



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:12 am GMT

PDB ID : 3UNA
Title : Crystal Structure of Bovine Milk Xanthine Dehydrogenase with NAD Bound
Authors : Eger, B.T.; Okamoto, K.; Nishino, T.; Pai, E.F.
Deposited on : 2011-11-15
Resolution : 1.90 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

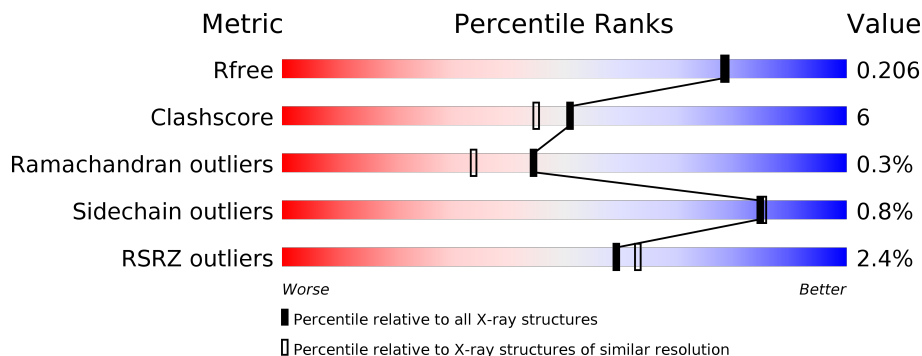
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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 $\leq 5\%$. 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	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div></div> </div> </div>
1	B	1332	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div></div> </div> </div>

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	X
4	MOS	B	1336	-	-	X	X
6	NAD	A	1338	-	-	-	X
6	NAD	B	1338	-	-	-	X
9	GOL	A	1341	-	-	-	X
9	GOL	A	1342	-	-	-	X
9	GOL	A	1343	-	-	-	X
9	GOL	A	1344	-	-	-	X
9	GOL	A	1347	-	-	-	X
9	GOL	A	1348	-	-	-	X
9	GOL	B	1341	-	-	-	X
9	GOL	B	1343	-	-	-	X
9	GOL	B	1345	-	-	-	X

2 Entry composition [i](#)

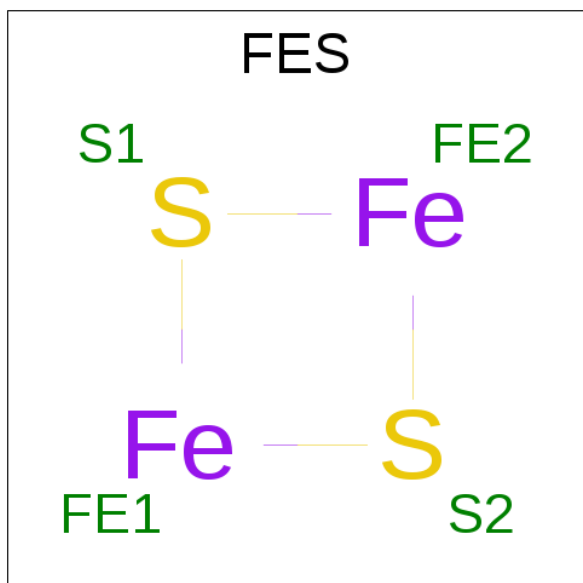
There are 11 unique types of molecules in this entry. The entry contains 21905 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

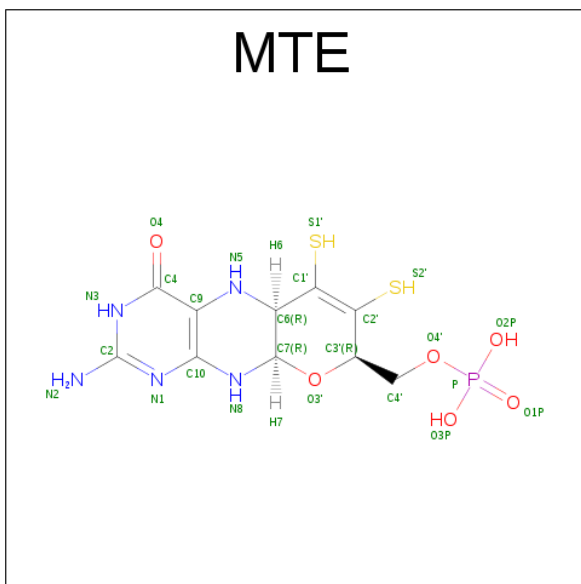
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1286	Total	C	N	O	S	0	7	0
			10036	6378	1717	1877	64			
1	B	1289	Total	C	N	O	S	0	4	0
			10035	6378	1717	1876	64			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



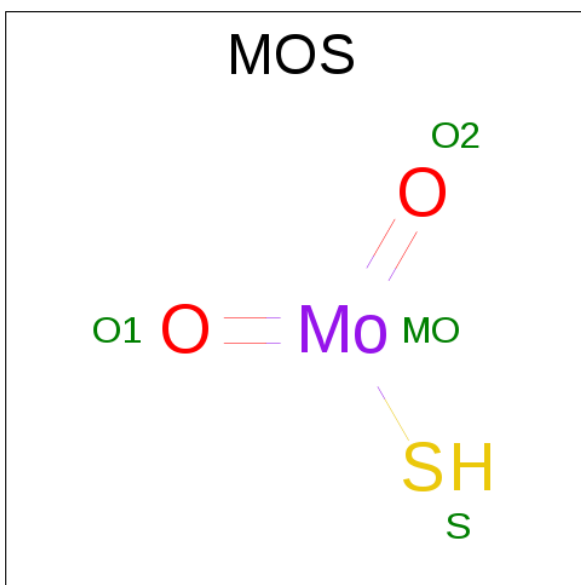
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

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



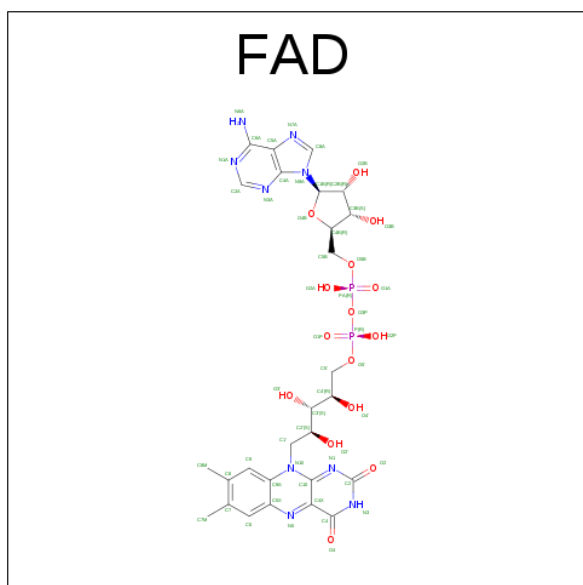
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
3	B	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

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



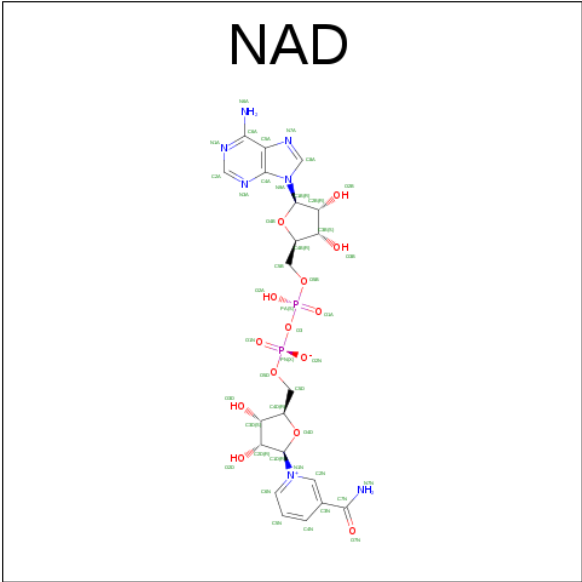
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
4	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

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



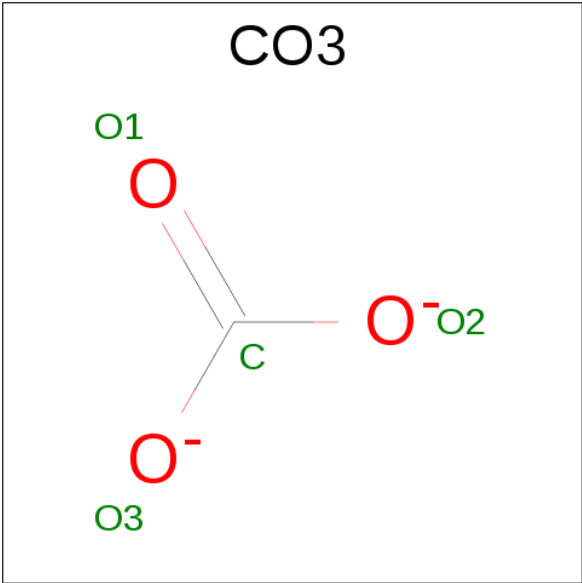
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



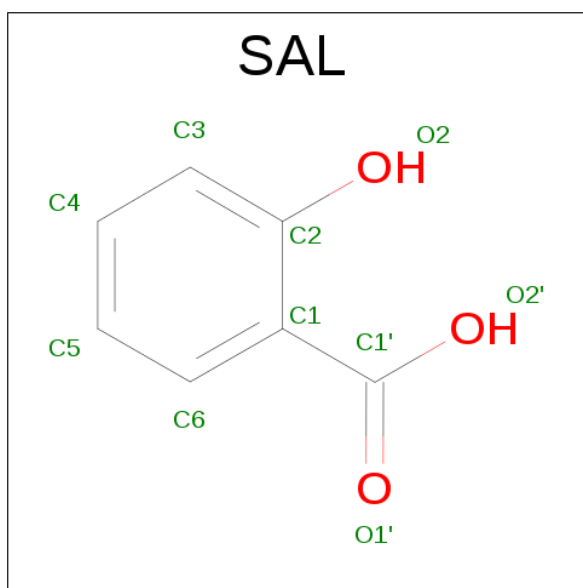
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
6	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 7 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



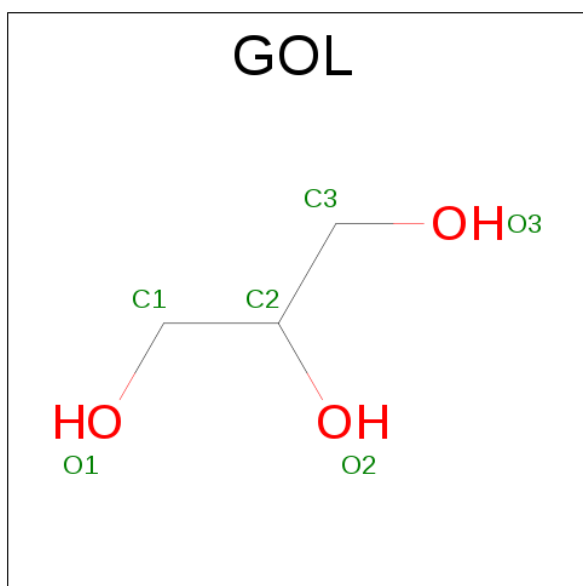
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	1	3		
7	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 8 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $C_7H_6O_3$).



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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

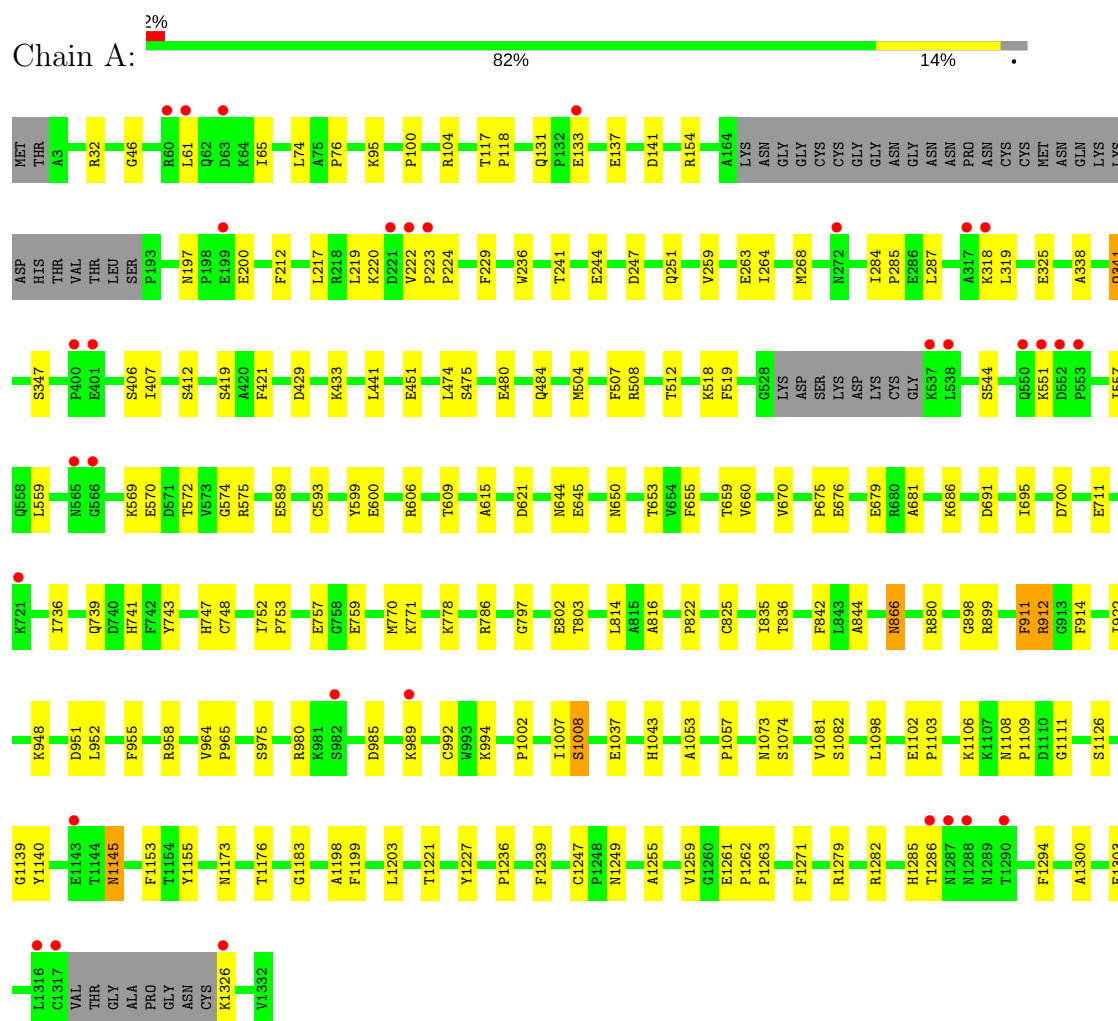
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	758	Total O 758 758	0	0
11	B	744	Total O 744 744	0	0

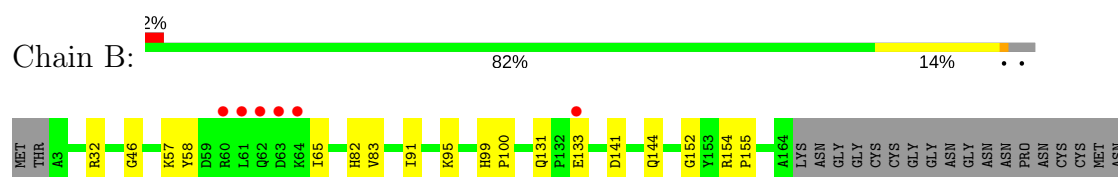
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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/oxidase



• Molecule 1: Xanthine dehydrogenase/oxidase



C1325	N1173	N925	E711	Q550	S376	GLN
K1326	L1174	E929	K721	K551	R377	LYS
P1327	R1175	K948	E725	P553	G378	LYS
V1332	T1176	D951	I736	Q558	T382	ASP
	G1183	F955	Q739	N565	E402	HIS
	A1189	V964	Y743	G566	L405	THR
	I1192	P965	H747	K569	L407	VAL
	F1199	K986	C748	E570	S412	THR
	V1200	F987	I752	D571	F418	LEU
	L1203	E990	P753	V572	D429	SER
	P1236	N991	E757	G574	K433	P193
	T1287	C992	K778	E589	R439	S194
	E1238	V993	R786	C593	V440	L195
	F1239	K995	G797	R598	L441	F212
	C1247	R996	P822	Y599	Q448	L216
	P1248	I1007	E802	F604	E451	L217
	N1249	S1008	L814	T609	E477	R218
	A1255	A1017	A815	S610	E480	L219
	V1259	E1037	A816	V628	Q484	K220
	G1260	H1043	P835	N644	L496	D221
	E1261	Q1048	T836	E645	M504	V222
	P1262	P1057	F842	N650	L506	P223
	R1279	V1081	L843	T653	E506	T241
	H1285	S1082	A844	V654	F507	E244
	T1286	Y1086	R880	K657	R509	E263
	N1287	E1102	M885	D658	T512	L264
	N1288	P1103	K890	V660	G528	K271
	N1289	M1118	G896	T661	LYS	N272
	T1290	Q1122	F899	C662	ASP	P281
	K1291	F1132	K902	V670	V316	E286
	F1294	G1139	N145	P675	LYS	L287
	P1299	E1145	F911	E676	ASP	P294
	A1300	F1153	R912	A681	LYS	E295
	T1301	T1154	G913	N705	CYS	K310
	K1312	Y1155	F914	S706	GLY	E314
	F1313	E1163	I922	Y708	LYS	A315
	T1314				LYS	V317
	V1318				ASP	A317
	T1319				LYS	K318
	GLY				ASP	T324
	ALA				CYS	E325
	PRO				GLY	A338
	GLY				LYS	L348
	ASN				GLY	L372
					LYS	S544

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.03Å 123.18Å 147.62Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-1.90) 96.0 (19.95-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.181 , 0.214 0.176 , 0.206	Depositor DCC
R_{free} test set	2214 reflections (1.00%)	DCC
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21905	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, NAD, SAL, MOS, CA, 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	0.31	0/10254	0.61	0/13876
1	B	0.31	0/10253	0.61	0/13876
All	All	0.31	0/20507	0.61	0/27752

There are no bond length outliers.

There are no bond angle outliers.

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	10036	0	10027	128	0
1	B	10035	0	10029	131	0
2	A	8	0	0	1	0
2	B	8	0	0	1	0
3	A	24	0	10	2	0
3	B	24	0	10	2	0
4	A	4	0	0	4	0
4	B	4	0	0	4	0
5	A	53	0	31	2	0
5	B	53	0	31	2	0
6	A	23	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	23	0	12	0	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
8	A	10	0	4	1	0
8	B	10	0	4	1	0
9	A	48	0	64	2	0
9	B	30	0	40	1	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	758	0	0	3	0
11	B	744	0	0	1	0
All	All	21905	0	20274	264	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 6.

All (264) 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:955:PHE:HA	1:A:1145:ASN:HD21	1.28	0.95
1:A:341:GLN:H	1:A:341:GLN:HE21	1.09	0.92
1:B:131:GLN:HE21	1:B:133:GLU:H	1.16	0.90
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.38	0.87
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.38	0.85
1:A:131:GLN:HE21	1:A:133:GLU:H	1.25	0.84
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.42	0.84
1:A:948:LYS:HG2	1:A:951:ASP:OD2	1.85	0.76
1:A:518:LYS:HE2	11:A:2094:HOH:O	1.84	0.76
1:B:1279:ARG:HG2	1:B:1294:PHE:HE2	1.52	0.74
1:A:341:GLN:NE2	1:A:341:GLN:H	1.83	0.74
1:B:1326:LYS:HD3	1:B:1326:LYS:H	1.53	0.72
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.53	0.71
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.58	0.69
1:A:341:GLN:HE21	1:A:341:GLN:N	1.90	0.66
1:A:1221:THR:HG22	1:A:1227:TYR:HB2	1.78	0.65
4:B:1336:MOS:MO	4:B:1336:MOS:O2	1.67	0.65
4:A:1336:MOS:O2	4:A:1336:MOS:MO	1.67	0.64
1:B:948:LYS:HG2	1:B:951:ASP:OD2	1.97	0.63
1:B:241:THR:OG1	1:B:244:GLU:HG3	1.98	0.63
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.80	0.62
1:B:131:GLN:HE21	1:B:133:GLU:N	1.94	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:ASP:O	1:A:989:LYS:HG3	2.00	0.61
4:B:1336:MOS:MO	4:B:1336:MOS:S	2.11	0.61
1:A:1279:ARG:HG2	1:A:1294:PHE:HE2	1.65	0.61
1:A:217:LEU:O	1:A:220:LYS:HG2	2.01	0.60
1:A:433:LYS:HE2	1:A:504:MET:SD	2.40	0.60
4:A:1336:MOS:S	4:A:1336:MOS:MO	2.11	0.60
1:A:621:ASP:HB3	1:A:686:LYS:HE2	1.84	0.60
1:A:264:ILE:HD11	5:A:1337:FAD:H3B	1.82	0.60
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.84	0.59
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.03	0.59
1:B:32:ARG:HH12	1:B:676:GLU:CD	2.06	0.58
1:A:318:LYS:HE2	1:A:319:LEU:HD21	1.84	0.58
1:B:131:GLN:NE2	1:B:133:GLU:H	1.94	0.58
1:A:557:ILE:HG22	1:A:559:LEU:CD1	2.33	0.58
1:B:552:ASP:HB3	1:B:553:PRO:HD2	1.86	0.58
1:B:281:PRO:HB2	1:B:287:LEU:HD12	1.85	0.58
1:A:441:LEU:HB3	1:A:451:GLU:HB2	1.86	0.57
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.86	0.57
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.05	0.57
1:A:593:CYS:HB3	1:A:748[B]:CYS:SG	2.44	0.57
1:A:559:LEU:HD13	11:A:1476:HOH:O	2.05	0.56
1:B:711:GLU:HA	1:B:899:ARG:HD2	1.87	0.56
1:B:1175:ARG:HG3	1:B:1238:GLU:HG2	1.86	0.56
1:B:570:GLU:OE2	1:B:1057:PRO:HG3	2.05	0.56
1:B:604:PHE:CD2	1:B:675:PRO:HG3	2.41	0.56
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.42	0.56
1:A:32:ARG:HH12	1:A:676:GLU:CD	2.08	0.55
1:A:1102:GLU:HB3	1:A:1103:PRO:HD3	1.88	0.55
1:A:407:ILE:N	1:A:407:ILE:HD12	2.22	0.55
1:B:310:LYS:O	1:B:314:GLU:HG3	2.07	0.55
1:B:433:LYS:HE3	1:B:433:LYS:HA	1.89	0.55
1:B:1008:SER:HA	1:B:1081:VAL:HG11	1.88	0.55
1:B:216:LEU:HD23	1:B:219:LEU:HD12	1.89	0.55
1:A:752:ILE:CD1	1:A:822:PRO:HB3	2.38	0.54
1:A:1008:SER:HA	1:A:1081:VAL:HG11	1.88	0.54
1:B:757:GLU:HB3	1:B:786:ARG:HE	1.70	0.54
1:B:377:ARG:HH11	1:B:377:ARG:HG3	1.71	0.54
1:B:318:LYS:N	1:B:318:LYS:HD2	2.22	0.54
1:B:1279:ARG:HG2	1:B:1294:PHE:CE2	2.39	0.54
1:A:474:LEU:O	1:A:475[A]:SER:HB2	2.07	0.53
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:ALA:O	1:A:659[A]:THR:HG23	2.09	0.52
1:B:281:PRO:HB2	1:B:287:LEU:CD1	2.39	0.52
1:A:141:ASP:OD1	1:A:551:LYS:NZ	2.42	0.52
1:B:752:ILE:CD1	1:B:822:PRO:HB3	2.39	0.52
1:A:406:SER:C	1:A:407:ILE:HD12	2.30	0.52
1:B:506:GLU:HG2	1:B:1319:THR:HG23	1.92	0.52
1:B:1326:LYS:N	1:B:1326:LYS:HD3	2.24	0.52
1:B:506:GLU:CG	1:B:1319:THR:HG23	2.40	0.51
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.46	0.51
1:A:421:PHE:CE2	1:A:518:LYS:NZ	2.79	0.51
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.92	0.51
1:B:264:ILE:HD11	5:B:1337:FAD:H3B	1.93	0.51
1:B:91:ILE:O	1:B:99:HIS:HB2	2.11	0.51
1:B:1314:THR:O	1:B:1318:VAL:HG13	2.11	0.51
3:B:1335:MTE:S1'	4:B:1336:MOS:S	3.09	0.50
1:A:544:SER:O	1:A:994:LYS:HE2	2.11	0.50
1:A:770[B]:MET:HE2	1:A:1073:ASN:C	2.31	0.50
1:A:247:ASP:O	1:A:251:GLN:HG3	2.12	0.50
1:B:711:GLU:HA	1:B:899:ARG:CD	2.41	0.50
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.46	0.50
1:A:284:ILE:CG2	1:A:287:LEU:HD23	2.42	0.50
1:A:770[B]:MET:HE2	1:A:1074:SER:O	2.12	0.50
1:A:1007:ILE:O	1:A:1008:SER:CB	2.60	0.50
1:A:1153:PHE:HB2	1:A:1155:TYR:CZ	2.46	0.49
1:A:100:PRO:O	1:A:104:ARG:HG3	2.12	0.49
1:B:1007:ILE:O	1:B:1008:SER:CB	2.60	0.49
1:A:1082:SER:HB2	3:A:1335:MTE:O3P	2.12	0.49
1:A:911:PHE:O	1:A:912:ARG:C	2.50	0.49
1:B:572:THR:OG1	1:B:1048:GLN:HG2	2.12	0.49
1:B:1082:SER:HB2	3:B:1335:MTE:O3P	2.13	0.49
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.95	0.49
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.78	0.49
1:B:217:LEU:O	1:B:220:LYS:HG2	2.13	0.48
1:B:82:HIS:NE2	1:B:219:LEU:HD13	2.27	0.48
1:A:32:ARG:NH1	1:A:676:GLU:OE2	2.43	0.48
1:B:348:LEU:HD13	1:B:407:ILE:CD1	2.43	0.48
1:A:1126:SER:HB2	1:B:1132:PHE:CD1	2.48	0.48
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.78	0.48
1:B:753:PRO:HD3	1:B:816:ALA:HB1	1.96	0.48
1:B:844:ALA:HB2	1:B:922:ILE:HD13	1.95	0.48
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992[A]:CYS:SG	1:A:1285:HIS:CE1	3.07	0.48
1:A:338:ALA:HA	1:A:429:ASP:OD1	2.13	0.48
1:A:197:ASN:ND2	1:A:200:GLU:HG3	2.29	0.48
1:B:992[A]:CYS:SG	1:B:1285:HIS:NE2	2.87	0.48
1:B:508:ARG:HD3	11:B:1385:HOH:O	2.14	0.47
1:A:219:LEU:O	1:A:222:VAL:HG12	2.13	0.47
1:A:263:GLU:HB2	5:A:1337:FAD:H52A	1.95	0.47
1:A:137:GLU:HG3	1:A:551:LYS:HD2	1.96	0.47
1:B:152:GLY:HA2	1:B:1200:VAL:HG21	1.96	0.47
1:A:770[B]:MET:HG3	1:A:1073:ASN:HA	1.96	0.47
1:B:376:SER:HB3	1:B:402:GLU:HG2	1.97	0.47
1:B:736:ILE:CG2	1:B:842:PHE:HB2	2.43	0.47
1:B:911:PHE:O	1:B:912:ARG:C	2.53	0.47
1:A:61:LEU:N	1:A:61:LEU:HD12	2.29	0.47
1:A:964:VAL:HB	1:A:965:PRO:HD3	1.95	0.47
1:A:480:GLU:O	1:A:484:GLN:HG3	2.14	0.47
1:A:606:ARG:CZ	1:A:679:GLU:HG3	2.45	0.47
1:B:721:LYS:O	1:B:725:GLU:HG3	2.15	0.47
1:A:569:LYS:NZ	1:A:569:LYS:HB3	2.29	0.47
1:B:433:LYS:HA	1:B:433:LYS:CE	2.46	0.46
1:B:593:CYS:HB3	1:B:748[B]:CYS:SG	2.55	0.46
1:B:348:LEU:HD13	1:B:407:ILE:HD11	1.95	0.46
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.96	0.46
1:B:1163:GLU:HB2	1:B:1174:LEU:HD11	1.98	0.46
1:B:263:GLU:HB2	5:B:1337:FAD:H52A	1.98	0.46
1:B:508:ARG:O	1:B:512:THR:HG23	2.16	0.46
1:A:992[A]:CYS:SG	1:A:1285:HIS:NE2	2.89	0.46
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.78	0.46
1:A:95:LYS:HG3	1:A:589:GLU:OE1	2.15	0.46
1:B:1153:PHE:HB2	1:B:1155:TYR:CZ	2.50	0.46
1:B:141:ASP:O	1:B:144:GLN:HG3	2.16	0.46
1:A:259:VAL:HG11	1:A:347:SER:HB3	1.97	0.46
1:B:338:ALA:HA	1:B:429:ASP:OD1	2.16	0.46
1:A:955:PHE:HA	1:A:1145:ASN:ND2	2.12	0.46
1:B:628:VAL:HG21	1:B:681:ALA:HA	1.98	0.46
1:A:1102:GLU:OE2	1:A:1106:LYS:HE3	2.16	0.46
1:A:1271:PHE:CE1	1:A:1300:ALA:HB2	2.51	0.45
1:B:1183:GLY:HA2	1:B:1247:CYS:O	2.17	0.45
1:B:377:ARG:HG3	1:B:377:ARG:NH1	2.29	0.45
1:B:992[A]:CYS:SG	1:B:1285:HIS:CE1	3.09	0.45
3:A:1335:MTE:S1'	4:A:1336:MOS:S	3.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1336:MOS:O1	4:B:1336:MOS:S	2.75	0.45
1:B:1173:ASN:O	1:B:1236:PRO:HA	2.16	0.45
1:B:1312:LYS:HE3	1:B:1313:PHE:CZ	2.52	0.45
1:B:655:PHE:CE1	1:B:814:LEU:HD23	2.52	0.45
1:A:1183:GLY:HA2	1:A:1247:CYS:O	2.16	0.45
1:B:195:LEU:HD22	1:B:1189:ALA:HA	1.98	0.45
1:B:287:LEU:HD23	1:B:405:LEU:HD12	1.97	0.45
1:B:46:GLY:HA2	2:B:1334:FES:S1	2.57	0.45
1:A:599:TYR:HA	1:B:599:TYR:HA	1.97	0.45
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.45
1:B:58:TYR:CE2	1:B:220:LYS:HD2	2.52	0.45
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.80	0.45
1:A:1176:THR:HG21	1:A:1199:PHE:CZ	2.51	0.45
1:A:736:ILE:CG2	1:A:842:PHE:HB2	2.47	0.45
1:A:711:GLU:HA	1:A:899:ARG:CD	2.47	0.45
1:B:286:GLU:HB3	1:B:405:LEU:HD11	1.98	0.44
1:A:711:GLU:HA	1:A:899:ARG:HD2	1.99	0.44
1:B:711:GLU:HB2	1:B:899:ARG:HD3	1.99	0.44
1:B:509:ARG:HG2	1:B:509:ARG:HH11	1.83	0.44
1:A:1203:LEU:C	1:A:1203:LEU:HD23	2.36	0.44
1:A:325:GLU:HB2	1:A:412:SER:HB3	2.00	0.44
1:A:644:ASN:O	1:A:653:THR:HA	2.17	0.44
1:B:1279:ARG:HB3	1:B:1279:ARG:NH1	2.32	0.44
1:B:271:LYS:N	1:B:271:LYS:HD2	2.33	0.44
1:B:294:PRO:HG2	1:B:295:GLU:OE1	2.18	0.44
1:B:325:GLU:HB2	1:B:412:SER:HB3	1.98	0.44
1:B:65:ILE:HD13	1:B:212:PHE:CB	2.48	0.44
1:A:844:ALA:HB2	1:A:922:ILE:HD13	2.00	0.44
1:B:433:LYS:HD3	1:B:504:MET:SD	2.57	0.44
4:A:1336:MOS:S	4:A:1336:MOS:O1	2.76	0.44
1:A:229:PHE:HB2	1:A:236:TRP:HB3	2.00	0.44
1:A:609:THR:HG21	1:A:835:ILE:HD11	1.99	0.43
1:A:325:GLU:HB2	1:A:412:SER:CB	2.48	0.43
1:B:1289:ASN:ND2	1:B:1291:LYS:H	2.16	0.43
1:B:802:GLU:OE1	8:B:1340:SAL:H3	2.18	0.43
1:A:1102:GLU:HG3	1:A:1106:LYS:HE3	1.99	0.43
1:A:284:ILE:HA	1:A:285:PRO:HD3	1.90	0.43
1:A:975:SER:O	1:A:980:ARG:HD3	2.19	0.43
1:A:268[B]:MET:CE	11:A:1781:HOH:O	2.67	0.43
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.53	0.43
1:B:372:LEU:O	1:B:382:THR:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:THR:HA	1:A:575:ARG:HD2	2.01	0.43
1:A:65:ILE:HD13	1:A:212:PHE:CB	2.49	0.43
1:B:1259:VAL:O	1:B:1259:VAL:HG22	2.19	0.43
1:B:986:LYS:HG2	1:B:990:GLU:OE2	2.19	0.43
1:A:1108:ASN:N	1:A:1109:PRO:HD3	2.33	0.43
1:B:1118:MET:O	1:B:1122:GLN:HG2	2.18	0.43
1:A:739:GLN:HG2	1:A:911:PHE:CE1	2.54	0.43
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.82	0.42
1:A:508:ARG:O	1:A:512:THR:HG23	2.18	0.42
1:A:802:GLU:HG2	1:A:803:THR:HG23	2.01	0.42
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	2.01	0.42
1:A:284:ILE:HG21	1:A:287:LEU:HD23	2.02	0.42
1:A:318:LYS:HG3	1:A:319:LEU:HG	2.02	0.42
1:A:621:ASP:CB	1:A:686:LYS:HE2	2.47	0.42
1:B:1176:THR:HG21	1:B:1199:PHE:CZ	2.54	0.42
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.20	0.42
1:A:1198:ALA:HB3	1:A:1263:PRO:HB2	2.00	0.42
1:B:544:SER:O	1:B:994:LYS:HE2	2.19	0.42
1:A:771:LYS:HD3	1:A:771:LYS:HA	1.87	0.42
1:A:866:ASN:C	1:A:866:ASN:HD22	2.22	0.42
1:A:1259:VAL:O	1:A:1259:VAL:HG22	2.19	0.42
1:A:46:GLY:HA2	2:A:1334:FES:S1	2.60	0.42
1:A:898:GLY:O	1:A:899:ARG:HD2	2.19	0.42
1:B:1326:LYS:HB2	1:B:1327:PRO:HD2	2.01	0.42
1:B:57:LYS:HE2	1:B:83:VAL:HG22	2.01	0.42
1:B:657:LYS:O	1:B:658:ASP:HB2	2.18	0.42
1:B:609:THR:HG21	1:B:835:ILE:HD11	2.01	0.42
1:B:890:LYS:HE2	1:B:951:ASP:CG	2.40	0.42
1:A:759:GLU:OE1	9:A:1348:GOL:H12	2.20	0.42
1:A:74:LEU:O	1:A:76:PRO:HD3	2.20	0.42
1:B:407:ILE:HG13	1:B:407:ILE:O	2.19	0.42
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.20	0.42
1:A:419:SER:HB2	1:A:519:PHE:CD1	2.55	0.42
1:A:574:GLY:CA	9:A:1345:GOL:H12	2.49	0.42
1:A:655:PHE:CE1	1:A:814:LEU:HD23	2.54	0.42
1:B:574:GLY:CA	9:B:1344:GOL:H12	2.50	0.42
1:B:418:PHE:CD1	1:B:439:ARG:HB2	2.54	0.42
1:B:95:LYS:HG3	1:B:589:GLU:OE1	2.20	0.42
1:B:661:THR:O	1:B:662:CYS:HB3	2.20	0.42
1:B:1299:PRO:HG2	1:B:1301:THR:HG23	2.01	0.41
1:B:448:GLN:HB2	1:B:477:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:GLU:HG3	1:B:484:GLN:HE21	1.85	0.41
1:B:885:MET:SD	1:B:896:GLY:HA3	2.59	0.41
1:B:644:ASN:O	1:B:653:THR:HA	2.21	0.41
1:A:600:GLU:OE2	1:B:598:ARG:HG2	2.20	0.41
1:B:890:LYS:HE2	1:B:951:ASP:OD2	2.19	0.41
1:B:316:VAL:HA	1:B:324:THR:HG21	2.02	0.41
1:B:752:ILE:HD13	1:B:822:PRO:HB3	2.02	0.41
1:B:987:PHE:CD2	1:B:996:ARG:HG3	2.56	0.41
1:A:1108:ASN:ND2	1:A:1111:GLY:HA3	2.36	0.41
1:A:154:ARG:C	1:A:154:ARG:HD2	2.41	0.41
1:A:675:PRO:HG2	1:A:676:GLU:OE1	2.20	0.41
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.54	0.41
1:B:65:ILE:HD13	1:B:212:PHE:HB2	2.03	0.41
1:A:570:GLU:CD	1:A:1057:PRO:HG3	2.41	0.41
1:A:1173:ASN:O	1:A:1236:PRO:HA	2.21	0.41
1:A:1282:ARG:O	1:A:1286:THR:HB	2.21	0.41
1:A:659[A]:THR:HG22	1:A:660:VAL:N	2.35	0.41
1:A:802:GLU:OE1	8:A:1340:SAL:H3	2.20	0.41
1:B:1102:GLU:HB3	1:B:1103:PRO:HD3	2.02	0.41
1:B:610:SER:HB2	1:B:660:VAL:HG11	2.03	0.41
1:B:705:ASN:HA	1:B:707:PHE:CE1	2.55	0.41
1:A:748[B]:CYS:HA	1:A:825:CYS:O	2.21	0.41
1:B:496:LEU:HB2	1:B:505:ILE:HG23	2.02	0.41
1:B:925:ASN:O	1:B:929:GLU:HG3	2.21	0.41
1:A:318:LYS:HG3	1:A:319:LEU:N	2.36	0.41
1:B:154:ARG:N	1:B:155:PRO:HD2	2.35	0.41
1:A:507:PHE:HB2	1:A:1303:GLU:HG3	2.03	0.41
1:A:952:LEU:HD23	1:A:958:ARG:HA	2.02	0.41
1:A:695:ILE:HG23	1:A:700:ASP:HB3	2.04	0.40
1:A:117:THR:HB	1:A:118:PRO:HD3	2.03	0.40
1:A:615:ALA:HB2	1:A:691:ASP:HA	2.02	0.40
1:A:955:PHE:HB2	1:A:1140:TYR:CE1	2.56	0.40
1:B:1203:LEU:HD23	1:B:1203:LEU:C	2.42	0.40
1:B:325:GLU:HB2	1:B:412:SER:CB	2.51	0.40
1:B:708:TYR:CE2	1:B:902:LYS:HD3	2.57	0.40
1:B:739:GLN:HG2	1:B:911:PHE:CE1	2.56	0.40
1:A:741:HIS:HA	1:A:911:PHE:CE1	2.56	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	1285/1332 (96%)	1241 (97%)	40 (3%)	4 (0%)	44	34
1	B	1285/1332 (96%)	1248 (97%)	33 (3%)	4 (0%)	44	34
All	All	2570/2664 (96%)	2489 (97%)	73 (3%)	8 (0%)	44	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	A	912	ARG
1	B	912	ARG
1	A	797	GLY
1	B	797	GLY
1	B	1139	GLY
1	A	1139	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	1098/1128 (97%)	1090 (99%)	8 (1%)	87	87
1	B	1098/1128 (97%)	1089 (99%)	9 (1%)	85	85
All	All	2196/2256 (97%)	2179 (99%)	17 (1%)	85	85

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	GLN
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	100	PRO
1	B	271	LYS
1	B	565	ASN
1	B	743	TYR
1	B	911	PHE
1	B	1145	ASN
1	B	1239	PHE
1	B	1289	ASN
1	B	1326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	251	GLN
1	A	272	ASN
1	A	341	GLN
1	A	471	GLN
1	A	473	GLN
1	A	650	ASN
1	A	683	HIS
1	A	866	ASN
1	A	1088	GLN
1	A	1145	ASN
1	A	1289	ASN
1	B	131	GLN
1	B	251	GLN
1	B	473	GLN
1	B	484	GLN
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	875	HIS
1	B	1088	GLN
1	B	1108	ASN

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Mol	Chain	Res	Type
1	B	1145	ASN
1	B	1288	ASN
1	B	1289	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 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	21,26,26	2.41	8 (38%)	19,40,40	2.75	7 (36%)
4	MOS	A	1336	3	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	A	1337	-	51,58,58	2.94	19 (37%)	54,89,89	2.99	18 (33%)
6	NAD	A	1338	-	22,25,48	2.87	8 (36%)	24,38,73	2.37	5 (20%)
7	CO3	A	1339	-	0,3,3	0.00	-	0,3,3	0.00	-
8	SAL	A	1340	-	7,10,10	1.82	3 (42%)	9,13,13	1.19	0
9	GOL	A	1341	-	5,5,5	0.60	0	5,5,5	0.38	0
9	GOL	A	1342	-	5,5,5	0.52	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	A	1343	-	5,5,5	0.61	0	5,5,5	0.30	0
9	GOL	A	1344	-	5,5,5	0.64	0	5,5,5	0.28	0
9	GOL	A	1345	-	5,5,5	0.60	0	5,5,5	0.34	0
9	GOL	A	1346	-	5,5,5	0.62	0	5,5,5	0.29	0
9	GOL	A	1347	-	5,5,5	0.56	0	5,5,5	0.31	0
9	GOL	A	1348	-	5,5,5	0.50	0	5,5,5	0.36	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	21,26,26	2.38	8 (38%)	19,40,40	2.75	7 (36%)
4	MOS	B	1336	3	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	B	1337	-	51,58,58	2.87	19 (37%)	54,89,89	2.96	19 (35%)
6	NAD	B	1338	-	22,25,48	2.87	8 (36%)	24,38,73	2.32	5 (20%)
7	CO3	B	1339	-	0,3,3	0.00	-	0,3,3	0.00	-
8	SAL	B	1340	-	7,10,10	1.85	3 (42%)	9,13,13	1.21	1 (11%)
9	GOL	B	1341	-	5,5,5	0.56	0	5,5,5	0.38	0
9	GOL	B	1342	-	5,5,5	0.58	0	5,5,5	0.30	0
9	GOL	B	1343	-	5,5,5	0.63	0	5,5,5	0.29	0
9	GOL	B	1344	-	5,5,5	0.60	0	5,5,5	0.34	0
9	GOL	B	1345	-	5,5,5	0.56	0	5,5,5	0.26	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	-	-	0/28/50/50	0/6/6/6
6	NAD	A	1338	-	-	0/6/26/62	0/3/3/5
7	CO3	A	1339	-	-	0/0/0/0	0/0/0/0
8	SAL	A	1340	-	-	0/0/4/4	0/1/1/1
9	GOL	A	1341	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1342	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1343	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1344	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1345	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1346	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1347	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1348	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	0/28/50/50	0/6/6/6
6	NAD	B	1338	-	-	0/6/26/62	0/3/3/5
7	CO3	B	1339	-	-	0/0/0/0	0/0/0/0
8	SAL	B	1340	-	-	0/0/4/4	0/1/1/1
9	GOL	B	1341	-	-	0/4/4/4	0/0/0/0
9	GOL	B	1342	-	-	0/4/4/4	0/0/0/0
9	GOL	B	1343	-	-	0/4/4/4	0/0/0/0
9	GOL	B	1344	-	-	0/4/4/4	0/0/0/0
9	GOL	B	1345	-	-	0/4/4/4	0/0/0/0

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1338	NAD	PA-O5B	-2.67	1.51	1.60
5	B	1337	FAD	C2B-C1B	-2.65	1.49	1.53
6	B	1338	NAD	PA-O5B	-2.64	1.51	1.60
5	A	1337	FAD	C2B-C1B	-2.54	1.49	1.53
8	A	1340	SAL	C3-C2	2.10	1.43	1.39
3	B	1335	MTE	C2-N1	2.15	1.39	1.35
8	B	1340	SAL	C3-C2	2.17	1.43	1.39
6	B	1338	NAD	O3B-C3B	2.22	1.48	1.43
6	B	1338	NAD	C6A-N6A	2.26	1.43	1.34
6	A	1338	NAD	O3B-C3B	2.29	1.48	1.43
3	A	1335	MTE	C2-N1	2.30	1.39	1.35
6	A	1338	NAD	C6A-N6A	2.32	1.43	1.34
8	B	1340	SAL	C6-C1	2.38	1.43	1.39
8	A	1340	SAL	C6-C1	2.44	1.43	1.39
3	B	1335	MTE	C7-C6	2.71	1.55	1.53
5	B	1337	FAD	C6-C5X	2.74	1.45	1.41
5	A	1337	FAD	C5A-C4A	2.77	1.46	1.40
5	B	1337	FAD	C5A-C4A	2.79	1.46	1.40
3	A	1335	MTE	C7-C6	2.85	1.55	1.53
5	B	1337	FAD	C9-C9A	2.90	1.46	1.40
5	A	1337	FAD	C4-C4X	2.94	1.47	1.41
5	B	1337	FAD	C4-C4X	2.97	1.47	1.41
8	A	1340	SAL	C5-C6	2.98	1.44	1.38
3	B	1335	MTE	C4-N3	3.00	1.38	1.33
8	B	1340	SAL	C5-C6	3.02	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1337	FAD	C6-C5X	3.03	1.46	1.41
3	A	1335	MTE	C4-N3	3.10	1.38	1.33
3	B	1335	MTE	C9-C10	3.14	1.47	1.41
5	A	1337	FAD	C9-C9A	3.15	1.47	1.40
3	A	1335	MTE	C9-C10	3.25	1.47	1.41
5	A	1337	FAD	C4X-N5	3.33	1.38	1.33
5	B	1337	FAD	O4B-C4B	3.59	1.53	1.45
5	B	1337	FAD	C4X-N5	3.62	1.38	1.33
5	A	1337	FAD	O4B-C4B	3.70	1.53	1.45
5	A	1337	FAD	C9A-C5X	3.70	1.50	1.42
5	B	1337	FAD	C8-C7	3.76	1.50	1.41
5	A	1337	FAD	C8-C7	3.77	1.50	1.41
5	A	1337	FAD	C2-N3	3.77	1.45	1.38
5	B	1337	FAD	C2-N3	3.78	1.45	1.38
6	A	1338	NAD	O4B-C1B	3.81	1.46	1.41
5	B	1337	FAD	C9A-C5X	3.85	1.50	1.42
3	A	1335	MTE	O3'-C7	3.91	1.49	1.43
6	B	1338	NAD	O4B-C1B	3.92	1.46	1.41
3	B	1335	MTE	O4-C4	3.94	1.34	1.24
5	B	1337	FAD	C5X-N5	4.00	1.41	1.35
5	A	1337	FAD	C2A-N1A	4.06	1.41	1.33
3	A	1335	MTE	O4-C4	4.07	1.34	1.24
5	A	1337	FAD	C5X-N5	4.09	1.41	1.35
3	B	1335	MTE	O3'-C7	4.14	1.49	1.43
5	B	1337	FAD	C2A-N1A	4.14	1.41	1.33
5	B	1337	FAD	C2A-N3A	4.34	1.39	1.32
6	B	1338	NAD	C8A-N7A	4.36	1.42	1.34
6	A	1338	NAD	C8A-N7A	4.38	1.42	1.34
5	B	1337	FAD	C4A-N3A	4.55	1.42	1.35
5	A	1337	FAD	C2A-N3A	4.57	1.39	1.32
5	B	1337	FAD	C10-N1	4.73	1.39	1.33
3	B	1335	MTE	C9-N5	4.79	1.48	1.37
5	A	1337	FAD	C4A-N3A	4.79	1.42	1.35
3	A	1335	MTE	C9-N5	4.80	1.48	1.37
3	A	1335	MTE	O3'-C3'	4.84	1.50	1.43
3	B	1335	MTE	O3'-C3'	4.89	1.50	1.43
5	B	1337	FAD	C4-N3	4.92	1.41	1.33
5	A	1337	FAD	C4-N3	4.97	1.42	1.33
5	A	1337	FAD	C10-N1	4.98	1.40	1.33
6	A	1338	NAD	C2A-N1A	5.05	1.43	1.33
6	B	1338	NAD	C2A-N1A	5.08	1.43	1.33
5	B	1337	FAD	C4X-C10	5.67	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1337	FAD	C4X-C10	5.81	1.51	1.41
6	A	1338	NAD	C2A-N3A	6.60	1.43	1.32
6	B	1338	NAD	C2A-N3A	6.64	1.43	1.32
6	A	1338	NAD	C4A-N3A	6.74	1.45	1.35
6	B	1338	NAD	C4A-N3A	6.75	1.45	1.35
5	B	1337	FAD	O4B-C1B	7.36	1.51	1.41
5	A	1337	FAD	O4B-C1B	7.43	1.51	1.41
5	B	1337	FAD	C9A-N10	9.18	1.50	1.38
5	A	1337	FAD	C9A-N10	9.59	1.51	1.38

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1337	FAD	N3A-C2A-N1A	-8.55	121.41	128.86
5	B	1337	FAD	N3A-C2A-N1A	-8.29	121.64	128.86
5	A	1337	FAD	C5X-C9A-N10	-7.96	111.75	117.66
5	B	1337	FAD	C5X-C9A-N10	-7.93	111.77	117.66
5	B	1337	FAD	C4-C4X-C10	-6.08	115.04	119.96
5	A	1337	FAD	C4-C4X-C10	-6.00	115.11	119.96
3	A	1335	MTE	N3-C2-N1	-5.24	116.96	125.45
5	A	1337	FAD	C4X-C10-N10	-5.22	116.90	120.52
3	B	1335	MTE	N3-C2-N1	-5.19	117.03	125.45
5	B	1337	FAD	C4X-C10-N10	-5.11	116.97	120.52
6	A	1338	NAD	C1B-N9A-C4A	-5.02	117.96	126.64
6	B	1338	NAD	C1B-N9A-C4A	-4.87	118.21	126.64
3	B	1335	MTE	O3'-C7-C6	-4.80	105.76	108.96
3	A	1335	MTE	O3'-C7-C6	-4.57	105.92	108.96
6	A	1338	NAD	N3A-C2A-N1A	-3.66	125.67	128.86
6	B	1338	NAD	N3A-C2A-N1A	-3.65	125.68	128.86
5	A	1337	FAD	C4X-C4-N3	-3.55	118.43	123.48
5	B	1337	FAD	C4X-C4-N3	-3.42	118.62	123.48
5	B	1337	FAD	C4'-C3'-C2'	-2.72	107.55	113.41
5	A	1337	FAD	C4'-C3'-C2'	-2.61	107.78	113.41
5	B	1337	FAD	O3B-C3B-C4B	-2.59	103.53	111.09
5	A	1337	FAD	O3B-C3B-C4B	-2.53	103.69	111.09
5	B	1337	FAD	C8M-C8-C9	-2.52	114.03	120.34
5	A	1337	FAD	C8M-C8-C9	-2.51	114.05	120.34
5	A	1337	FAD	C1'-N10-C9A	-2.47	116.08	118.35
5	B	1337	FAD	C1'-N10-C9A	-2.42	116.12	118.35
5	B	1337	FAD	C4B-O4B-C1B	-2.30	107.32	109.77
5	A	1337	FAD	C4B-O4B-C1B	-2.12	107.51	109.77
5	B	1337	FAD	O4B-C4B-C5B	-2.06	102.44	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1337	FAD	O5'-C5'-C4'	-2.06	103.87	109.36
5	A	1337	FAD	O4B-C4B-C5B	-2.01	102.60	109.40
5	B	1337	FAD	O2'-C2'-C3'	2.01	114.09	109.09
8	B	1340	SAL	C3-C2-C1	2.02	123.65	120.36
5	A	1337	FAD	O2'-C2'-C3'	2.07	114.22	109.09
3	B	1335	MTE	C4-C9-C10	2.16	116.52	114.56
6	A	1338	NAD	O5B-PA-O1A	2.27	112.85	106.47
6	B	1338	NAD	O5B-PA-O1A	2.29	112.90	106.47
3	A	1335	MTE	C4-C9-C10	2.31	116.66	114.56
5	B	1337	FAD	C4A-C5A-N7A	2.31	111.65	109.41
5	A	1337	FAD	O3'-C3'-C4'	2.43	114.84	108.82
5	B	1337	FAD	O3'-C3'-C4'	2.44	114.85	108.82
5	A	1337	FAD	C4A-C5A-N7A	2.47	111.80	109.41
5	A	1337	FAD	C8M-C8-C7	3.41	127.88	120.72
5	B	1337	FAD	C8M-C8-C7	3.41	127.88	120.72
6	B	1338	NAD	C4B-O4B-C1B	3.57	113.57	109.77
3	B	1335	MTE	N8-C10-N1	3.63	123.93	116.90
3	A	1335	MTE	N8-C10-N1	3.63	123.93	116.90
6	A	1338	NAD	C4B-O4B-C1B	4.10	114.14	109.77
3	A	1335	MTE	C4-N3-C2	4.48	122.50	116.06
3	B	1335	MTE	C4-N3-C2	4.66	122.77	116.06
3	B	1335	MTE	N2-C2-N3	4.73	124.80	117.24
3	A	1335	MTE	N2-C2-N3	4.83	124.96	117.24
3	B	1335	MTE	C2-N1-C10	4.83	125.40	114.51
5	B	1337	FAD	C4X-N5-C5X	4.88	121.92	116.76
3	A	1335	MTE	C2-N1-C10	4.91	125.57	114.51
5	A	1337	FAD	C4X-N5-C5X	4.98	122.02	116.76
5	A	1337	FAD	C4-C4X-N5	5.61	124.83	118.68
5	B	1337	FAD	C4-C4X-N5	5.72	124.95	118.68
6	A	1338	NAD	O5B-C5B-C4B	7.69	136.26	109.00
6	B	1338	NAD	O5B-C5B-C4B	7.72	136.37	109.00
5	B	1337	FAD	C4-N3-C2	10.63	124.45	115.16
5	A	1337	FAD	C4-N3-C2	10.86	124.66	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1334	FES	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1335	MTE	2	0
4	A	1336	MOS	4	0
5	A	1337	FAD	2	0
8	A	1340	SAL	1	0
9	A	1345	GOL	1	0
9	A	1348	GOL	1	0
2	B	1334	FES	1	0
3	B	1335	MTE	2	0
4	B	1336	MOS	4	0
5	B	1337	FAD	2	0
8	B	1340	SAL	1	0
9	B	1344	GOL	1	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, 95th 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	1286/1332 (96%)	-0.12	32 (2%) 58 62	9, 18, 33, 53	0
1	B	1289/1332 (96%)	-0.07	31 (2%) 59 63	9, 18, 33, 52	0
All	All	2575/2664 (96%)	-0.10	63 (2%) 59 63	9, 18, 33, 53	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1325	CYS	7.2
1	A	1288	ASN	7.0
1	B	1288	ASN	6.8
1	A	61	LEU	6.8
1	B	1318	VAL	5.8
1	B	537	LYS	5.6
1	B	61	LEU	5.3
1	B	1319	THR	4.8
1	B	565	ASN	4.7
1	A	565	ASN	4.6
1	B	222	VAL	4.3
1	B	528	GLY	4.3
1	A	221	ASP	4.3
1	B	566	GLY	4.0
1	B	221	ASP	3.9
1	A	537	LYS	3.8
1	B	63	ASP	3.7
1	A	1290	THR	3.7
1	A	553	PRO	3.5
1	A	63	ASP	3.5
1	B	1326	LYS	3.5
1	A	1286	THR	3.4
1	A	223	PRO	3.3
1	A	566	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	378	GLY	3.2
1	B	552	ASP	3.2
1	A	1287	ASN	3.0
1	B	272	ASN	3.0
1	A	272	ASN	3.0
1	A	551	LYS	3.0
1	B	540	PRO	2.9
1	A	222	VAL	2.8
1	B	553	PRO	2.8
1	B	1290	THR	2.7
1	A	1316	LEU	2.7
1	B	1287	ASN	2.7
1	A	199	GLU	2.7
1	B	1286	THR	2.7
1	A	60	ARG	2.6
1	B	60	ARG	2.6
1	B	217	LEU	2.6
1	A	550	GLN	2.6
1	B	318	LYS	2.5
1	A	538	LEU	2.5
1	B	62	GLN	2.5
1	A	401	GLU	2.5
1	B	64	LYS	2.5
1	B	223	PRO	2.4
1	B	550	GLN	2.3
1	B	538	LEU	2.3
1	A	1143	GLU	2.3
1	B	569	LYS	2.3
1	A	318	LYS	2.3
1	A	989	LYS	2.3
1	A	133	GLU	2.2
1	A	400	PRO	2.2
1	A	982	SER	2.2
1	A	721	LYS	2.1
1	A	552	ASP	2.1
1	A	1317	CYS	2.1
1	A	317	ALA	2.0
1	B	133	GLU	2.0
1	A	1326	LYS	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, 95th 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
9	GOL	B	1343	6/6	0.71	0.28	29.71	50,52,53,54	0
9	GOL	A	1347	6/6	0.79	0.24	12.65	40,43,44,47	0
9	GOL	A	1342	6/6	0.64	0.32	12.09	44,46,47,49	0
9	GOL	A	1348	6/6	0.88	0.23	9.39	28,29,32,34	0
9	GOL	A	1343	6/6	0.77	0.20	8.18	35,39,40,41	0
9	GOL	B	1345	6/6	0.94	0.17	6.53	21,24,24,26	0
4	MOS	A	1336	4/4	0.99	0.12	4.13	21,23,24,30	0
6	NAD	A	1338	23/44	0.79	0.19	3.65	45,50,59,59	0
9	GOL	B	1341	6/6	0.93	0.15	3.58	17,21,23,24	0
6	NAD	B	1338	23/44	0.78	0.20	3.52	46,50,59,61	0
9	GOL	A	1341	6/6	0.94	0.12	2.86	16,18,18,19	0
4	MOS	B	1336	4/4	0.99	0.11	2.12	20,22,23,28	0
9	GOL	A	1344	6/6	0.84	0.14	2.09	35,38,39,39	0
8	SAL	B	1340	10/10	0.91	0.11	1.46	23,25,27,27	0
9	GOL	A	1345	6/6	0.90	0.15	1.17	30,33,34,35	0
9	GOL	B	1342	6/6	0.91	0.13	1.13	18,25,26,31	0
9	GOL	A	1346	6/6	0.91	0.14	0.78	25,30,30,31	0
8	SAL	A	1340	10/10	0.95	0.10	0.77	19,22,25,26	0
3	MTE	B	1335	24/24	0.97	0.09	0.50	13,17,19,20	0
9	GOL	B	1344	6/6	0.92	0.15	0.45	28,30,32,33	0
5	FAD	B	1337	53/53	0.97	0.09	-0.24	12,15,18,19	0
5	FAD	A	1337	53/53	0.97	0.09	-0.25	13,16,19,19	0
3	MTE	A	1335	24/24	0.97	0.08	-0.40	14,17,19,20	0
7	CO3	B	1339	4/4	0.98	0.07	-1.68	15,15,16,16	0
7	CO3	A	1339	4/4	0.99	0.07	-1.69	11,12,13,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FES	B	1333	4/4	0.99	0.04	-2.10	12,12,12,12	0
2	FES	B	1334	4/4	0.99	0.05	-2.23	11,11,11,12	0
2	FES	A	1333	4/4	0.99	0.04	-2.33	12,12,12,13	0
2	FES	A	1334	4/4	1.00	0.04	-2.37	11,12,12,13	0
10	CA	A	1349	1/1	1.00	0.05	-2.52	14,14,14,14	0
10	CA	B	1346	1/1	0.99	0.04	-4.21	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.