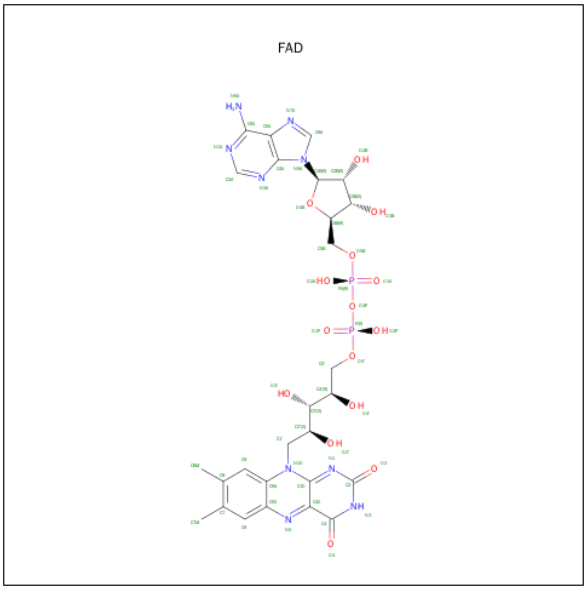


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

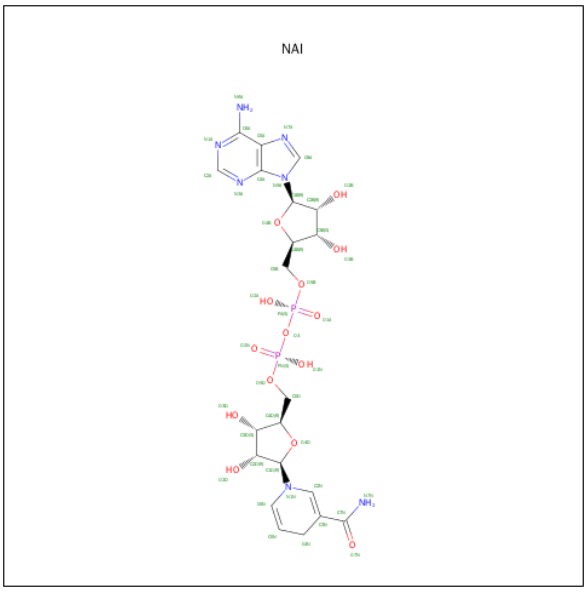
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0

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



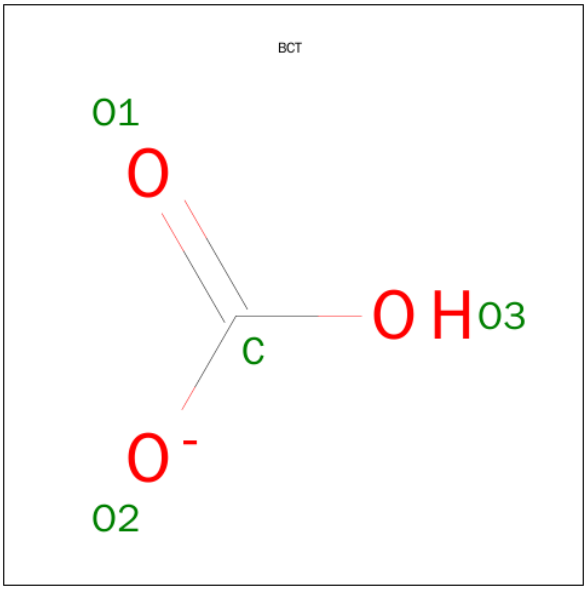
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 53 27 9 15 2	0	0
4	B	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 5 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



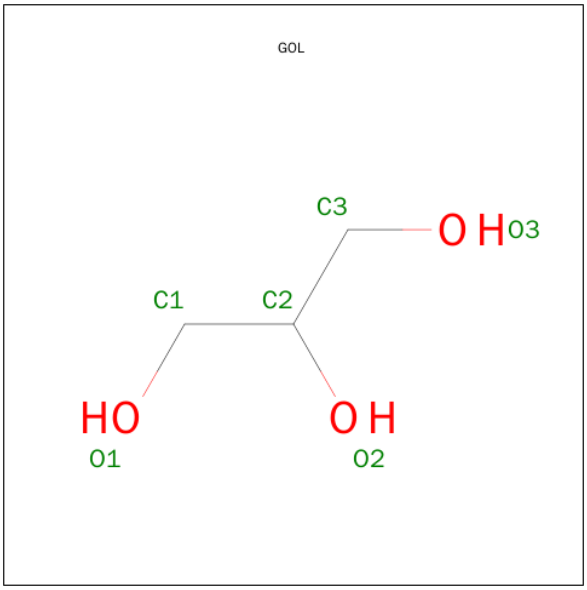
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



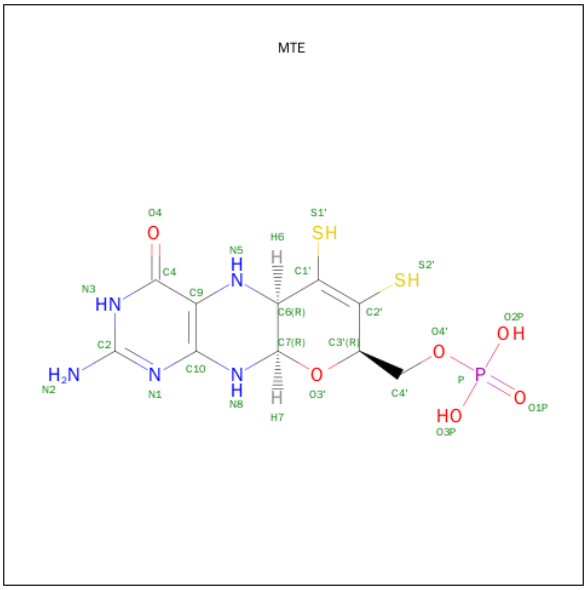
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O		0	0
			4	1	3			
6	B	1	Total	C	O		0	0
			4	1	3			

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



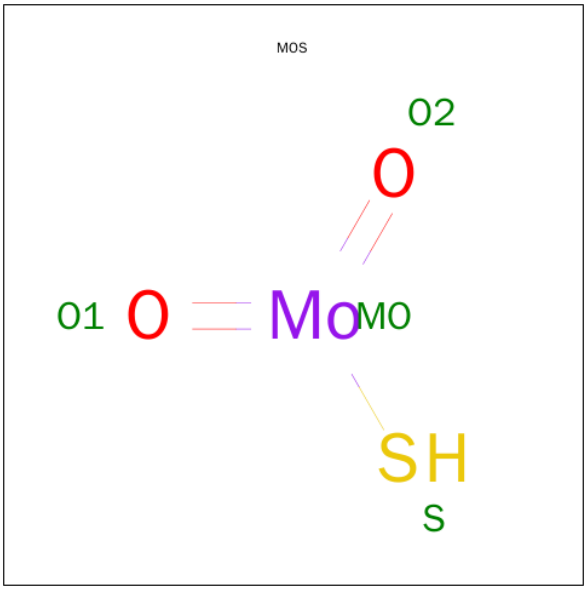
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0

- Molecule 8 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



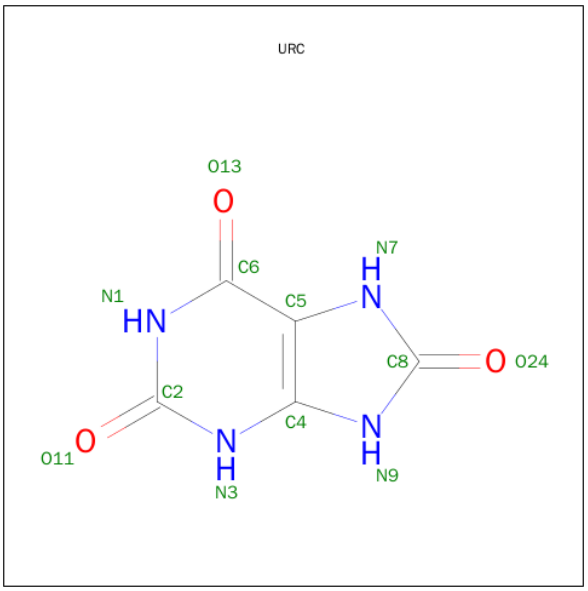
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
8	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 9 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: $HMoO_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	Mo	O	S	0	0
			3	1	1	1		
9	B	1	Total	Mo	O	S	0	0
			3	1	1	1		

- Molecule 10 is URIC ACID (three-letter code: URC) (formula: $C_5H_4N_4O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N O 12 5 4 3	0	0
10	B	1	Total C N O 12 5 4 3	0	0

- Molecule 11 is water.

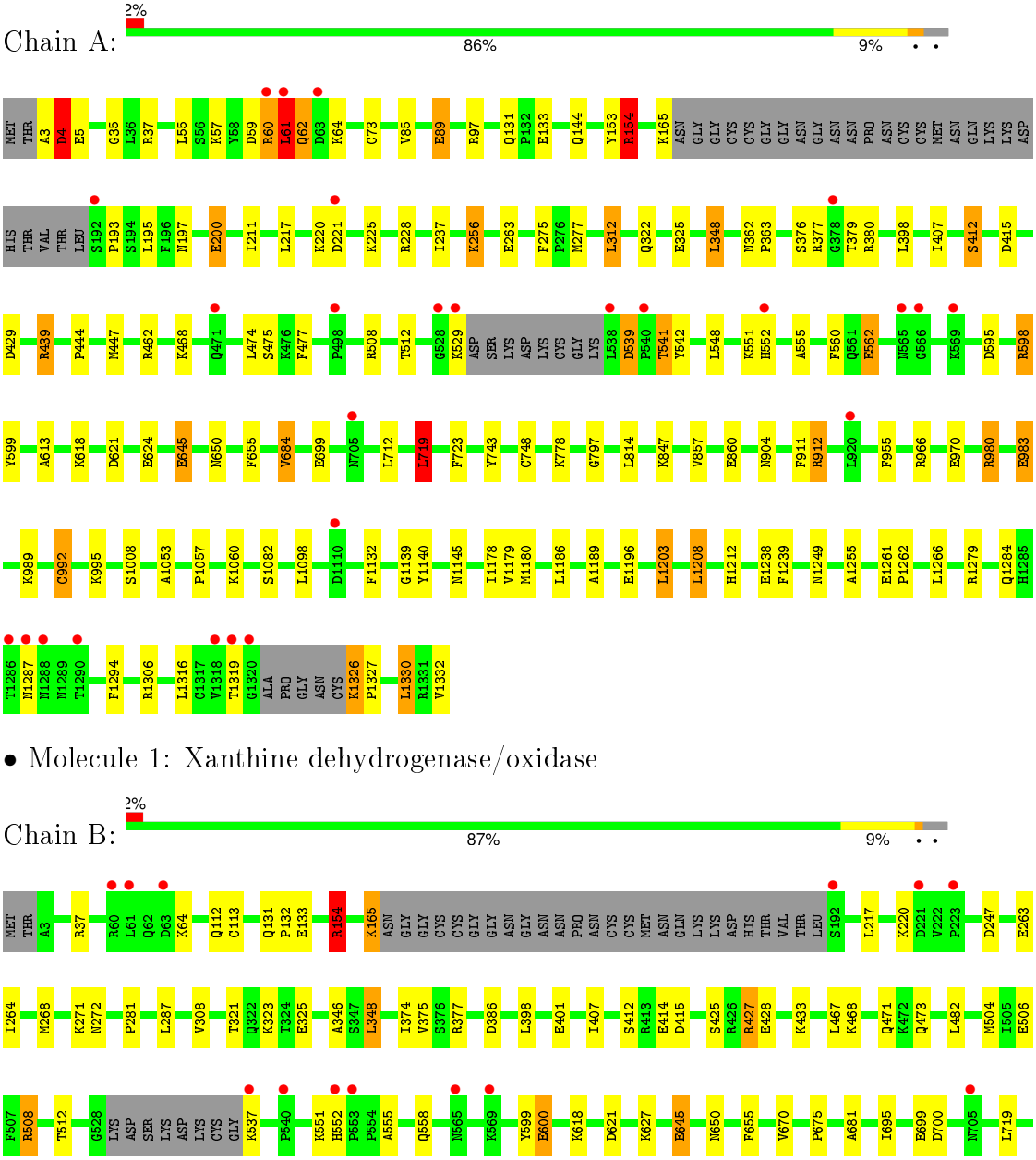
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1019	Total O 1019 1019	0	0
11	B	1010	Total O 1010 1010	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

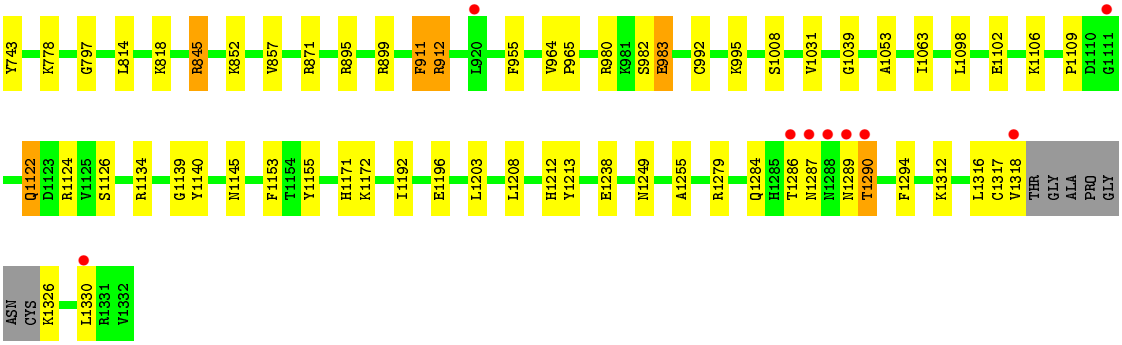
- Molecule 1: Xanthine dehydrogenase/oxidase

Chain A:



- Molecule 1: Xanthine dehydrogenase/oxidase

Chain B:


Y743
K778
G797
L814
K818
R845
K852
V857
R871
R895
R899
F911
R912
L920
F955
V964
P965
R980
K981
S982
E983
C992
K995
S1008
V1031
G1039
A1053
I1063
L1098
E1102
K1106
P1109
D1110
G1111
Q1122
D1123
R1124
V1125
S1126
R1134
G1139
Y1140
N1145
F1153
T1154
Y1155
H1171
K1172
I1192
E1196
L1203
L1208
H1212
Y1213
E1238
N1249
A1255
R1279
Q1284
H1285
T1286
N1287
N1288
N1289
T1290
F1294
K1312
L1316
C1317
V1318
THR
GLY
ALA
PRO
GLY
ASN
CYS
K1326
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	168.21Å 124.53Å 148.03Å 90.00° 91.07° 90.00°	Depositor
Resolution (Å)	34.83 – 2.10 34.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.83-2.10) 99.4 (34.83-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.151 , 0.202 0.152 , 0.203	Depositor DCC
R_{free} test set	8872 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.9	EDS
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 177440 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	22382	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, URC, MOS, CA, NAI, FES, BCT, FAD, MTE

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	1.09	9/10243 (0.1%)	0.96	31/13863 (0.2%)
1	B	1.07	6/10232 (0.1%)	0.94	15/13848 (0.1%)
All	All	1.08	15/20475 (0.1%)	0.95	46/27711 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	0	1
All	All	1	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	992	CYS	CB-SG	-8.12	1.68	1.82
1	A	983	GLU	CG-CD	7.98	1.64	1.51
1	B	992	CYS	CB-SG	-7.79	1.69	1.82
1	B	699	GLU	CG-CD	7.34	1.62	1.51
1	A	412	SER	CB-OG	-6.95	1.33	1.42
1	B	645	GLU	CD-OE2	6.73	1.33	1.25
1	A	73	CYS	CB-SG	6.12	1.92	1.82
1	A	645	GLU	CG-CD	5.93	1.60	1.51
1	A	153	TYR	CD2-CE2	5.64	1.47	1.39
1	B	645	GLU	CG-CD	5.61	1.60	1.51
1	B	983	GLU	CG-CD	5.58	1.60	1.51
1	A	645	GLU	CD-OE2	5.44	1.31	1.25
1	A	699	GLU	CG-CD	5.25	1.59	1.51
1	A	983	GLU	CD-OE2	5.10	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	508	ARG	CD-NE	-5.07	1.37	1.46

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	ARG	NE-CZ-NH2	-16.98	111.81	120.30
1	B	154	ARG	NE-CZ-NH2	-16.20	112.20	120.30
1	B	154	ARG	NE-CZ-NH1	15.12	127.86	120.30
1	A	97	ARG	NE-CZ-NH2	-14.60	113.00	120.30
1	B	508	ARG	NE-CZ-NH2	-14.59	113.00	120.30
1	B	508	ARG	NE-CZ-NH1	14.14	127.37	120.30
1	B	427	ARG	NE-CZ-NH2	-12.93	113.84	120.30
1	A	980	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	A	154	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	A	980	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	A	97	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	B	427	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	A	1332	VAL	CB-CA-C	7.77	126.16	111.40
1	B	1124	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	A	61	LEU	CA-CB-CG	7.03	131.46	115.30
1	B	1316	LEU	CA-CB-CG	7.01	131.42	115.30
1	A	398	LEU	CA-CB-CG	6.96	131.30	115.30
1	A	1306	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	386	ASP	CB-CG-OD1	6.76	124.38	118.30
1	B	1330	LEU	CA-CB-CG	6.65	130.60	115.30
1	A	684	VAL	CG1-CB-CG2	6.56	121.40	110.90
1	A	719	LEU	CA-CB-CG	-6.54	100.27	115.30
1	A	1203	LEU	CA-CB-CG	6.39	130.00	115.30
1	B	621	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	4	ASP	CB-CA-C	6.24	122.88	110.40
1	B	621	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	B	1124	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	1332	VAL	CG1-CB-CG2	-5.98	101.33	110.90
1	A	97	ARG	CG-CD-NE	-5.95	99.30	111.80
1	A	598	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	412	SER	N-CA-CB	-5.90	101.65	110.50
1	A	89	GLU	CA-CB-CG	5.82	126.20	113.40
1	B	845	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	598	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	621	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	1306	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	A	380	ARG	NE-CZ-NH2	-5.54	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	871	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	312	LEU	CB-CG-CD1	5.19	119.82	111.00
1	A	966	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	1208	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	1208	LEU	CB-CG-CD1	5.11	119.68	111.00
1	A	1186	LEU	CB-CG-CD1	-5.09	102.34	111.00
1	A	748	CYS	CA-CB-SG	-5.05	104.91	114.00
1	A	97	ARG	CD-NE-CZ	5.01	130.62	123.60
1	A	4	ASP	CB-CG-OD1	5.01	122.81	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1332	VAL	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1286	THR	Peptide

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	10024	0	10027	92	0
1	B	10013	0	10017	76	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	31	4	0
4	B	53	0	31	6	0
5	A	44	0	25	4	0
5	B	44	0	27	3	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	6	0	8	1	0
8	A	24	0	10	1	0
8	B	24	0	10	0	0
9	A	3	0	0	2	0
9	B	3	0	0	1	0
10	A	12	0	4	0	0
10	B	12	0	4	0	0
11	A	1019	0	0	18	0
11	B	1010	0	0	19	0
All	All	22382	0	20210	173	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 4.

All (173) 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:3:ALA:HB1	1:A:228:ARG:H	1.08	1.09
1:A:60:ARG:O	1:A:61:LEU:HB2	1.47	1.08
1:B:272:ASN:HB3	11:B:1988:HOH:O	1.65	0.95
1:B:217:LEU:O	1:B:220:LYS:HG2	1.70	0.92
1:A:3:ALA:HB1	1:A:228:ARG:N	1.86	0.90
4:A:3005:FAD:C4X	5:A:1333:NAI:C6N	2.50	0.90
4:B:4005:FAD:C4X	5:B:1333:NAI:C6N	2.52	0.88
1:B:37:ARG:HD3	11:B:1467:HOH:O	1.74	0.88
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.77	0.85
1:A:377:ARG:NE	11:A:2032:HOH:O	2.09	0.84
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.41	0.83
1:A:60:ARG:O	1:A:61:LEU:CB	2.27	0.83
1:A:237:ILE:HD12	1:A:277:MET:HE2	1.61	0.82
1:B:131:GLN:HE21	1:B:133:GLU:H	1.27	0.80
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.44	0.80
1:A:154:ARG:CD	1:A:1196:GLU:OE2	2.29	0.80
1:A:57:LYS:HD2	11:A:1470:HOH:O	1.81	0.79
1:A:1330:LEU:HG	11:A:2358:HOH:O	1.83	0.78
1:B:165:LYS:HE3	1:B:165:LYS:O	1.84	0.77
1:B:506:GLU:HG3	11:B:1384:HOH:O	1.86	0.76
1:A:552:HIS:HB2	11:A:2208:HOH:O	1.85	0.75
1:A:3:ALA:O	1:A:4:ASP:C	2.23	0.75
1:B:323:LYS:NZ	11:B:1485:HOH:O	2.18	0.75
1:B:552:HIS:CE1	1:B:1172:LYS:HZ2	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.51	0.74
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	1.85	0.73
1:A:154:ARG:HD2	11:A:1444:HOH:O	1.89	0.72
1:A:1279:ARG:HG2	1:A:1294:PHE:HE2	1.56	0.70
1:A:3:ALA:O	1:A:5:GLU:N	2.25	0.69
1:A:439:ARG:HB3	1:A:439:ARG:HH11	1.58	0.68
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.57	0.68
1:B:467:LEU:O	1:B:471:GLN:HG2	1.94	0.67
1:A:415:ASP:OD2	1:A:444:PRO:HA	1.95	0.66
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	1.95	0.66
1:A:1178:ILE:CG2	1:A:1180:MET:HE2	2.26	0.66
1:A:131:GLN:HE21	1:A:133:GLU:H	1.44	0.66
1:A:237:ILE:HD12	1:A:277:MET:CE	2.25	0.66
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	1.92	0.65
1:B:1212:HIS:HD2	11:B:2345:HOH:O	1.80	0.64
1:B:154:ARG:HD2	11:B:1705:HOH:O	1.98	0.63
1:A:1249:ASN:O	1:A:1255:ALA:HA	1.98	0.63
1:B:433:LYS:HE2	1:B:504:MET:SD	2.38	0.63
1:B:1312:LYS:HE2	11:B:2314:HOH:O	1.99	0.62
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.64	0.62
1:A:1319:THR:HG22	11:A:2095:HOH:O	2.00	0.62
1:A:995:LYS:HZ3	1:A:1284:GLN:HE21	1.48	0.61
1:B:627:LYS:NZ	11:B:2302:HOH:O	2.28	0.61
1:A:154:ARG:HD2	1:A:1196:GLU:OE2	2.00	0.61
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.50	0.60
1:A:624:GLU:HB3	11:A:2199:HOH:O	2.00	0.60
9:A:1338:MOS:MO	9:A:1338:MOS:O1	1.72	0.59
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.85	0.58
1:B:348:LEU:HD13	1:B:407:ILE:HD13	1.84	0.58
4:A:3005:FAD:C4	5:A:1333:NAI:C6N	2.81	0.58
1:A:562:GLU:HB2	11:A:2245:HOH:O	2.04	0.58
1:B:425:SER:OG	1:B:433:LYS:NZ	2.38	0.57
1:B:427:ARG:NH2	1:B:1171:HIS:O	2.37	0.57
1:B:645:GLU:HG2	1:B:650:ASN:ND2	2.16	0.57
1:A:237:ILE:CD1	1:A:277:MET:CE	2.82	0.57
4:B:4005:FAD:C4	5:B:1333:NAI:C6N	2.83	0.57
1:A:645:GLU:HG2	1:A:650:ASN:ND2	2.19	0.57
1:B:552:HIS:CE1	1:B:1172:LYS:NZ	2.73	0.57
1:A:144:GLN:HE21	1:A:429:ASP:H	1.53	0.56
1:B:695:ILE:HG23	1:B:700:ASP:HB3	1.87	0.56
1:A:541:THR:HG23	1:A:992:CYS:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:LYS:N	1:A:1327:PRO:CD	2.70	0.55
1:B:980:ARG:HD2	11:B:2278:HOH:O	2.07	0.55
1:A:197:ASN:O	1:A:200:GLU:HG3	2.06	0.54
1:B:154:ARG:CD	1:B:1196:GLU:OE2	2.55	0.54
1:B:1106:LYS:O	1:B:1109:PRO:HD3	2.08	0.54
1:B:264:ILE:HD11	4:B:4005:FAD:H3B	1.89	0.54
1:A:322:GLN:O	1:A:412:SER:HB3	2.08	0.54
1:B:346:ALA:HB1	4:B:4005:FAD:H4'	1.90	0.53
1:A:1140:TYR:OH	1:A:1145:ASN:ND2	2.41	0.53
1:A:508:ARG:O	1:A:512:THR:HG23	2.08	0.52
1:A:655:PHE:HE1	1:A:814:LEU:CD2	2.23	0.52
1:A:256:LYS:HG3	1:A:275:PHE:CD2	2.45	0.52
1:A:220:LYS:HG2	1:A:221:ASP:N	2.25	0.51
1:A:719:LEU:HD22	1:A:860:GLU:HG3	1.93	0.51
1:A:37:ARG:HD3	1:A:595:ASP:O	2.11	0.51
1:A:980:ARG:HD2	11:A:2318:HOH:O	2.12	0.50
1:B:508:ARG:O	1:B:512:THR:HG23	2.11	0.50
1:A:263:GLU:HB2	11:A:2103:HOH:O	2.11	0.50
1:A:655:PHE:CE1	1:A:814:LEU:HD23	2.44	0.50
1:A:59:ASP:OD2	1:A:62:GLN:HB2	2.12	0.50
1:A:193:PRO:HG2	1:A:560:PHE:CE1	2.47	0.49
1:A:220:LYS:HE3	11:A:2267:HOH:O	2.11	0.49
1:A:1057:PRO:HD2	1:A:1060:LYS:HD2	1.95	0.49
1:A:237:ILE:CD1	1:A:277:MET:HE3	2.43	0.48
1:A:1212:HIS:HD2	11:A:1528:HOH:O	1.95	0.48
1:B:401:GLU:HB2	11:B:1713:HOH:O	2.13	0.48
1:A:35:GLY:N	11:A:2071:HOH:O	2.47	0.48
1:B:473:GLN:HE21	1:B:482:LEU:HD12	1.79	0.48
1:B:428:GLU:HG2	11:B:1891:HOH:O	2.12	0.48
1:A:529:LYS:HG2	11:A:2066:HOH:O	2.13	0.48
1:B:271:LYS:HE2	11:B:2010:HOH:O	2.13	0.48
1:B:414:GLU:O	1:B:415:ASP:HB2	2.13	0.48
1:A:539:ASP:OD1	1:A:541:THR:HB	2.14	0.48
1:B:1203:LEU:C	1:B:1203:LEU:HD23	2.34	0.48
4:A:3005:FAD:C4	5:A:1333:NAI:H6N	2.44	0.48
1:A:1178:ILE:CG2	1:A:1180:MET:CE	2.92	0.47
1:A:1132:PHE:CD1	1:B:1126:SER:HB2	2.49	0.47
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.96	0.47
1:A:376:SER:HB3	1:A:379:THR:OG1	2.15	0.47
1:B:247:ASP:OD1	1:B:377:ARG:HD3	2.14	0.46
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1289:ASN:O	1:B:1290:THR:HB	2.16	0.46
1:B:912:ARG:N	9:B:1337:MOS:S	2.89	0.46
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.80	0.46
1:A:154:ARG:HD3	1:A:1196:GLU:CD	2.35	0.46
1:B:468:LYS:HG3	11:B:1428:HOH:O	2.15	0.46
1:B:555:ALA:O	1:B:1238:GLU:HA	2.16	0.46
1:B:263:GLU:HB3	4:B:4005:FAD:H52A	1.98	0.45
1:B:281:PRO:HB2	1:B:287:LEU:CD1	2.47	0.45
1:A:723:PHE:CE2	1:A:847:LYS:HG2	2.51	0.45
1:A:474:LEU:O	1:A:475:SER:HB2	2.16	0.45
1:A:217:LEU:O	1:A:220:LYS:HD3	2.16	0.45
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.97	0.45
1:A:618:LYS:HA	1:A:618:LYS:HD2	1.67	0.45
1:B:1213:TYR:HD1	11:B:2360:HOH:O	2.00	0.45
1:B:1153:PHE:HB2	1:B:1155:TYR:CZ	2.52	0.45
1:B:1122:GLN:NE2	11:B:1906:HOH:O	2.50	0.44
1:A:217:LEU:HA	1:A:217:LEU:HD12	1.77	0.44
1:B:112:GLN:HB3	1:B:1039:GLY:O	2.17	0.44
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.44
1:A:1082:SER:HB2	8:A:1337:MTE:O3P	2.17	0.44
1:A:723:PHE:CZ	1:A:847:LYS:HG2	2.53	0.44
1:A:35:GLY:HA2	11:A:2071:HOH:O	2.17	0.44
4:A:3005:FAD:C4X	5:A:1333:NAI:C5N	2.96	0.44
1:A:1212:HIS:HE1	11:A:1816:HOH:O	2.00	0.44
1:A:970:GLU:HG2	1:A:1179:VAL:HG21	2.00	0.44
1:A:195:LEU:HD22	1:A:1189:ALA:HA	2.00	0.44
1:A:256:LYS:HE2	1:A:275:PHE:CE2	2.52	0.43
1:B:325:GLU:HB2	1:B:412:SER:HB3	2.00	0.43
1:A:613:ALA:O	1:A:904:ASN:HB3	2.19	0.43
1:B:1212:HIS:HE1	11:B:2011:HOH:O	2.00	0.43
1:A:598:ARG:HG3	1:B:600:GLU:HG2	2.00	0.43
1:B:268:MET:CE	11:B:2245:HOH:O	2.67	0.43
1:B:113:CYS:HA	1:B:1039:GLY:HA2	2.00	0.43
1:B:1140:TYR:OH	1:B:1145:ASN:ND2	2.51	0.43
1:B:374:ILE:HD13	1:B:398:LEU:HD22	2.01	0.43
1:B:1279:ARG:HG2	1:B:1294:PHE:HE2	1.84	0.43
1:A:55:LEU:CD2	1:A:85:VAL:HG22	2.49	0.43
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.18	0.43
1:A:362:ASN:N	1:A:363:PRO:CD	2.82	0.43
1:A:348:LEU:HD13	1:A:407:ILE:HD13	2.01	0.43
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.84	0.43
1:B:308:VAL:HG21	1:B:348:LEU:HG	2.01	0.43
1:A:712:LEU:HG	11:A:1380:HOH:O	2.19	0.42
4:B:4005:FAD:C4	5:B:1333:NAI:H6N	2.49	0.42
1:A:325:GLU:HB2	1:A:412:SER:OG	2.19	0.42
1:A:995:LYS:NZ	1:A:1284:GLN:NE2	2.63	0.42
1:B:911:PHE:O	1:B:912:ARG:C	2.57	0.42
1:B:1031:VAL:HB	1:B:1063:ILE:HG12	2.01	0.42
1:A:599:TYR:HA	1:B:599:TYR:HA	2.02	0.42
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.20	0.41
1:A:1178:ILE:HG21	1:A:1180:MET:CE	2.50	0.41
1:A:447:MET:O	1:A:477:PHE:HA	2.20	0.41
1:A:995:LYS:HZ1	1:A:1284:GLN:HE21	1.64	0.41
1:A:1180:MET:HE1	1:A:1266:LEU:HD12	2.02	0.41
1:B:1134:ARG:HG2	11:B:1419:HOH:O	2.20	0.41
1:A:912:ARG:N	9:A:1338:MOS:S	2.94	0.41
1:A:541:THR:HG22	1:A:542:TYR:HD1	1.84	0.41
1:A:35:GLY:CA	11:A:2071:HOH:O	2.69	0.41
1:B:272:ASN:CB	11:B:1988:HOH:O	2.42	0.41
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.86	0.41
1:B:645:GLU:CG	1:B:650:ASN:HD22	2.26	0.40
1:B:675:PRO:HB3	7:B:1335:GOL:H12	2.03	0.40
1:B:1102:GLU:OE1	1:B:1106:LYS:HD2	2.22	0.40
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	2.02	0.40
1:A:555:ALA:O	1:A:1238:GLU:HA	2.20	0.40
1:B:618:LYS:HD2	1:B:618:LYS:HA	1.91	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	1283/1332 (96%)	1234 (96%)	42 (3%)	7 (0%)	34	30
1	B	1281/1332 (96%)	1239 (97%)	37 (3%)	5 (0%)	39	37
All	All	2564/2664 (96%)	2473 (96%)	79 (3%)	12 (0%)	34	30

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	539	ASP
1	A	61	LEU
1	A	912	ARG
1	A	1008	SER
1	B	1008	SER
1	B	912	ARG
1	A	1139	GLY
1	A	797	GLY
1	B	797	GLY
1	B	1139	GLY
1	B	1290	THR

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	1095/1128 (97%)	1061 (97%)	34 (3%)	47	50
1	B	1094/1128 (97%)	1069 (98%)	25 (2%)	58	62
All	All	2189/2256 (97%)	2130 (97%)	59 (3%)	52	56

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	61	LEU
1	A	62	GLN
1	A	64	LYS

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Mol	Chain	Res	Type
1	A	89	GLU
1	A	154	ARG
1	A	165	LYS
1	A	200	GLU
1	A	211	ILE
1	A	225	LYS
1	A	256	LYS
1	A	312	LEU
1	A	348	LEU
1	A	439	ARG
1	A	462	ARG
1	A	468	LYS
1	A	541	THR
1	A	548	LEU
1	A	551	LYS
1	A	562	GLU
1	A	684	VAL
1	A	719	LEU
1	A	743	TYR
1	A	857	VAL
1	A	911	PHE
1	A	983	GLU
1	A	989	LYS
1	A	1203	LEU
1	A	1208	LEU
1	A	1239	PHE
1	A	1287	ASN
1	A	1316	LEU
1	A	1326	LYS
1	A	1330	LEU
1	B	64	LYS
1	B	132	PRO
1	B	154	ARG
1	B	165	LYS
1	B	321	THR
1	B	348	LEU
1	B	375	VAL
1	B	537	LYS
1	B	551	LYS
1	B	600	GLU
1	B	743	TYR
1	B	818	LYS

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Mol	Chain	Res	Type
1	B	845	ARG
1	B	852	LYS
1	B	857	VAL
1	B	899	ARG
1	B	911	PHE
1	B	982	SER
1	B	983	GLU
1	B	1122	GLN
1	B	1208	LEU
1	B	1287	ASN
1	B	1317	CYS
1	B	1318	VAL
1	B	1326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	144	GLN
1	A	251	GLN
1	A	473	GLN
1	A	567	GLN
1	A	650	ASN
1	A	728	ASN
1	A	1088	GLN
1	A	1145	ASN
1	A	1212	HIS
1	A	1284	GLN
1	B	131	GLN
1	B	146	ASN
1	B	251	GLN
1	B	333	GLN
1	B	471	GLN
1	B	473	GLN
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	1088	GLN
1	B	1122	GLN
1	B	1145	ASN
1	B	1212	HIS
1	B	1284	GLN

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Mol	Chain	Res	Type
1	B	1288	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	$\#\|Z\| > 2$
5	NAI	A	1333	-	38,48,48	1.32	4 (10%)	48,73,73	2.65	10 (20%)
6	BCT	A	1334	-	0,3,3	0.00	-	0,3,3	0.00	-
7	GOL	A	1335	-	5,5,5	1.00	0	5,5,5	1.71	1 (20%)
7	GOL	A	1336	-	5,5,5	0.32	0	5,5,5	0.53	0
8	MTE	A	1337	9	19,26,26	1.43	4 (21%)	19,40,40	2.03	9 (47%)
9	MOS	A	1338	8,10	0,2,3	0.00	-	0,1,3	0.00	-
10	URC	A	1339	9	12,13,13	6.52	10 (83%)	10,19,19	11.08	5 (50%)
2	FES	A	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	A	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	A	3005	-	48,58,58	1.20	5 (10%)	54,89,89	2.67	16 (29%)
5	NAI	B	1333	-	38,48,48	1.26	5 (13%)	48,73,73	2.57	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BCT	B	1334	-	0,3,3	0.00	-	0,3,3	0.00	-
7	GOL	B	1335	-	5,5,5	0.52	0	5,5,5	0.74	0
8	MTE	B	1336	9	19,26,26	1.96	6 (31%)	19,40,40	1.84	5 (26%)
9	MOS	B	1337	8,10	0,2,3	0.00	-	0,1,3	0.00	-
10	URC	B	1338	9	12,13,13	6.30	8 (66%)	10,19,19	11.72	9 (90%)
2	FES	B	4001	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	B	4002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	B	4005	-	48,58,58	1.39	5 (10%)	54,89,89	2.52	13 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAI	A	1333	-	-	0/25/72/72	0/4/5/5
6	BCT	A	1334	-	-	0/0/0/0	0/0/0/0
7	GOL	A	1335	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1336	-	-	0/4/4/4	0/0/0/0
8	MTE	A	1337	9	-	0/6/34/34	0/3/3/3
9	MOS	A	1338	8,10	-	0/0/0/0	0/0/0/0
10	URC	A	1339	9	-	0/0/24/24	0/2/2/2
2	FES	A	3001	1	-	0/0/4/4	0/1/1/1
2	FES	A	3002	1	-	0/0/4/4	0/1/1/1
4	FAD	A	3005	-	-	0/30/50/50	0/6/6/6
5	NAI	B	1333	-	-	0/25/72/72	0/4/5/5
6	BCT	B	1334	-	-	0/0/0/0	0/0/0/0
7	GOL	B	1335	-	-	0/4/4/4	0/0/0/0
8	MTE	B	1336	9	-	0/6/34/34	0/3/3/3
9	MOS	B	1337	8,10	-	0/0/0/0	0/0/0/0
10	URC	B	1338	9	-	0/0/24/24	0/2/2/2
2	FES	B	4001	1	-	0/0/4/4	0/1/1/1
2	FES	B	4002	1	-	0/0/4/4	0/1/1/1
4	FAD	B	4005	-	-	0/30/50/50	0/6/6/6

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1338	URC	C4-N3	-7.89	1.37	1.46
10	A	1339	URC	C4-N3	-7.29	1.37	1.46
10	B	1338	URC	C4-N9	-5.03	1.38	1.44
10	A	1339	URC	C5-C6	-4.96	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1339	URC	C4-N9	-4.88	1.38	1.44
10	B	1338	URC	C5-C6	-4.76	1.44	1.53
5	A	1333	NAI	C4N-C5N	-3.95	1.40	1.49
5	B	1333	NAI	C4N-C5N	-3.66	1.41	1.49
5	A	1333	NAI	C7N-N7N	-3.18	1.24	1.33
5	B	1333	NAI	C7N-N7N	-2.54	1.25	1.33
10	A	1339	URC	C5-N7	-2.45	1.40	1.45
10	B	1338	URC	C5-N7	-2.38	1.40	1.45
8	B	1336	MTE	C10-N1	2.04	1.38	1.34
10	A	1339	URC	C2-N3	2.07	1.39	1.34
10	B	1338	URC	O11-C2	2.15	1.27	1.23
4	A	3005	FAD	C9A-N10	2.16	1.41	1.38
4	B	4005	FAD	C5X-N5	2.18	1.38	1.35
8	A	1337	MTE	C6-N5	2.19	1.48	1.45
8	A	1337	MTE	C4-N3	2.20	1.37	1.33
8	B	1336	MTE	C10-N8	2.28	1.39	1.35
4	A	3005	FAD	C4-N3	2.37	1.37	1.33
8	A	1337	MTE	C10-N8	2.41	1.39	1.35
5	B	1333	NAI	C6N-N1N	2.44	1.44	1.37
5	B	1333	NAI	C2A-N3A	2.50	1.36	1.32
10	A	1339	URC	C6-N1	2.56	1.41	1.37
8	B	1336	MTE	C4-N3	2.70	1.38	1.33
4	A	3005	FAD	C2A-N1A	2.77	1.39	1.33
4	A	3005	FAD	C2A-N3A	2.80	1.37	1.32
4	B	4005	FAD	C9A-N10	2.89	1.42	1.38
8	B	1336	MTE	C7-C6	2.96	1.55	1.53
5	A	1333	NAI	O4B-C1B	3.00	1.45	1.41
8	B	1336	MTE	C6-N5	3.08	1.49	1.45
4	B	4005	FAD	C4-N3	3.09	1.38	1.33
5	A	1333	NAI	C6N-C5N	3.26	1.39	1.33
10	A	1339	URC	O11-C2	3.29	1.30	1.23
5	B	1333	NAI	C6N-C5N	3.49	1.40	1.33
8	A	1337	MTE	O4-C4	3.88	1.34	1.24
4	B	4005	FAD	C2A-N1A	4.11	1.41	1.33
4	A	3005	FAD	C4X-N5	4.19	1.39	1.33
4	B	4005	FAD	C2A-N3A	4.20	1.39	1.32
8	B	1336	MTE	O4-C4	5.23	1.37	1.24
10	A	1339	URC	O24-C8	8.52	1.40	1.23
10	B	1338	URC	O24-C8	8.59	1.40	1.23
10	B	1338	URC	C8-N9	9.78	1.48	1.35
10	A	1339	URC	C8-N9	10.54	1.50	1.35
10	B	1338	URC	C8-N7	13.40	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1339	URC	C8-N7	13.79	1.54	1.35

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1339	URC	O24-C8-N9	-25.38	96.44	125.90
10	B	1338	URC	O24-C8-N9	-23.68	98.41	125.90
5	A	1333	NAI	N3A-C2A-N1A	-14.70	117.64	128.89
5	B	1333	NAI	N3A-C2A-N1A	-14.13	118.08	128.89
4	B	4005	FAD	N3A-C2A-N1A	-13.17	118.81	128.89
4	A	3005	FAD	N3A-C2A-N1A	-12.84	119.06	128.89
10	B	1338	URC	N7-C8-N9	-12.46	100.28	108.88
10	A	1339	URC	N7-C8-N9	-12.33	100.37	108.88
4	A	3005	FAD	O3'-C3'-C2'	-4.99	96.18	108.75
4	A	3005	FAD	C4X-C4-N3	-4.31	117.69	123.59
5	B	1333	NAI	O3-PA-O5B	-4.21	91.77	102.94
5	A	1333	NAI	C1D-N1N-C2N	-4.19	113.61	120.91
5	B	1333	NAI	C1D-N1N-C2N	-4.14	113.70	120.91
4	B	4005	FAD	O3'-C3'-C2'	-3.65	99.55	108.75
4	B	4005	FAD	C4X-C4-N3	-3.47	118.85	123.59
4	A	3005	FAD	C9A-C5X-N5	-3.38	117.36	122.36
7	A	1335	GOL	O2-C2-C3	-3.35	93.27	108.65
8	B	1336	MTE	N3-C2-N1	-2.95	120.70	125.53
10	B	1338	URC	O13-C6-N1	-2.92	115.46	120.93
5	B	1333	NAI	C4N-C5N-C6N	-2.79	117.98	122.58
4	A	3005	FAD	O3P-PA-O5B	-2.76	95.61	102.94
8	A	1337	MTE	O2P-P-O4'	-2.75	98.66	106.56
4	B	4005	FAD	O2'-C2'-C3'	-2.63	102.40	109.02
10	B	1338	URC	O11-C2-N3	-2.61	116.80	122.86
5	A	1333	NAI	O4D-C4D-C3D	-2.58	99.94	105.15
4	B	4005	FAD	C9A-C5X-N5	-2.54	118.60	122.36
5	A	1333	NAI	C1B-N9A-C4A	-2.53	123.12	126.94
8	A	1337	MTE	C10-N8-C7	-2.41	118.95	123.67
4	B	4005	FAD	O3P-P-O5'	-2.41	96.54	102.94
4	A	3005	FAD	O2'-C2'-C3'	-2.39	103.01	109.02
4	B	4005	FAD	O4B-C1B-N9A	-2.32	103.23	108.10
5	A	1333	NAI	C4N-C5N-C6N	-2.29	118.80	122.58
8	A	1337	MTE	N3-C2-N1	-2.29	121.79	125.53
5	B	1333	NAI	C1D-N1N-C6N	-2.26	115.74	120.81
8	A	1337	MTE	O3'-C7-C6	-2.22	107.44	108.96
5	A	1333	NAI	PN-O3-PA	-2.22	126.50	132.73
4	A	3005	FAD	C4A-C5A-N7A	-2.19	107.46	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3005	FAD	O3P-P-O5'	-2.16	97.21	102.94
4	B	4005	FAD	O3B-C3B-C4B	-2.07	104.86	111.05
8	A	1337	MTE	C10-C9-N5	2.02	121.40	118.85
4	A	3005	FAD	C2B-C1B-N9A	2.11	117.52	114.29
4	A	3005	FAD	C1'-N10-C9A	2.16	121.29	118.86
10	B	1338	URC	N1-C2-N3	2.24	118.59	116.14
4	A	3005	FAD	C4-C4X-N5	2.24	121.44	118.72
8	A	1337	MTE	C4-N3-C2	2.35	119.20	115.94
8	B	1336	MTE	C2-N1-C10	2.40	119.93	114.54
8	B	1336	MTE	O2P-P-O1P	2.44	118.44	110.58
5	B	1333	NAI	O4D-C1D-N1N	2.46	113.26	108.07
8	A	1337	MTE	C9-C10-N8	2.46	120.92	118.34
5	A	1333	NAI	C2A-N1A-C6A	2.51	123.25	118.77
4	B	4005	FAD	C6-C5X-C9A	2.55	122.34	118.98
4	B	4005	FAD	C2B-C1B-N9A	2.60	118.27	114.29
8	A	1337	MTE	C2-N1-C10	2.74	120.69	114.54
4	A	3005	FAD	C6-C5X-C9A	2.82	122.69	118.98
4	A	3005	FAD	O4'-C4'-C3'	2.85	116.18	109.02
8	B	1336	MTE	C4-N3-C2	2.87	119.92	115.94
5	B	1333	NAI	O1N-PN-O2N	3.02	128.91	112.53
5	B	1333	NAI	C5N-C4N-C3N	3.04	120.91	112.52
5	A	1333	NAI	C5N-C4N-C3N	3.05	120.93	112.52
5	B	1333	NAI	C2A-N1A-C6A	3.13	124.36	118.77
10	B	1338	URC	O13-C6-C5	3.23	124.69	119.47
5	A	1333	NAI	O1N-PN-O2N	3.36	130.75	112.53
8	A	1337	MTE	O2P-P-O1P	3.48	121.77	110.58
4	A	3005	FAD	O2'-C2'-C1'	3.56	118.69	109.94
10	A	1339	URC	O24-C8-N7	3.72	130.23	125.90
5	A	1333	NAI	C2B-C1B-N9A	3.78	120.07	114.29
4	B	4005	FAD	C1'-N10-C9A	3.84	123.17	118.86
10	B	1338	URC	O24-C8-N7	3.88	130.41	125.90
4	B	4005	FAD	C4-N3-C2	4.09	118.78	115.25
8	B	1336	MTE	C4-C9-C10	4.44	118.58	114.56
10	B	1338	URC	N9-C4-N3	5.33	122.55	112.36
4	B	4005	FAD	C4X-N5-C5X	5.61	123.22	116.76
4	A	3005	FAD	C4-N3-C2	5.70	120.18	115.25
4	A	3005	FAD	C4X-N5-C5X	5.90	123.55	116.76
10	A	1339	URC	N9-C4-N3	5.95	123.74	112.36
10	A	1339	URC	C5-C4-N9	19.26	111.24	102.69
10	B	1338	URC	C5-C4-N9	24.13	113.40	102.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1333	NAI	4	0
8	A	1337	MTE	1	0
9	A	1338	MOS	2	0
4	A	3005	FAD	4	0
5	B	1333	NAI	3	0
7	B	1335	GOL	1	0
9	B	1337	MOS	1	0
4	B	4005	FAD	6	0

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	1291/1332 (96%)	-0.42	26 (2%)	68	73	12, 22, 39, 66	0
1	B	1289/1332 (96%)	-0.46	22 (1%)	73	78	12, 22, 39, 65	0
All	All	2580/2664 (96%)	-0.44	48 (1%)	70	75	12, 22, 39, 66	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1288	ASN	7.6
1	B	1288	ASN	5.9
1	B	1287	ASN	5.8
1	B	565	ASN	4.8
1	A	565	ASN	4.7
1	A	1287	ASN	4.5
1	A	1320	GLY	4.5
1	A	1319	THR	4.4
1	A	1318	VAL	4.2
1	A	552	HIS	4.1
1	A	528	GLY	4.1
1	A	378	GLY	4.0
1	A	60	ARG	3.7
1	B	1318	VAL	3.7
1	A	192	SER	3.7
1	B	60	ARG	3.7
1	A	566	GLY	3.6
1	B	192	SER	3.5
1	B	61	LEU	3.4
1	A	529	LYS	3.3
1	B	223	PRO	3.3
1	A	538	LEU	3.3
1	B	537	LYS	3.2
1	B	552	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	1286	THR	2.9
1	B	1289	ASN	2.9
1	A	540	PRO	2.7
1	A	61	LEU	2.6
1	B	540	PRO	2.6
1	B	1111	GLY	2.4
1	B	553	PRO	2.4
1	A	221	ASP	2.4
1	A	471	GLN	2.4
1	A	1290	THR	2.4
1	A	63	ASP	2.4
1	B	221	ASP	2.3
1	A	498	PRO	2.3
1	A	1286	THR	2.2
1	B	1290	THR	2.2
1	A	705	ASN	2.2
1	B	1330	LEU	2.1
1	A	920	LEU	2.1
1	B	569	LYS	2.1
1	A	569	LYS	2.1
1	B	920	LEU	2.0
1	A	1110	ASP	2.0
1	B	705	ASN	2.0
1	B	63	ASP	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
7	GOL	A	1335	6/6	0.91	0.14	3.79	28,39,39,41	0
7	GOL	B	1335	6/6	0.93	0.12	2.78	29,35,39,40	0
10	URC	B	1338	12/12	0.91	0.16	2.06	31,38,41,43	0
7	GOL	A	1336	6/6	0.96	0.11	0.81	23,27,31,32	0
10	URC	A	1339	12/12	0.88	0.13	0.59	30,34,37,39	0
4	FAD	B	4005	53/53	0.98	0.10	-0.19	15,18,21,28	0
4	FAD	A	3005	53/53	0.98	0.11	-0.31	14,19,24,28	0
6	BCT	A	1334	4/4	0.98	0.11	-0.43	17,20,20,22	0
5	NAI	A	1333	44/44	0.96	0.08	-0.68	18,25,29,33	0
2	FES	A	3002	4/4	1.00	0.07	-0.75	15,15,17,18	0
8	MTE	A	1337	24/24	0.98	0.09	-0.85	14,19,24,25	0
5	NAI	B	1333	44/44	0.98	0.07	-0.91	18,25,28,31	0
6	BCT	B	1334	4/4	0.99	0.09	-1.17	16,17,18,19	0
3	CA	B	4008	1/1	1.00	0.05	-1.19	19,19,19,19	0
2	FES	A	3001	4/4	1.00	0.05	-1.41	15,15,16,17	0
3	CA	A	3008	1/1	1.00	0.05	-1.43	20,20,20,20	0
2	FES	B	4001	4/4	1.00	0.05	-1.51	14,15,16,16	0
8	MTE	B	1336	24/24	0.99	0.07	-1.54	15,20,23,25	0
2	FES	B	4002	4/4	1.00	0.06	-1.79	14,15,16,16	0
9	MOS	A	1338	3/4	1.00	0.06	-1.97	25,25,27,40	0
9	MOS	B	1337	3/4	1.00	0.06	-2.48	27,27,27,39	0

6.5 Other polymers (i)

There are no such residues in this entry.