Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:43 PM GMT

PDB ID	:	3UNI
Title	:	Crystal Structure of Bovine Milk Xanthine Dehydrogenase with NADH Bound
Authors	:	Eger, B.T.; Okamoto, K.; Nishino, T.; Pai, E.F.
Deposited on	:	2011-11-15
Resolution	:	2.20 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:

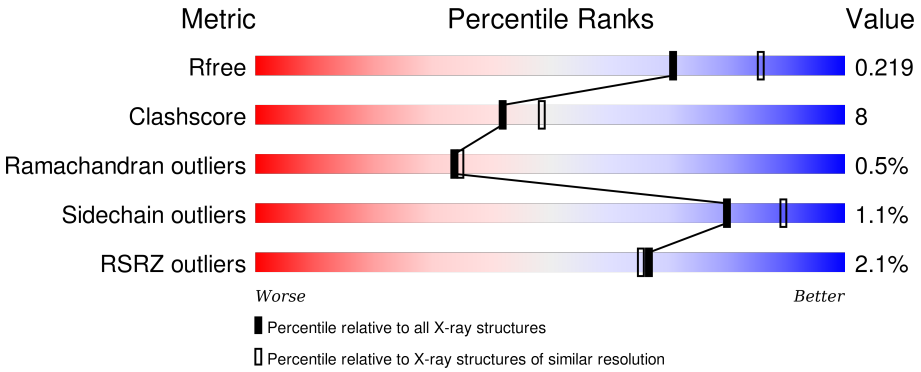
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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% 77% 19%
1	B	1332	2% 78% 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
4	MOS	A	1336	-	-	X	-
4	MOS	B	1336	-	-	X	-
7	GOL	A	1341	-	-	-	X
7	GOL	B	1339	-	-	-	X

2 Entry composition

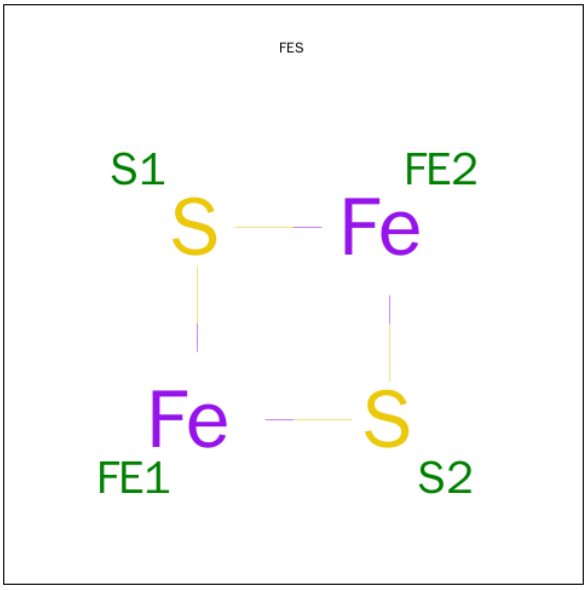
There are 11 unique types of molecules in this entry. The entry contains 21491 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

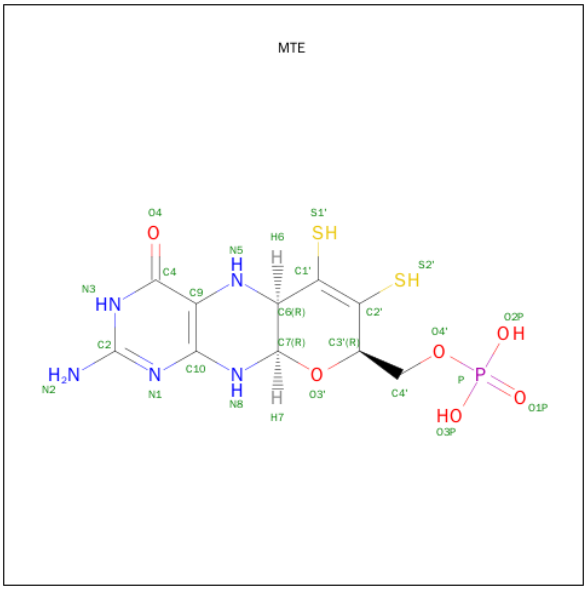
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1289	Total	C	N	O	S	0	0	0
			10003	6360	1712	1871	60			
1	B	1288	Total	C	N	O	S	0	0	0
			9998	6357	1711	1870	60			

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



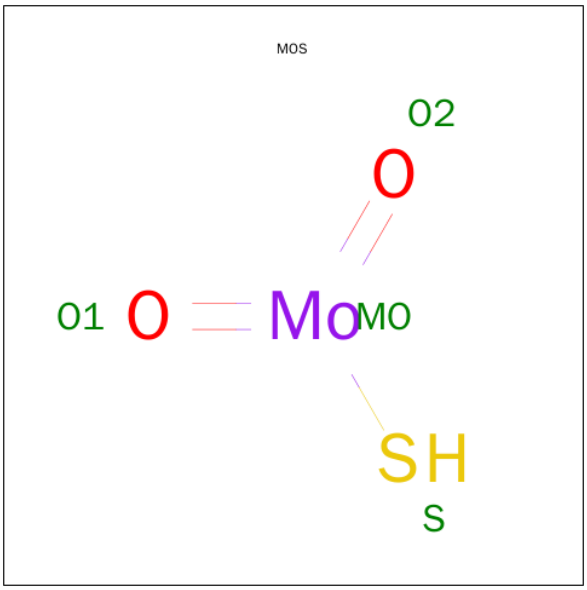
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is 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: $C_{10}H_{14}N_5O_6PS_2$).



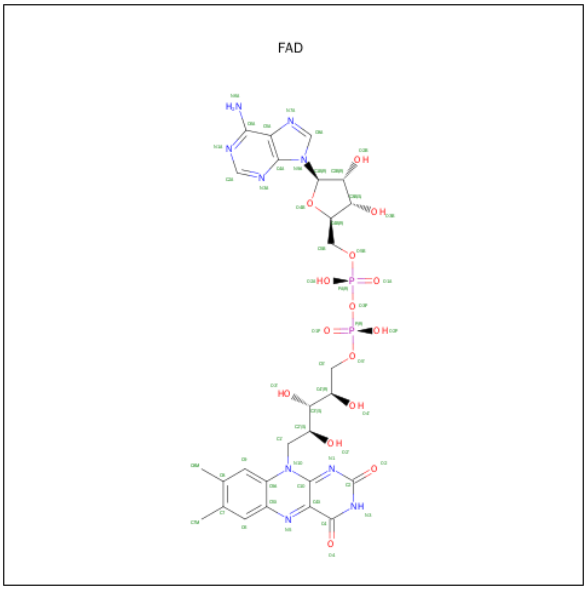
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 4 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: $HMoO_2S$).



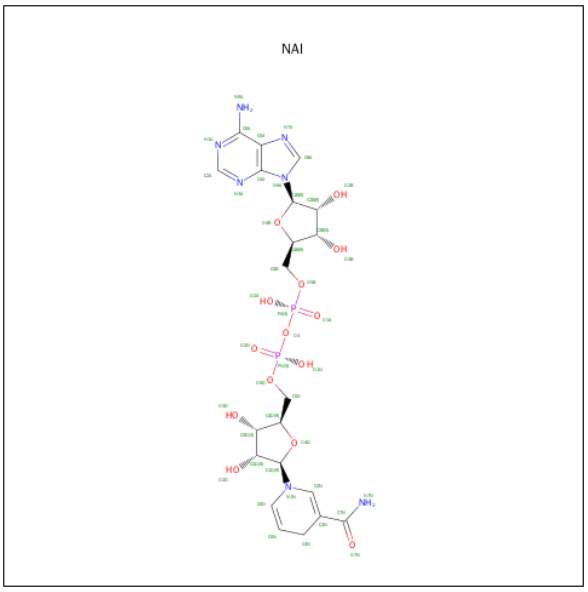
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
4	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

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



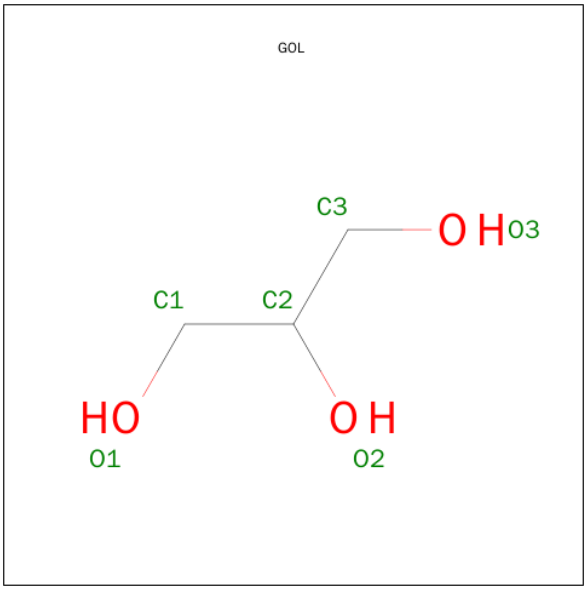
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is 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
6	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
6	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- 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		0	0
			6	3	3			
7	A	1	Total	C	O		0	0
			6	3	3			

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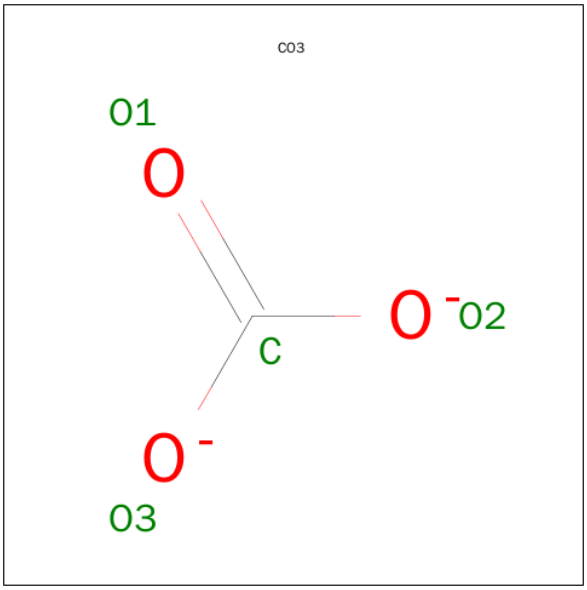
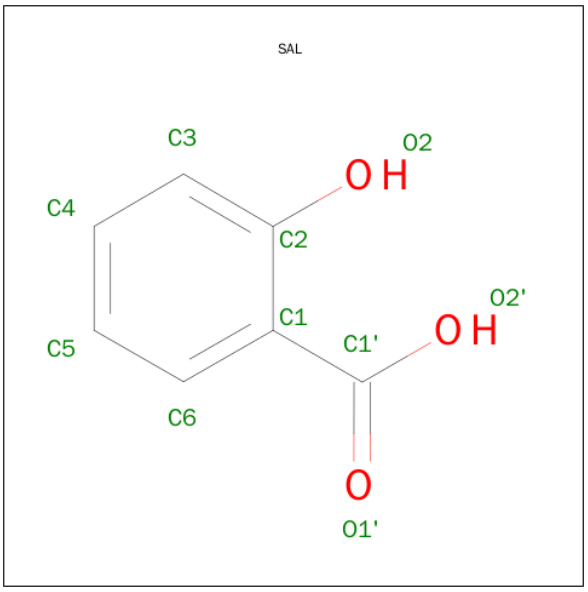
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0

- Molecule 8 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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

- Molecule 9 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $C_7H_6O_3$).



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

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 11 is water.

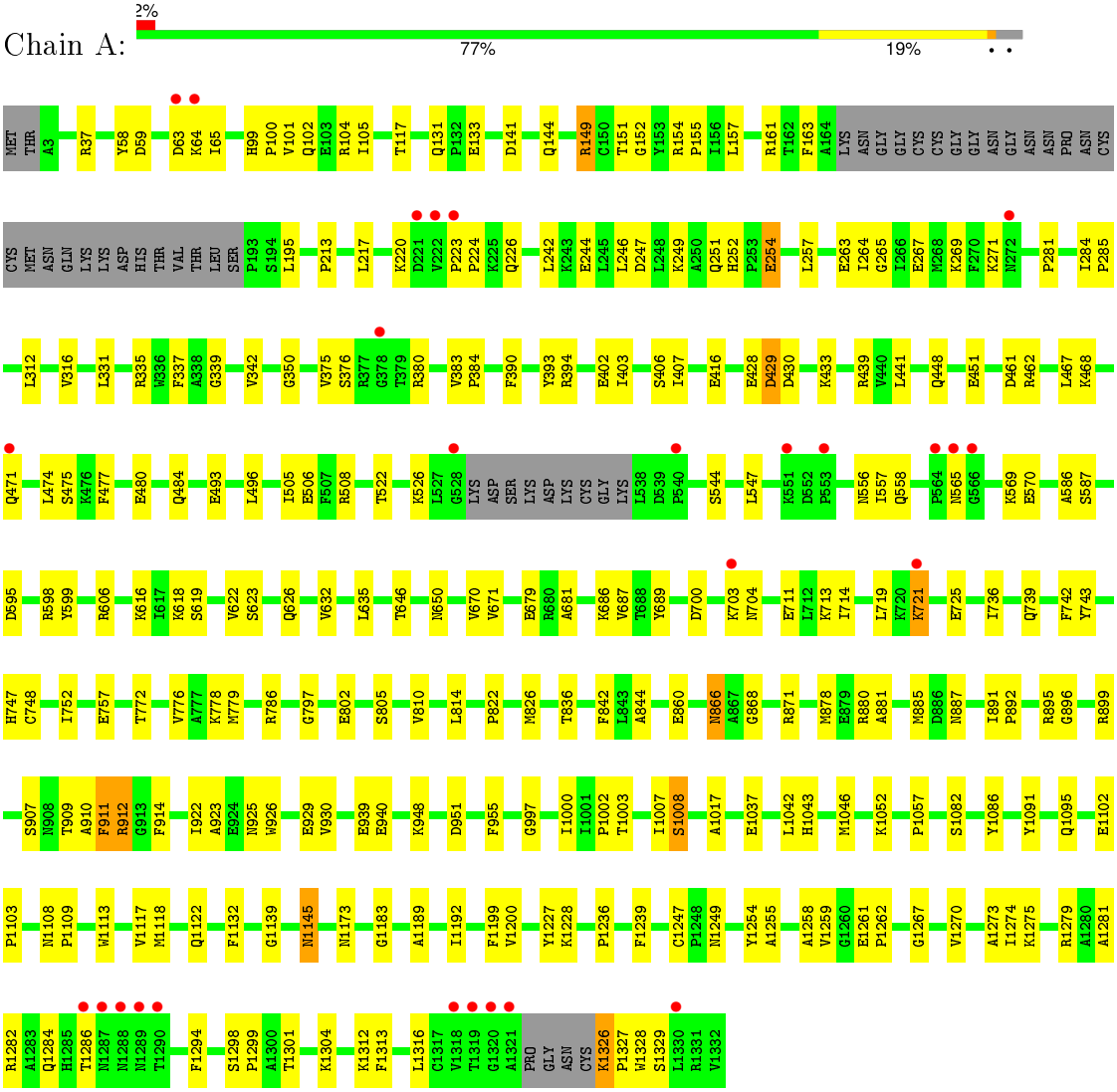
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	587	Total O 587 587	0	0
11	B	553	Total O 553 553	0	0

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.

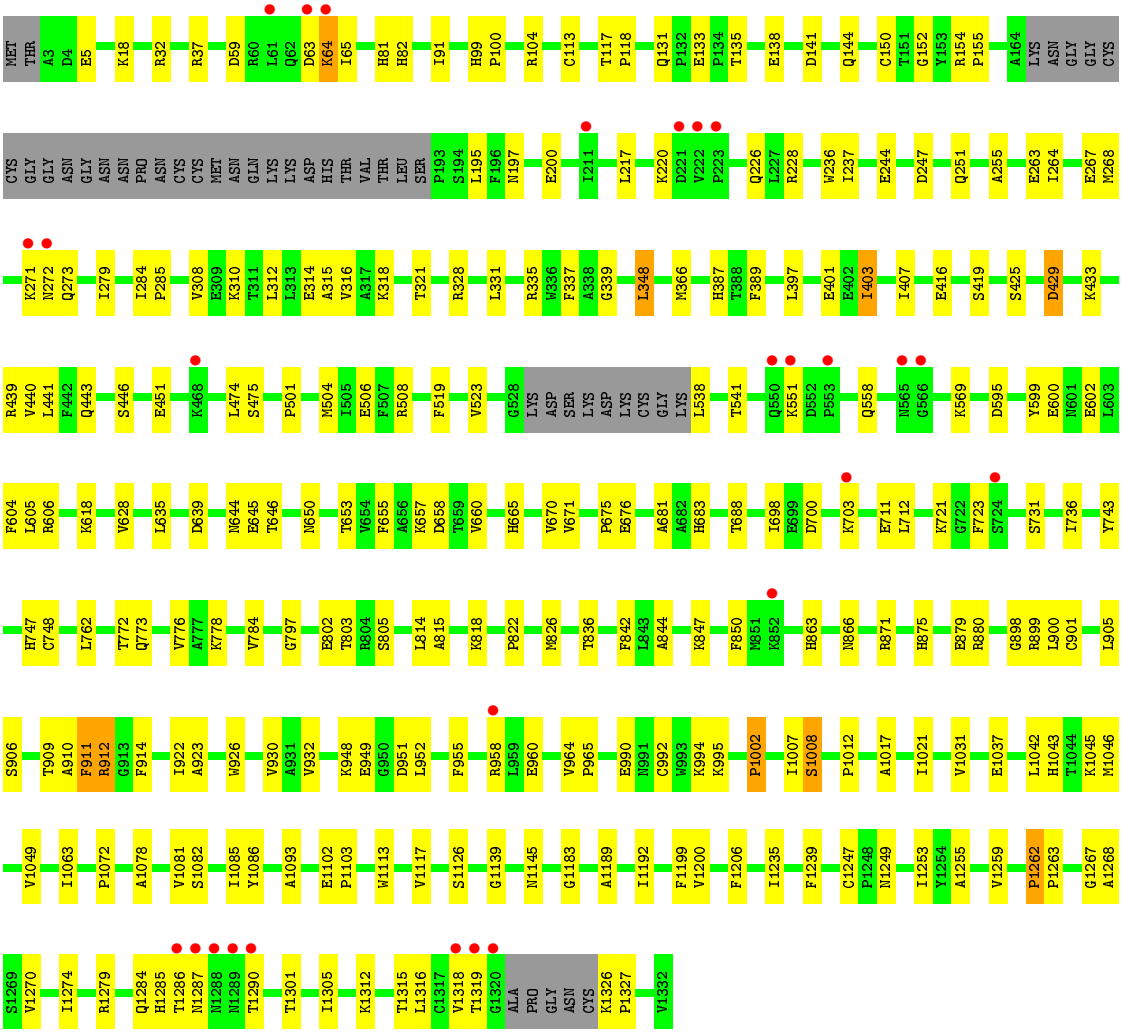
- Molecule 1: Xanthine dehydrogenase/oxidase

Chain A:



- Molecule 1: Xanthine dehydrogenase/oxidase

Chain B:


MET THR A3 D4 E5 K18 R32 R37 D59 R60 L61 Q62 D63 K64 I65 H81 H82 I91 H99 P100 R104 C113 T117 P118 Q131 P132 E133 P134 T135 E138 D141 Q144 C150 V151 G152 Y153 R154 P155 A164 LYS 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 SER P193 S194 L195 F196 N197 E200 I211 L217 K220 D221 V222 P223 Q226 L227 R228 W236 I237 E244 D247 Q251 A255 E263 I264 E267 M268
K271 N272 Q273 I279 I284 P285 V308 E309 K310 T311 L312 L313 E314 A315 V316 A317 K318 T321 R328 L331 R335 W336 F337 A338 G339 L348 M366 H387 T388 F389 L397 E401 E402 I403 I407 E416 S419 S425 D429 K433
R439 V440 L441 F442 Q443 S446 E451 K468 L474 S475 P501 M504 I505 E506 F507 R508 F519 V523 G528 LYS ASP SER LYS ASP LYS CYS GLY LYS L538 T541 Q550 K551 D552 P553 Q558 W565 G566 K569 D595 Y599 E600 W601 E602 L603
F604 L605 R606 K618 V628 L635 D639 N644 E645 T646 N650 T653 V654 F655 A656 K657 D658 T659 V660 H665 V670 V671 P675 E676 A681 A682 H683 T688 I698 E699 D700 K703 E711 L712 K721 G722 F723 S724 S731 I736 Y743
H747 C748 L762 T772 Q773 V776 A777 K778 V784 G797 E802 T803 R804 S805 L814 A815 K818 P822 M826 T836 F842 L843 A844 K847 F850 M851 K852 H863 N866 R871 H875 E879 R880 G898 R899 L900 C901 L905
S906 T909 A910 F911 R912 G913 F914 I922 A923 W926 V930 A931 V932 K948 E949 G950 D951 L952 F965 R958 L959 E960 V964 P965 E990 N991 C992 W993 K994 K995 P1002 I1007 S1008 P1012 A1017 I1021 V1031 E1037 L1042 H1043 T1044 K1045 M1046
V1049 I1063 P1072 A1078 V1081 S1082 I1085 Y1086 A1093 E1102 P1103 W1113 V1117 S1126 G1139 N1145 G1183 A1189 I1192 F1199 V1200 F1206 I1235 F1239 C1247 P1248 N1249 I1253 Y1254 A1255 V1259 P1262 P1263 G1267 A1268
S1269 V1270 I1274 R1279 Q1284 H1285 T1286 N1287 N1288 N1289 T1290 T1301 I1305 K1312 T1315 L1316 C1317 V1318 T1319 G1320 ALA PRO GLY ASN CYS K1326 P1327 V1332

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.04Å 146.70Å 107.02Å 90.00° 106.03° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.20) 95.9 (19.95-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 2.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.240 0.184 , 0.219	Depositor DCC
R_{free} test set	2293 reflections (1.62%)	DCC
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 149817 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21491	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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, CO3, SAL, MOS, CA, NAI, FES, 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	0.34	0/10221	0.61	1/13835 (0.0%)
1	B	0.33	0/10216	0.60	0/13828
All	All	0.34	0/20437	0.61	1/27663 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	151	THR	N-CA-C	5.26	125.20	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10003	0	9999	173	0
1	B	9998	0	9994	168	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	24	0	10	1	0
3	B	24	0	10	1	0
4	A	4	0	0	2	0
4	B	4	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	53	0	31	3	0
5	B	53	0	31	3	0
6	A	44	0	27	0	0
6	B	44	0	27	1	0
7	A	24	0	32	0	0
7	B	30	0	40	1	0
8	A	4	0	0	0	0
8	B	4	0	0	0	0
9	A	10	0	4	1	0
9	B	10	0	4	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	587	0	0	4	0
11	B	553	0	0	5	0
All	All	21491	0	20209	340	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 8.

All (340) 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:B:955:PHE:HA	1:B:1145:ASN:HD21	1.28	0.97
1:A:131:GLN:HE21	1:A:133:GLU:H	1.11	0.96
1:B:1286:THR:HG22	1:B:1287:ASN:H	1.31	0.94
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.36	0.91
1:A:700:ASP:HA	1:A:703:LYS:HE3	1.53	0.89
1:A:1279:ARG:HG2	1:A:1294:PHE:HE2	1.37	0.85
1:A:506:GLU:CD	1:A:506:GLU:H	1.90	0.74
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.53	0.73
1:A:1118:MET:O	1:A:1122:GLN:HG2	1.90	0.72
1:B:131:GLN:HE21	1:B:133:GLU:H	1.38	0.71
1:A:1279:ARG:HG2	1:A:1294:PHE:CE2	2.25	0.71
1:A:556:ASN:C	1:A:557:ILE:HD12	2.15	0.67
1:B:1249:ASN:O	1:B:1255:ALA:HA	1.95	0.67
1:A:844:ALA:HB2	1:A:922:ILE:HD13	1.77	0.66
4:A:1336:MOS:O2	4:A:1336:MOS:MO	1.66	0.65
1:A:622:VAL:O	1:A:626:GLN:HG3	1.96	0.65
1:B:948:LYS:HG2	1:B:951:ASP:OD2	1.96	0.65
1:B:312:LEU:O	1:B:316:VAL:HG23	1.98	0.64
1:B:267:GLU:HA	1:B:271:LYS:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1336:MOS:MO	4:B:1336:MOS:O2	1.68	0.64
1:B:639:ASP:HB3	1:B:818:LYS:HE3	1.81	0.63
1:A:131:GLN:HE21	1:A:133:GLU:N	1.91	0.63
1:A:1326:LYS:HA	1:A:1326:LYS:HE3	1.80	0.63
1:A:635:LEU:HD13	1:A:814:LEU:CD1	2.28	0.63
1:A:131:GLN:NE2	1:A:133:GLU:H	1.91	0.63
1:B:618:LYS:HE2	1:B:618:LYS:HA	1.79	0.63
1:B:1286:THR:HG22	1:B:1287:ASN:N	2.09	0.63
1:B:994:LYS:HE3	7:B:1342:GOL:O2	1.99	0.63
1:A:1249:ASN:O	1:A:1255:ALA:HA	1.97	0.63
1:A:1299:PRO:O	1:A:1304:LYS:HE2	1.98	0.62
1:A:441:LEU:HB3	1:A:451:GLU:HB2	1.81	0.61
1:A:152:GLY:HA2	1:A:1200:VAL:HG21	1.82	0.61
1:A:1316:LEU:O	1:A:1316:LEU:HD23	2.00	0.60
1:B:1315:THR:O	1:B:1318:VAL:HG22	2.01	0.60
1:A:58:TYR:CE2	1:A:220:LYS:HD2	2.36	0.60
1:A:939:GLU:HG2	1:A:940:GLU:N	2.17	0.59
1:B:64:LYS:HG2	1:B:65:ILE:N	2.16	0.59
1:A:598:ARG:O	1:B:600:GLU:HG2	2.02	0.59
1:A:375:VAL:HG12	1:A:380:ARG:HG3	1.83	0.59
1:A:141:ASP:O	1:A:144:GLN:HG3	2.03	0.59
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.38	0.59
1:B:712:LEU:HD21	1:B:879:GLU:HG2	1.85	0.58
1:B:264:ILE:O	1:B:268:MET:HG2	2.04	0.58
1:A:474:LEU:O	1:A:475:SER:HB2	2.04	0.58
1:B:1318:VAL:HG23	1:B:1319:THR:N	2.20	0.57
1:B:1279:ARG:HH11	1:B:1279:ARG:HG3	1.70	0.57
1:B:712:LEU:HD21	1:B:879:GLU:CG	2.33	0.57
1:B:932:VAL:HG13	1:B:1279:ARG:NH2	2.19	0.57
1:A:635:LEU:HD13	1:A:814:LEU:HD12	1.86	0.56
1:B:1262:PRO:HB2	1:B:1263:PRO:HD3	1.87	0.56
1:A:149:ARG:HG3	1:A:742:PHE:O	2.05	0.56
1:A:100:PRO:O	1:A:104:ARG:HG3	2.05	0.56
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.21	0.56
1:A:713:LYS:HG2	1:A:714:ILE:N	2.19	0.56
1:B:37:ARG:HD3	1:B:595:ASP:O	2.06	0.56
1:A:719:LEU:HD13	1:A:860:GLU:OE2	2.06	0.55
1:B:433:LYS:HE2	1:B:504:MET:SD	2.47	0.55
1:B:618:LYS:HB2	1:B:688:THR:HG22	1.88	0.55
1:B:711:GLU:HA	1:B:899:ARG:HD2	1.89	0.55
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LYS:HG2	1:A:65:ILE:N	2.22	0.54
1:A:1279:ARG:NH1	1:A:1279:ARG:HB3	2.22	0.54
1:B:310:LYS:O	1:B:314:GLU:HG3	2.08	0.54
1:B:1102:GLU:HB3	1:B:1103:PRO:HD3	1.90	0.54
1:B:635:LEU:HD11	1:B:815:ALA:HA	1.88	0.54
1:A:599:TYR:HA	1:B:599:TYR:HA	1.88	0.53
1:A:157:LEU:O	1:A:161:ARG:HG3	2.08	0.53
1:A:195:LEU:HD22	1:A:1189:ALA:HA	1.90	0.53
1:A:508:ARG:HD3	11:A:1547:HOH:O	2.09	0.53
1:A:1082:SER:HB2	3:A:1335:MTE:O3P	2.08	0.53
1:A:1282:ARG:O	1:A:1286:THR:HB	2.09	0.53
1:A:461:ASP:OD1	1:A:462:ARG:HG2	2.08	0.53
1:A:217:LEU:O	1:A:220:LYS:HG2	2.08	0.53
1:A:748:CYS:HB2	1:A:826:MET:HG3	1.90	0.53
1:B:1316:LEU:HD23	1:B:1316:LEU:O	2.08	0.53
1:B:263:GLU:HB2	5:B:1337:FAD:H52A	1.91	0.52
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.74	0.52
1:A:739:GLN:HG2	1:A:911:PHE:CE1	2.44	0.52
1:A:247:ASP:HB3	1:A:251:GLN:NE2	2.24	0.52
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.07	0.52
1:A:249:LYS:HD3	1:A:257:LEU:HD11	1.92	0.52
1:A:406:SER:C	1:A:407:ILE:HD12	2.29	0.52
1:A:407:ILE:N	1:A:407:ILE:HD12	2.24	0.52
1:B:1007:ILE:O	1:B:1008:SER:CB	2.58	0.52
1:B:419:SER:HB2	1:B:519:PHE:CD1	2.45	0.52
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.73	0.52
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.75	0.52
1:A:448:GLN:HB2	1:A:477:PHE:CE2	2.44	0.51
1:B:863:HIS:O	1:B:898:GLY:HA2	2.11	0.51
1:A:264:ILE:HD11	5:A:1337:FAD:H3B	1.93	0.51
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.92	0.51
1:B:1270:VAL:O	1:B:1274:ILE:HG13	2.11	0.51
1:A:719:LEU:HD11	1:A:895:ARG:CB	2.40	0.51
1:B:443:GLN:HB2	1:B:446:SER:OG	2.10	0.51
1:A:948:LYS:HG2	1:A:951:ASP:OD2	2.10	0.51
1:B:197:ASN:HD22	1:B:200:GLU:HG3	1.75	0.51
1:B:425:SER:HB3	11:B:1525:HOH:O	2.09	0.51
1:B:1312:LYS:HG2	11:B:1856:HOH:O	2.11	0.50
1:A:911:PHE:O	1:A:912:ARG:C	2.49	0.50
1:A:814:LEU:C	1:A:814:LEU:HD13	2.32	0.50
1:B:312:LEU:HB2	1:B:331:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1279:ARG:NH2	1:B:1290:THR:O	2.45	0.50
1:A:144:GLN:HB2	1:A:339:GLY:HA2	1.94	0.50
1:B:416:GLU:OE1	1:B:439:ARG:HD2	2.12	0.50
1:A:719:LEU:HD11	1:A:895:ARG:HB3	1.93	0.50
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.75	0.50
1:A:1007:ILE:O	1:A:1008:SER:CB	2.60	0.50
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.47	0.50
1:A:390:PHE:HB3	11:A:1552:HOH:O	2.10	0.50
1:B:389:PHE:HA	1:B:397:LEU:HG	1.94	0.50
1:B:911:PHE:O	1:B:912:ARG:C	2.50	0.50
1:B:711:GLU:HA	1:B:899:ARG:CD	2.42	0.49
1:B:197:ASN:ND2	1:B:200:GLU:HG3	2.27	0.49
1:B:267:GLU:HA	1:B:271:LYS:CG	2.41	0.49
1:B:474:LEU:O	1:B:475:SER:HB2	2.13	0.49
1:B:569:LYS:NZ	1:B:569:LYS:HB3	2.28	0.49
1:A:1052:LYS:HD3	1:A:1254:TYR:CE1	2.48	0.49
1:B:698:ILE:HG23	1:B:901:CYS:SG	2.53	0.49
1:A:1326:LYS:HB3	1:A:1327:PRO:HD3	1.94	0.49
1:B:605:LEU:C	1:B:605:LEU:HD23	2.32	0.49
1:A:544:SER:HA	1:A:547:LEU:HD12	1.93	0.49
1:A:1017:ALA:HB1	1:A:1086:TYR:CD2	2.48	0.49
1:B:628:VAL:HG21	1:B:681:ALA:HA	1.93	0.49
1:B:871:ARG:HH11	1:B:871:ARG:HG3	1.78	0.48
1:B:308:VAL:HG21	1:B:348:LEU:HG	1.95	0.48
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.48	0.48
1:A:467:LEU:O	1:A:471:GLN:HB2	2.14	0.48
1:A:249:LYS:HD3	1:A:257:LEU:CD1	2.44	0.48
1:A:871:ARG:HG3	1:A:871:ARG:HH11	1.78	0.48
1:B:1007:ILE:HG22	1:B:1081:VAL:HG12	1.95	0.48
1:A:1091:TYR:O	1:A:1095:GLN:HG2	2.13	0.48
1:A:686:LYS:HD3	1:A:687:VAL:N	2.29	0.48
1:B:1082:SER:HB2	3:B:1335:MTE:O3P	2.14	0.48
1:A:430:ASP:CG	1:A:1228:LYS:HE2	2.34	0.48
1:B:676:GLU:CD	1:B:676:GLU:H	2.17	0.48
1:A:1279:ARG:HB3	1:A:1279:ARG:CZ	2.44	0.47
1:B:655:PHE:CE1	1:B:814:LEU:HD23	2.49	0.47
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.95	0.47
1:A:1183:GLY:HA2	1:A:1247:CYS:O	2.15	0.47
1:A:711:GLU:HB2	1:A:899:ARG:HD3	1.97	0.47
1:B:506:GLU:H	1:B:506:GLU:CD	2.17	0.47
1:A:721:LYS:NZ	1:A:721:LYS:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:ARG:HD3	11:B:1785:HOH:O	2.13	0.47
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.95	0.47
1:A:265:GLY:O	1:A:269:LYS:HB2	2.13	0.47
1:A:281:PRO:HB2	1:A:284:ILE:HD12	1.97	0.47
1:B:646:THR:O	1:B:650:ASN:HA	2.14	0.47
1:A:1102:GLU:HB3	1:A:1103:PRO:HD3	1.97	0.47
1:A:480:GLU:O	1:A:484:GLN:HG3	2.15	0.47
1:A:926:TRP:O	1:A:930:VAL:HG23	2.15	0.47
1:B:909:THR:OG1	1:B:910:ALA:N	2.47	0.47
1:A:154:ARG:N	1:A:155:PRO:HD2	2.30	0.47
1:A:752:ILE:CD1	1:A:822:PRO:HB3	2.44	0.47
1:B:723:PHE:CZ	1:B:847:LYS:HE3	2.50	0.47
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.12	0.47
1:A:267:GLU:O	1:A:271:LYS:HB2	2.15	0.47
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.96	0.47
1:B:1199:PHE:CE1	1:B:1267:GLY:HA2	2.50	0.47
1:B:335:ARG:HH21	1:B:551:LYS:NZ	2.13	0.47
1:B:1279:ARG:NH1	1:B:1279:ARG:HG3	2.28	0.47
1:B:604:PHE:CD2	1:B:675:PRO:HG3	2.51	0.46
1:B:644:ASN:O	1:B:653:THR:HA	2.16	0.46
1:A:1270:VAL:O	1:A:1274:ILE:HG13	2.16	0.46
1:B:773:GLN:HG2	1:B:784:VAL:HG13	1.97	0.46
1:A:263:GLU:HB3	5:A:1337:FAD:H52A	1.96	0.46
1:B:1017:ALA:HB2	1:B:1085:ILE:HD12	1.96	0.46
1:B:401:GLU:OE2	1:B:401:GLU:N	2.39	0.46
1:A:416:GLU:OE1	1:A:439:ARG:HD2	2.16	0.46
1:B:949:GLU:OE2	1:B:960:GLU:HA	2.16	0.46
1:B:660:VAL:HA	1:B:665:HIS:ND1	2.31	0.46
1:A:955:PHE:CA	1:A:1145:ASN:HD21	2.18	0.46
1:A:1326:LYS:HB3	1:A:1327:PRO:CD	2.46	0.46
1:A:99:HIS:CE1	1:A:101:VAL:HG23	2.51	0.46
1:B:1206:PHE:CE1	1:B:1268:ALA:HB2	2.51	0.46
1:B:772:THR:O	1:B:776:VAL:HG23	2.16	0.46
1:A:99:HIS:CE1	1:A:100:PRO:HD2	2.50	0.45
1:B:700:ASP:HA	1:B:703:LYS:NZ	2.32	0.45
1:B:255:ALA:HB1	1:B:279:ILE:HG13	1.97	0.45
1:A:885:MET:SD	1:A:896:GLY:HA3	2.56	0.45
1:A:242:LEU:O	1:A:246:LEU:HG	2.16	0.45
1:B:226:GLN:HB2	1:B:244:GLU:OE1	2.17	0.45
1:B:321:THR:O	1:B:328:ARG:NH2	2.49	0.45
1:B:135:THR:OG1	1:B:138:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:LYS:O	1:A:619:SER:HB3	2.17	0.45
1:A:342:VAL:HG23	11:A:1746:HOH:O	2.16	0.45
1:A:104:ARG:HD2	1:A:163:PHE:CE1	2.51	0.45
1:A:646:THR:O	1:A:650:ASN:HA	2.16	0.45
1:B:541:THR:HA	1:B:990:GLU:O	2.17	0.45
1:B:992:CYS:O	1:B:1285:HIS:HE1	2.00	0.45
1:B:403:ILE:C	1:B:403:ILE:HD13	2.37	0.45
1:B:144:GLN:HB2	1:B:339:GLY:HA2	1.99	0.45
1:B:195:LEU:HD22	1:B:1189:ALA:HA	1.99	0.45
1:A:1042:LEU:O	1:A:1046:MET:HG2	2.17	0.45
1:B:1301:THR:O	1:B:1305:ILE:HG13	2.16	0.45
1:B:141:ASP:O	1:B:144:GLN:HG3	2.17	0.44
1:A:725:GLU:HG2	1:A:725:GLU:O	2.16	0.44
1:A:1312:LYS:HE3	1:A:1313:PHE:CZ	2.52	0.44
1:B:1045:LYS:O	1:B:1049:VAL:HG23	2.17	0.44
1:A:312:LEU:O	1:A:316:VAL:HG23	2.17	0.44
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.65	0.44
1:A:997:GLY:HA3	1:A:1273:ALA:O	2.17	0.44
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.98	0.44
1:A:506:GLU:CD	1:A:506:GLU:N	2.67	0.44
1:A:686:LYS:HD3	1:A:686:LYS:C	2.38	0.44
1:B:602:GLU:HG3	1:B:822:PRO:HB2	2.00	0.44
1:A:703:LYS:NZ	1:A:704:ASN:HD21	2.16	0.44
1:B:1183:GLY:HA2	1:B:1247:CYS:O	2.18	0.44
1:B:154:ARG:HD2	1:B:154:ARG:C	2.38	0.44
1:B:440:VAL:O	1:B:440:VAL:HG13	2.17	0.44
1:A:376:SER:HB3	1:A:402:GLU:HG2	1.99	0.44
1:B:1312:LYS:O	1:B:1316:LEU:HB2	2.18	0.44
1:B:875:HIS:HA	1:B:900:LEU:HD11	1.99	0.44
1:B:154:ARG:N	1:B:155:PRO:HD2	2.33	0.44
1:A:1108:ASN:N	1:A:1109:PRO:HD3	2.33	0.44
1:A:736:ILE:HG23	1:A:736:ILE:O	2.18	0.44
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.32	0.44
1:B:657:LYS:O	1:B:658:ASP:HB2	2.18	0.44
1:A:496:LEU:HB2	1:A:505:ILE:HG23	1.99	0.44
1:B:315:ALA:HA	1:B:318:LYS:NZ	2.31	0.44
1:B:519:PHE:O	1:B:523:VAL:HG23	2.18	0.43
1:A:736:ILE:HG13	1:A:1298:SER:HB3	2.00	0.43
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	2.00	0.43
1:A:1000:ILE:O	1:A:1000:ILE:HG23	2.17	0.43
1:A:154:ARG:C	1:A:154:ARG:HD2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:ILE:CG2	1:A:842:PHE:HB2	2.48	0.43
1:A:1281:ALA:O	1:A:1284:GLN:HB3	2.18	0.43
1:A:779:MET:HG3	1:A:810:VAL:CG1	2.48	0.43
1:B:721:LYS:HD2	1:B:721:LYS:O	2.18	0.43
1:A:772:THR:O	1:A:776:VAL:HG23	2.19	0.43
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.00	0.43
1:A:117:THR:CG2	1:A:586:ALA:HA	2.48	0.43
1:A:383:VAL:HA	1:A:384:PRO:HD3	1.91	0.43
1:A:226:GLN:HB2	1:A:244:GLU:OE1	2.18	0.43
1:B:844:ALA:HB2	1:B:922:ILE:HD13	2.01	0.43
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.84	0.43
1:A:254:GLU:H	1:A:254:GLU:CD	2.21	0.43
1:B:59:ASP:O	1:B:63:ASP:N	2.51	0.43
1:B:762:LEU:HD12	1:B:762:LEU:N	2.32	0.43
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.54	0.43
1:A:616:LYS:O	1:A:689:TYR:HA	2.18	0.43
1:B:228:ARG:HG3	1:B:237:ILE:CD1	2.49	0.43
1:B:1008:SER:HA	1:B:1081:VAL:HG11	2.01	0.43
1:A:267:GLU:HA	1:A:271:LYS:HB2	1.99	0.43
1:B:113:CYS:HB3	1:B:150:CYS:SG	2.58	0.43
1:B:1253:ILE:O	1:B:1253:ILE:HG23	2.18	0.43
1:A:844:ALA:CB	1:A:922:ILE:HD13	2.47	0.43
1:A:152:GLY:CA	1:A:1200:VAL:HG21	2.47	0.43
1:B:1017:ALA:HB1	1:B:1086:TYR:CE2	2.54	0.43
1:A:284:ILE:HA	1:A:285:PRO:HD3	1.88	0.43
1:A:752:ILE:HD13	1:A:822:PRO:HB3	2.00	0.43
1:B:731:SER:OG	1:B:847:LYS:HG3	2.19	0.43
1:A:522:THR:HG22	1:A:526:LYS:HE3	2.00	0.43
1:B:802:GLU:HG2	1:B:803:THR:HG23	2.01	0.43
1:B:1113:TRP:O	1:B:1117:VAL:HG23	2.19	0.43
1:B:247:ASP:O	1:B:251:GLN:HG3	2.19	0.42
1:B:366:MET:CE	1:B:387:HIS:HA	2.49	0.42
1:B:736:ILE:CG2	1:B:842:PHE:HB2	2.49	0.42
1:B:217:LEU:O	1:B:220:LYS:HG2	2.19	0.42
1:A:312:LEU:HB2	1:A:331:LEU:HD21	2.00	0.42
1:B:1042:LEU:O	1:B:1046:MET:HG2	2.19	0.42
1:A:58:TYR:CZ	1:A:220:LYS:HD2	2.54	0.42
1:A:868:GLY:HA3	1:A:907:SER:HA	2.02	0.42
1:A:37:ARG:HD2	1:A:595:ASP:O	2.19	0.42
1:A:1227:TYR:C	1:A:1228:LYS:HD2	2.39	0.42
1:A:331:LEU:O	1:A:335:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:O	1:A:63:ASP:N	2.50	0.42
1:A:606:ARG:HG2	1:A:679:GLU:HA	2.00	0.42
1:B:850:PHE:CD2	1:B:850:PHE:N	2.87	0.42
1:B:1259:VAL:O	1:B:1259:VAL:HG22	2.18	0.42
1:B:331:LEU:O	1:B:335:ARG:HG3	2.20	0.42
1:B:1012:PRO:HB2	11:B:1817:HOH:O	2.18	0.42
1:B:747:HIS:ND1	1:B:805:SER:HA	2.35	0.42
1:A:878:MET:O	1:A:881:ALA:HB3	2.19	0.42
1:A:1132:PHE:CD1	1:B:1126:SER:HB2	2.55	0.42
1:A:1007:ILE:HD12	1:A:1258:ALA:HB3	2.01	0.42
1:A:909:THR:OG1	1:A:910:ALA:N	2.51	0.42
1:A:102:GLN:NE2	1:A:587:SER:HA	2.35	0.42
1:B:1031:VAL:HB	1:B:1063:ILE:HG12	2.01	0.42
1:B:905:LEU:O	1:B:906:SER:C	2.56	0.42
1:B:117:THR:HB	1:B:118:PRO:HD3	2.01	0.42
1:A:912:ARG:N	4:A:1336:MOS:S	2.93	0.42
1:A:1173:ASN:O	1:A:1236:PRO:HA	2.19	0.42
1:B:407:ILE:HD12	1:B:407:ILE:N	2.35	0.42
1:A:1275:LYS:O	1:A:1279:ARG:HG3	2.20	0.42
1:A:1299:PRO:HG2	1:A:1301:THR:HG23	2.02	0.42
1:A:393:TYR:CE2	1:A:394:ARG:HD2	2.55	0.42
1:B:712:LEU:HD21	1:B:879:GLU:HG3	2.02	0.41
1:A:558:GLN:HB3	1:A:1192:ILE:HD13	2.02	0.41
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.90	0.41
1:B:952:LEU:HD23	1:B:958:ARG:HA	2.01	0.41
1:B:926:TRP:O	1:B:930:VAL:HG23	2.20	0.41
1:A:1199:PHE:CE1	1:A:1267:GLY:HA2	2.55	0.41
1:B:748:CYS:HB2	1:B:826:MET:HG3	2.02	0.41
1:A:105:ILE:HA	11:A:1766:HOH:O	2.20	0.41
1:A:891:ILE:HA	1:A:892:PRO:HD2	1.87	0.41
1:B:131:GLN:HE21	1:B:133:GLU:N	2.13	0.41
1:B:429:ASP:OD1	5:B:1337:FAD:H6	2.20	0.41
1:A:721:LYS:HD2	1:A:721:LYS:O	2.21	0.41
1:A:403:ILE:HD12	1:A:403:ILE:C	2.39	0.41
1:A:1328:TRP:CE3	1:A:1329:SER:HB3	2.55	0.41
1:B:1078:ALA:HB1	4:B:1336:MOS:O1	2.21	0.41
5:B:1337:FAD:HM73	11:B:1589:HOH:O	2.20	0.41
1:A:866:ASN:C	1:A:866:ASN:HD22	2.23	0.41
1:B:91:ILE:O	1:B:99:HIS:HB2	2.20	0.41
1:A:802:GLU:OE1	9:A:1344:SAL:H3	2.20	0.41
1:A:623:SER:HA	1:A:626:GLN:HE21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ARG:HG3	1:B:600:GLU:HG2	2.03	0.41
1:B:284:ILE:HA	1:B:285:PRO:HD3	1.91	0.41
1:A:252:HIS:HB3	1:A:254:GLU:OE2	2.21	0.41
1:B:5:GLU:OE2	1:B:18:LYS:HE2	2.21	0.41
1:B:152:GLY:HA2	1:B:1200:VAL:HG21	2.03	0.41
1:A:632:VAL:HB	1:A:671:VAL:O	2.21	0.41
1:B:236:TRP:C	1:B:236:TRP:CD1	2.93	0.41
1:B:272:ASN:CG	1:B:683:HIS:HE1	2.24	0.41
1:B:1326:LYS:CG	1:B:1327:PRO:HD2	2.50	0.41
1:A:899:ARG:HA	1:A:899:ARG:HD2	1.91	0.41
1:A:468:LYS:HB2	1:A:493:GLU:OE2	2.21	0.41
1:B:605:LEU:HD23	1:B:606:ARG:N	2.36	0.41
1:A:1113:TRP:O	1:A:1117:VAL:HG23	2.21	0.41
1:B:1318:VAL:CG2	1:B:1319:THR:N	2.83	0.41
1:B:604:PHE:O	1:B:671:VAL:HA	2.20	0.41
1:B:1286:THR:CG2	1:B:1287:ASN:N	2.78	0.40
1:A:471:GLN:HA	1:A:471:GLN:NE2	2.36	0.40
1:B:100:PRO:O	1:B:104:ARG:HG3	2.22	0.40
1:A:887:ASN:OD1	1:A:1003:THR:HA	2.21	0.40
1:B:81:HIS:O	1:B:82:HIS:HB2	2.21	0.40
1:A:428:GLU:O	1:A:429:ASP:C	2.60	0.40
1:B:64:LYS:CB	1:B:64:LYS:NZ	2.84	0.40
1:A:747:HIS:ND1	1:A:805:SER:HA	2.37	0.40
1:B:501:PRO:HD2	6:B:1338:NAI:C6A	2.51	0.40
1:A:433:LYS:HA	1:A:433:LYS:HD3	1.91	0.40
1:A:1259:VAL:O	1:A:1259:VAL:HG22	2.20	0.40
1:A:570:GLU:OE2	1:A:1057:PRO:HG3	2.21	0.40
1:B:271:LYS:HB2	1:B:273:GLN:HG2	2.02	0.40
1:A:350:GLY:C	5:A:1337:FAD:H5'1	2.42	0.40
1:B:32:ARG:NH2	1:B:676:GLU:OE2	2.54	0.40
1:A:925:ASN:O	1:A:929:GLU:HG3	2.21	0.40
1:B:912:ARG:N	4:B:1336:MOS:S	2.95	0.40
1:B:152:GLY:O	1:B:1235:ILE:HG21	2.22	0.40
1:B:1021:ILE:HD12	1:B:1093:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1281/1332 (96%)	1229 (96%)	46 (4%)	6 (0%)	34 35
1	B	1280/1332 (96%)	1228 (96%)	46 (4%)	6 (0%)	34 35
All	All	2561/2664 (96%)	2457 (96%)	92 (4%)	12 (0%)	34 35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	A	429	ASP
1	A	912	ARG
1	B	429	ASP
1	B	912	ARG
1	B	1002	PRO
1	A	797	GLY
1	A	1139	GLY
1	B	1139	GLY
1	A	213	PRO
1	B	797	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1092/1128 (97%)	1079 (99%)	13 (1%)	78 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	1092/1128 (97%)	1080 (99%)	12 (1%)	80 89
All	All	2184/2256 (97%)	2159 (99%)	25 (1%)	80 89

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ARG
1	A	254	GLU
1	A	337	PHE
1	A	565	ASN
1	A	569	LYS
1	A	721	LYS
1	A	743	TYR
1	A	866	ASN
1	A	911	PHE
1	A	1002	PRO
1	A	1145	ASN
1	A	1239	PHE
1	A	1326	LYS
1	B	64	LYS
1	B	337	PHE
1	B	348	LEU
1	B	403	ILE
1	B	538	LEU
1	B	743	TYR
1	B	866	ASN
1	B	911	PHE
1	B	1002	PRO
1	B	1072	PRO
1	B	1239	PHE
1	B	1262	PRO

Some 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	471	GLN
1	A	473	GLN
1	A	565	ASN
1	A	626	GLN

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Mol	Chain	Res	Type
1	A	650	ASN
1	A	704	ASN
1	A	866	ASN
1	A	875	HIS
1	A	1088	GLN
1	A	1145	ASN
1	A	1212	HIS
1	A	1284	GLN
1	A	1289	ASN
1	B	131	GLN
1	B	144	GLN
1	B	197	ASN
1	B	272	ASN
1	B	471	GLN
1	B	473	GLN
1	B	556	ASN
1	B	626	GLN
1	B	650	ASN
1	B	683	HIS
1	B	866	ASN
1	B	869	ASN
1	B	1088	GLN
1	B	1095	GLN
1	B	1108	ASN
1	B	1122	GLN
1	B	1145	ASN
1	B	1284	GLN

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 (i)

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 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	$\#\|Z\|>2$
2	FES	A	1333	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	A	1334	1	0,4,4	0.00	-	0,4,4	0.00	-
3	MTE	A	1335	4	19,26,26	2.90	8 (42%)	19,40,40	2.78	8 (42%)
4	MOS	A	1336	3	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	A	1337	-	48,58,58	2.92	17 (35%)	54,89,89	3.10	17 (31%)
6	NAI	A	1338	-	38,48,48	1.23	4 (10%)	48,73,73	1.93	4 (8%)
7	GOL	A	1339	-	5,5,5	0.38	0	5,5,5	0.34	0
7	GOL	A	1340	-	5,5,5	0.19	0	5,5,5	0.18	0
7	GOL	A	1341	-	5,5,5	0.34	0	5,5,5	0.37	0
7	GOL	A	1342	-	5,5,5	0.40	0	5,5,5	0.40	0
8	CO3	A	1343	-	0,3,3	0.00	-	0,3,3	0.00	-
9	SAL	A	1344	-	7,10,10	1.69	3 (42%)	10,13,13	1.17	0
2	FES	B	1333	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	B	1334	1	0,4,4	0.00	-	0,4,4	0.00	-
3	MTE	B	1335	4	19,26,26	2.93	8 (42%)	19,40,40	2.78	7 (36%)
4	MOS	B	1336	3	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	B	1337	-	48,58,58	2.88	17 (35%)	54,89,89	3.11	16 (29%)
6	NAI	B	1338	-	38,48,48	1.23	3 (7%)	48,73,73	1.93	4 (8%)
7	GOL	B	1339	-	5,5,5	0.28	0	5,5,5	0.23	0
7	GOL	B	1340	-	5,5,5	0.39	0	5,5,5	0.36	0
7	GOL	B	1341	-	5,5,5	0.27	0	5,5,5	0.32	0
7	GOL	B	1342	-	5,5,5	0.32	0	5,5,5	0.29	0
7	GOL	B	1343	-	5,5,5	0.32	0	5,5,5	0.33	0
8	CO3	B	1344	-	0,3,3	0.00	-	0,3,3	0.00	-
9	SAL	B	1345	-	7,10,10	1.84	3 (42%)	10,13,13	1.21	0

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
2	FES	A	1333	1	-	0/0/4/4	0/1/1/1
2	FES	A	1334	1	-	0/0/4/4	0/1/1/1
3	MTE	A	1335	4	-	0/6/34/34	0/3/3/3
4	MOS	A	1336	3	-	0/0/0/0	0/0/0/0
5	FAD	A	1337	-	-	0/30/50/50	0/6/6/6
6	NAI	A	1338	-	-	0/25/72/72	0/5/5/5
7	GOL	A	1339	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1340	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1341	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1342	-	-	0/4/4/4	0/0/0/0
8	CO3	A	1343	-	-	0/0/0/0	0/0/0/0
9	SAL	A	1344	-	-	0/0/4/4	0/1/1/1
2	FES	B	1333	1	-	0/0/4/4	0/1/1/1
2	FES	B	1334	1	-	0/0/4/4	0/1/1/1
3	MTE	B	1335	4	-	0/6/34/34	0/3/3/3
4	MOS	B	1336	3	-	0/0/0/0	0/0/0/0
5	FAD	B	1337	-	-	0/30/50/50	0/6/6/6
6	NAI	B	1338	-	-	0/25/72/72	0/5/5/5
7	GOL	B	1339	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1340	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1341	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1342	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1343	-	-	0/4/4/4	0/0/0/0
8	CO3	B	1344	-	-	0/0/0/0	0/0/0/0
9	SAL	B	1345	-	-	0/0/4/4	0/1/1/1

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1338	NAI	C4N-C5N	-3.76	1.41	1.49
6	B	1338	NAI	C4N-C5N	-3.57	1.41	1.49
9	A	1344	SAL	C3-C2	2.10	1.43	1.39
6	A	1338	NAI	C2N-C3N	2.13	1.39	1.34
3	A	1335	MTE	C7-C6	2.14	1.55	1.53
9	A	1344	SAL	C6-C1	2.17	1.43	1.39
6	B	1338	NAI	C2N-C3N	2.28	1.40	1.34
9	B	1345	SAL	C6-C1	2.35	1.43	1.39
9	B	1345	SAL	C3-C2	2.37	1.43	1.39
6	A	1338	NAI	O4B-C1B	2.45	1.44	1.41
3	A	1335	MTE	C4-N3	2.70	1.38	1.33
3	A	1335	MTE	C9-C10	2.70	1.47	1.41
3	B	1335	MTE	C9-C10	2.73	1.47	1.41
9	A	1344	SAL	C5-C6	2.78	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1337	FAD	C5A-C4A	2.86	1.47	1.40
5	A	1337	FAD	C5A-C4A	2.87	1.47	1.40
3	B	1335	MTE	C4-N3	2.89	1.38	1.33
5	A	1337	FAD	C6-C5X	2.89	1.46	1.41
9	B	1345	SAL	C5-C6	2.91	1.44	1.38
3	B	1335	MTE	C7-C6	2.99	1.55	1.53
5	A	1337	FAD	C9-C9A	3.00	1.47	1.40
5	A	1337	FAD	C10-N1	3.08	1.40	1.35
5	B	1337	FAD	C10-N1	3.10	1.40	1.35
5	B	1337	FAD	C6-C5X	3.20	1.46	1.41
5	B	1337	FAD	C4X-N5	3.27	1.38	1.33
5	B	1337	FAD	C9-C9A	3.33	1.48	1.40
5	A	1337	FAD	C4X-N5	3.37	1.38	1.33
5	B	1337	FAD	O4B-C4B	3.42	1.52	1.45
5	A	1337	FAD	C9A-C5X	3.50	1.49	1.42
5	A	1337	FAD	C8-C7	3.51	1.50	1.41
5	B	1337	FAD	C4-C4X	3.59	1.48	1.41
5	B	1337	FAD	C8-C7	3.60	1.50	1.41
5	B	1337	FAD	C9A-C5X	3.61	1.50	1.42
6	A	1338	NAI	C6N-C5N	3.75	1.40	1.33
3	B	1335	MTE	O3'-C7	3.80	1.49	1.43
5	A	1337	FAD	C4-C4X	3.88	1.49	1.41
5	A	1337	FAD	O4B-C4B	3.91	1.54	1.45
5	B	1337	FAD	C2A-N1A	4.05	1.41	1.33
3	A	1335	MTE	O3'-C7	4.06	1.49	1.43
6	B	1338	NAI	C6N-C5N	4.08	1.41	1.33
5	B	1337	FAD	C2A-N3A	4.14	1.39	1.32
5	A	1337	FAD	C2A-N1A	4.16	1.41	1.33
5	A	1337	FAD	C2A-N3A	4.27	1.39	1.32
5	A	1337	FAD	C5X-N5	4.27	1.42	1.35
3	A	1335	MTE	O4-C4	4.30	1.35	1.24
3	B	1335	MTE	O4-C4	4.33	1.35	1.24
5	B	1337	FAD	C4-N3	4.53	1.41	1.33
5	A	1337	FAD	C4-N3	4.55	1.41	1.33
3	B	1335	MTE	C9-N5	4.74	1.49	1.38
5	B	1337	FAD	C5X-N5	4.77	1.43	1.35
5	B	1337	FAD	C4A-N3A	4.81	1.42	1.35
3	A	1335	MTE	C9-N5	4.91	1.49	1.38
5	A	1337	FAD	C4A-N3A	4.97	1.43	1.35
5	A	1337	FAD	C4X-C10	5.26	1.50	1.41
5	B	1337	FAD	C4X-C10	5.31	1.51	1.41
3	B	1335	MTE	O3'-C3'	5.60	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1335	MTE	O3'-C3'	5.81	1.52	1.43
3	A	1335	MTE	C10-N8	6.16	1.46	1.35
3	B	1335	MTE	C10-N8	6.38	1.47	1.35
5	B	1337	FAD	O4B-C1B	8.22	1.51	1.41
5	A	1337	FAD	O4B-C1B	8.70	1.52	1.41
5	B	1337	FAD	C9A-N10	9.09	1.51	1.38
5	A	1337	FAD	C9A-N10	9.32	1.51	1.38

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1338	NAI	N3A-C2A-N1A	-10.83	120.60	128.89
6	A	1338	NAI	N3A-C2A-N1A	-10.68	120.72	128.89
5	A	1337	FAD	N3A-C2A-N1A	-9.72	121.45	128.89
5	B	1337	FAD	N3A-C2A-N1A	-9.56	121.58	128.89
5	B	1337	FAD	C4-C4X-C10	-7.73	115.00	119.94
5	B	1337	FAD	C5X-C9A-N10	-7.63	111.82	117.62
5	A	1337	FAD	C4-C4X-C10	-7.49	115.14	119.94
5	A	1337	FAD	C5X-C9A-N10	-7.36	112.03	117.62
5	A	1337	FAD	C4X-C10-N10	-5.97	117.00	120.52
5	B	1337	FAD	C4X-C10-N10	-5.76	117.12	120.52
3	B	1335	MTE	N3-C2-N1	-5.40	116.69	125.53
3	A	1335	MTE	N3-C2-N1	-5.31	116.82	125.53
6	B	1338	NAI	O4D-C1D-N1N	-4.33	98.92	108.07
6	A	1338	NAI	O4D-C1D-N1N	-4.22	99.16	108.07
5	B	1337	FAD	O4B-C1B-N9A	-4.08	99.57	108.10
5	A	1337	FAD	O4B-C1B-N9A	-3.80	100.15	108.10
3	A	1335	MTE	O3'-C7-C6	-3.74	106.41	108.96
5	A	1337	FAD	C4X-C4-N3	-3.61	118.65	123.59
3	B	1335	MTE	O3'-C7-C6	-3.61	106.50	108.96
5	B	1337	FAD	C4X-C4-N3	-3.56	118.72	123.59
6	A	1338	NAI	PN-O3-PA	-3.36	123.30	132.73
6	B	1338	NAI	PN-O3-PA	-3.27	123.56	132.73
6	A	1338	NAI	C3N-C2N-N1N	-2.67	119.31	123.14
5	B	1337	FAD	C1'-N10-C9A	-2.59	115.95	118.86
6	B	1338	NAI	C3N-C2N-N1N	-2.51	119.55	123.14
5	B	1337	FAD	O3B-C3B-C4B	-2.46	103.67	111.05
5	A	1337	FAD	C1'-N10-C9A	-2.44	116.12	118.86
5	B	1337	FAD	C8M-C8-C9	-2.38	113.81	120.28
5	A	1337	FAD	O3B-C3B-C4B	-2.34	104.05	111.05
5	A	1337	FAD	C4B-O4B-C1B	-2.32	107.17	109.72
5	A	1337	FAD	C8M-C8-C9	-2.31	113.99	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1335	MTE	C10-C9-N5	-2.09	116.21	118.85
3	A	1335	MTE	C4-C9-C10	2.01	116.39	114.56
3	B	1335	MTE	C4-C9-C10	2.28	116.63	114.56
5	B	1337	FAD	P-O3P-PA	2.31	139.22	132.73
5	B	1337	FAD	O3'-C3'-C4'	2.33	114.62	108.75
5	B	1337	FAD	C4A-C5A-N7A	2.42	111.70	109.48
5	A	1337	FAD	O3'-C3'-C4'	2.46	114.94	108.75
5	A	1337	FAD	C4A-C5A-N7A	2.47	111.75	109.48
5	A	1337	FAD	P-O3P-PA	2.58	139.98	132.73
5	A	1337	FAD	C8M-C8-C7	3.35	128.08	120.73
5	B	1337	FAD	C8M-C8-C7	3.42	128.25	120.73
5	B	1337	FAD	C4X-N5-C5X	4.41	121.84	116.76
3	A	1335	MTE	N8-C10-N1	4.49	123.77	116.62
5	A	1337	FAD	C4X-N5-C5X	4.64	122.10	116.76
3	B	1335	MTE	N2-C2-N3	4.66	124.92	117.20
3	B	1335	MTE	N8-C10-N1	4.68	124.07	116.62
3	A	1335	MTE	N2-C2-N3	4.77	125.10	117.20
3	B	1335	MTE	C2-N1-C10	4.87	125.48	114.54
3	A	1335	MTE	C2-N1-C10	4.92	125.60	114.54
3	B	1335	MTE	C4-N3-C2	4.92	122.77	115.94
3	A	1335	MTE	C4-N3-C2	4.96	122.82	115.94
5	A	1337	FAD	C4-C4X-N5	5.10	124.91	118.72
5	B	1337	FAD	C4-C4X-N5	5.23	125.06	118.72
5	A	1337	FAD	C4-N3-C2	10.54	124.36	115.25
5	B	1337	FAD	C4-N3-C2	10.86	124.63	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1335	MTE	1	0
4	A	1336	MOS	2	0
5	A	1337	FAD	3	0
9	A	1344	SAL	1	0
3	B	1335	MTE	1	0
4	B	1336	MOS	3	0
5	B	1337	FAD	3	0
6	B	1338	NAI	1	0
7	B	1342	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	1289/1332 (96%)	-0.24	27 (2%)	67	65	7, 22, 40, 65	0
1	B	1288/1332 (96%)	-0.22	27 (2%)	67	65	7, 23, 39, 65	0
All	All	2577/2664 (96%)	-0.23	54 (2%)	67	65	7, 22, 40, 65	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1288	ASN	7.7
1	A	1288	ASN	6.8
1	A	565	ASN	5.6
1	A	1286	THR	4.9
1	B	223	PRO	4.7
1	A	1320	GLY	4.6
1	B	1287	ASN	4.5
1	B	1286	THR	4.5
1	A	1290	THR	4.1
1	A	1318	VAL	3.9
1	A	1321	ALA	3.8
1	A	221	ASP	3.5
1	B	1290	THR	3.4
1	A	272	ASN	3.4
1	B	1318	VAL	3.3
1	A	1319	THR	3.2
1	A	223	PRO	3.1
1	A	378	GLY	3.0
1	B	1319	THR	2.9
1	B	566	GLY	2.8
1	A	553	PRO	2.8
1	A	222	VAL	2.7
1	B	553	PRO	2.7
1	B	852	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1320	GLY	2.7
1	A	540	PRO	2.5
1	B	221	ASP	2.5
1	A	551	LYS	2.5
1	A	564	PRO	2.5
1	A	566	GLY	2.5
1	B	222	VAL	2.5
1	B	272	ASN	2.5
1	B	271	LYS	2.4
1	A	1289	ASN	2.4
1	B	64	LYS	2.3
1	B	565	ASN	2.3
1	A	1287	ASN	2.3
1	B	550	GLN	2.2
1	A	721	LYS	2.2
1	B	1289	ASN	2.2
1	A	703	LYS	2.2
1	B	551	LYS	2.2
1	B	63	ASP	2.2
1	A	528	GLY	2.2
1	A	64	LYS	2.1
1	B	724	SER	2.1
1	B	703	LYS	2.1
1	A	1330	LEU	2.1
1	B	958	ARG	2.0
1	A	63	ASP	2.0
1	B	468	LYS	2.0
1	A	471	GLN	2.0
1	B	61	LEU	2.0
1	B	211	ILE	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

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	1341	6/6	0.96	0.13	3.21	18,20,21,25	0
7	GOL	B	1339	6/6	0.93	0.14	2.77	22,23,25,25	0
7	GOL	A	1340	6/6	0.93	0.13	1.68	25,26,28,28	0
7	GOL	A	1339	6/6	0.91	0.15	1.52	37,38,40,40	0
7	GOL	B	1342	6/6	0.95	0.14	1.24	30,31,31,32	0
7	GOL	A	1342	6/6	0.93	0.14	0.95	28,30,31,34	0
7	GOL	B	1340	6/6	0.93	0.12	0.32	25,29,29,33	0
9	SAL	B	1345	10/10	0.93	0.11	0.19	26,27,29,29	0
6	NAI	B	1338	44/44	0.93	0.12	0.13	16,23,27,31	0
3	MTE	A	1335	24/24	0.98	0.09	-0.07	9,15,20,24	0
7	GOL	B	1343	6/6	0.94	0.13	-0.10	30,33,35,38	0
6	NAI	A	1338	44/44	0.94	0.11	-0.10	18,24,30,33	0
7	GOL	B	1341	6/6	0.96	0.10	-0.11	16,16,18,19	0
3	MTE	B	1335	24/24	0.98	0.09	-0.18	12,17,20,24	0
5	FAD	A	1337	53/53	0.96	0.10	-0.39	16,19,25,30	0
5	FAD	B	1337	53/53	0.97	0.10	-0.54	16,20,24,26	0
9	SAL	A	1344	10/10	0.97	0.09	-0.70	17,21,23,25	0
10	CA	A	1345	1/1	1.00	0.07	-1.48	17,17,17,17	0
8	CO3	A	1343	4/4	0.98	0.07	-1.81	12,13,14,15	0
4	MOS	A	1336	4/4	1.00	0.06	-1.90	17,19,23,28	0
4	MOS	B	1336	4/4	0.99	0.06	-2.05	19,22,22,29	0
10	CA	B	1346	1/1	0.99	0.07	-2.23	21,21,21,21	0
2	FES	B	1334	4/4	0.99	0.05	-2.23	14,14,16,17	0
8	CO3	B	1344	4/4	0.98	0.07	-2.31	12,13,14,16	0
2	FES	B	1333	4/4	0.99	0.04	-3.30	11,11,12,13	0
2	FES	A	1333	4/4	0.99	0.05	-3.41	12,13,13,13	0
2	FES	A	1334	4/4	0.99	0.04	-3.53	14,15,16,17	0

6.5 Other polymers

There are no such residues in this entry.