



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:14 am 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](mailto: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.

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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

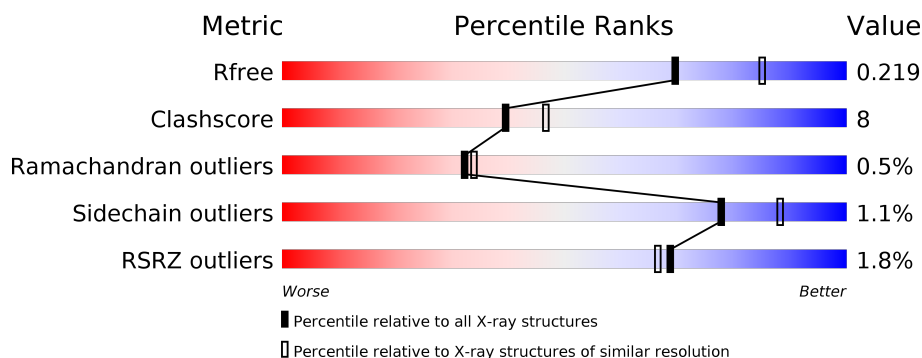
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (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  $\geq 3$ , 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>77%</div> <div>19%</div> <div>••</div> </div> </div>
1	B	1332	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>18%</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	-
4	MOS	B	1336	-	-	X	-
7	GOL	A	1341	-	-	-	X
7	GOL	B	1339	-	-	-	X

## 2 Entry composition [i](#)

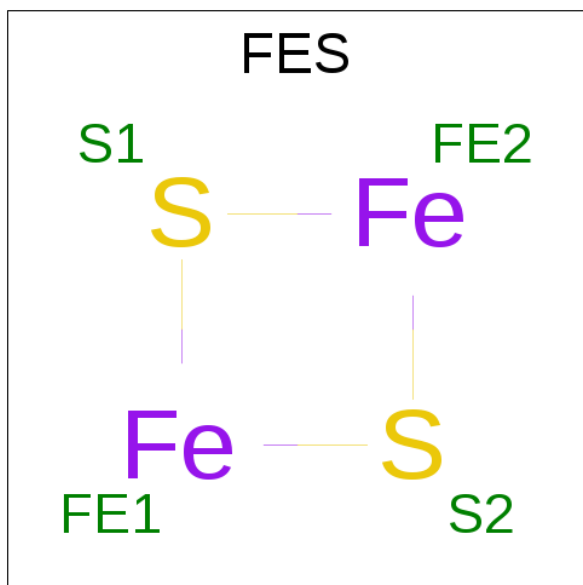
There are 11 unique types of molecules in this entry. The entry contains 21491 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

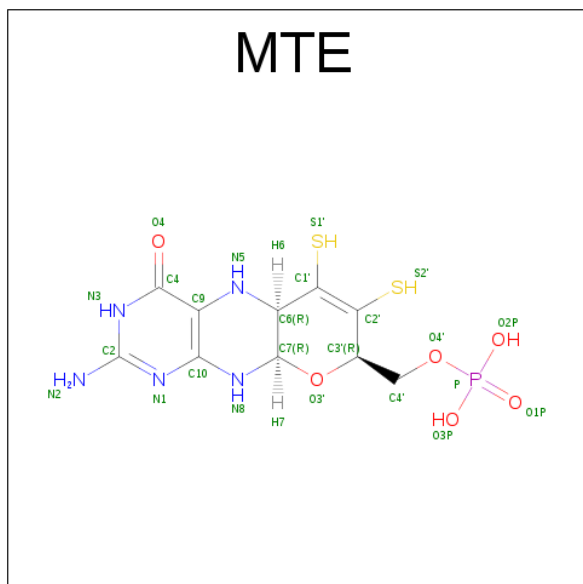
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1289	Total	C	N	O	S	0	0	0
			10003	6360	1712	1871	60			
1	B	1288	Total	C	N	O	S	0	0	0
			9998	6357	1711	1870	60			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



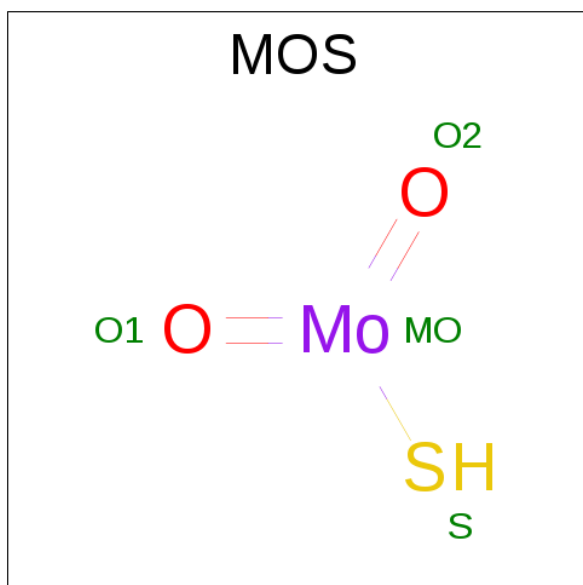
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

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



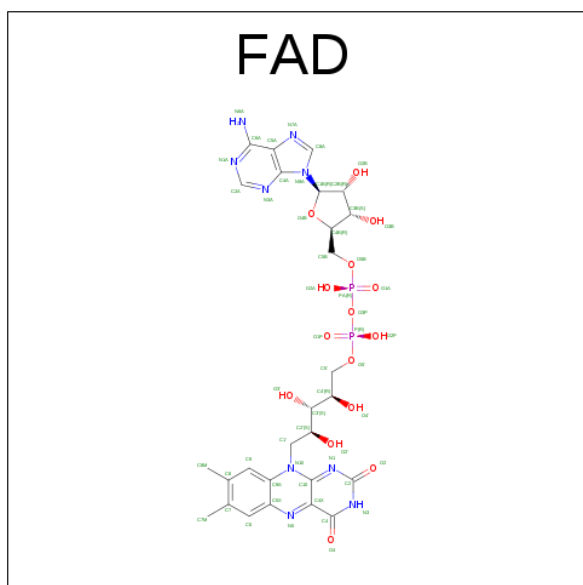
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

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



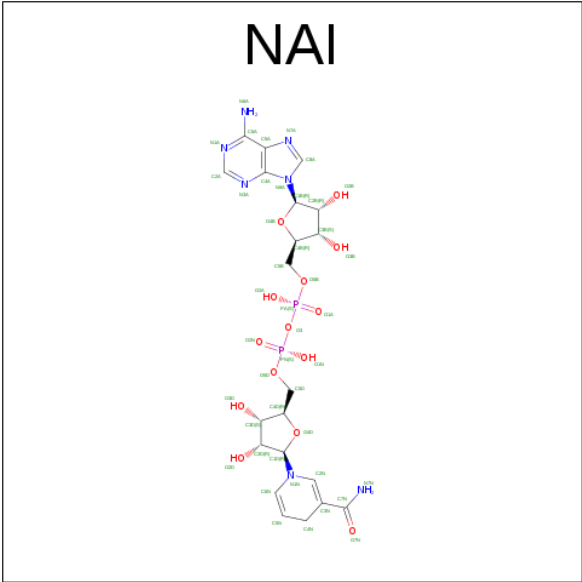
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
4	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

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



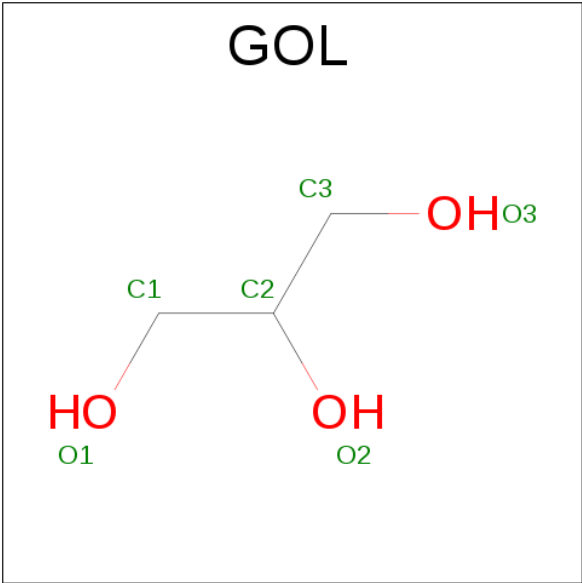
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0
			53	27	9	15	2	0
5	B	1	Total	C	N	O	P	0
			53	27	9	15	2	0

- 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<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



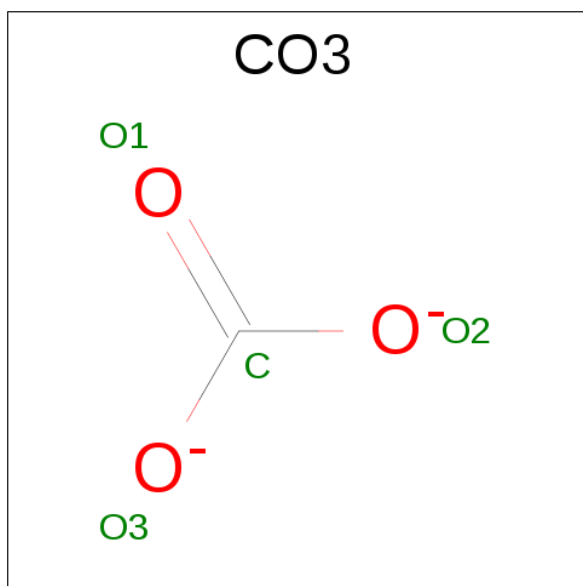
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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

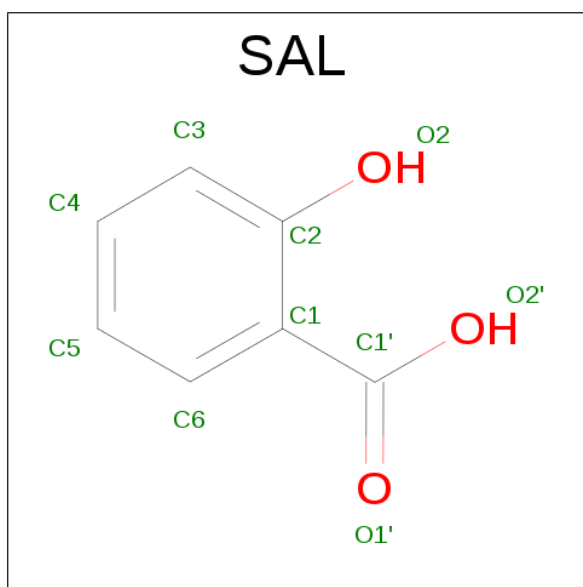
- Molecule 8 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



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

- Molecule 9 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: C<sub>7</sub>H<sub>6</sub>O<sub>3</sub>).





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

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

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

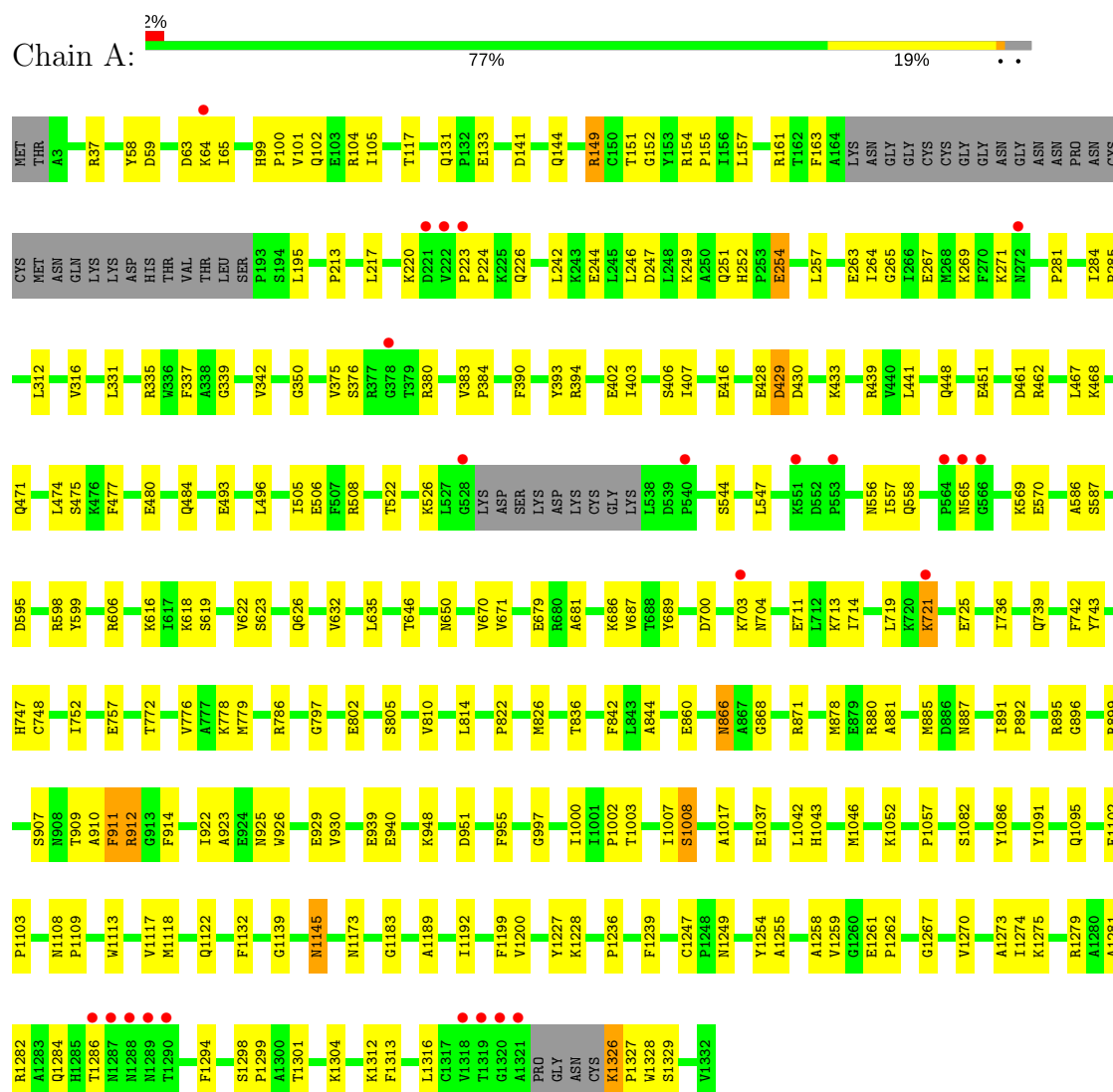
- Molecule 11 is water.

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

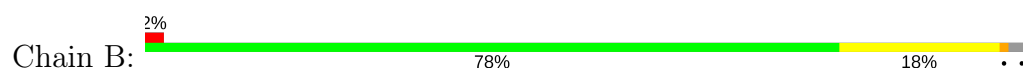
### 3 Residue-property plots

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



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Q1284	H1285	T1286	N1287	N1288	N1289	T1290	T1301	I1305	K1312	T1315	L1316	G1317	V1318	T1319	G1320	ALA	PRO	GLY	ASN	CYS	K1326	P1327	V1332																						
A1078	V1081	S1082	T1085	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										
G913	F914	I922	A923	W926	V930	A931	V932	K948	E949	G950	D951	L952	F955	R958	L959	E960	V964	P965	A1189	I1192	F1199	V1200	F1206	I1235	F1239	C1247	P1248	N1249	I1253	Y1254	A1255	V1259	P1262	P1263	G1267	A1268	S1269	V1270	I1274	R1279					
T772	Q773	V776	A777	K778	V784	G797	N650	T653	R654	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					
V628	L635	D639	N644	E645	T646	N650	T653	R654	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						
Q443	S446	E451	L474	S475	F501	M504	I505	E506	F507	R508	F519	V523	G528	L538	T541	G550	K551	D552	P553	Q558	N565	G566	K569	D595	Y599	E600	R601	L602	F604	L605	R606	K618													
I279	I284	P285	V308	E309	T311	L312	L313	A314	A315	V316	K318	T321	R328	L331	R335	R336	F337	A338	G339	L348	M366	H387	T388	F389	L397	E401	E402	I403	I407	E416	S419	S425	D429	K433	R439	V440	L441	F442							
GLY	ASN	GLY	ASN	ASN	PRO	ASN	CYS	K310	MET	ASN	GLN	LYS	LYS	ASP	HIS	THR	VAL	THR	LEU	SER	P193	S194	L195	F196	N197	E200	L217	K220	D221	V222	P223	Q226	L227	R228	W236	I237	Q251	A255	E263	I264	E267	N268	K271	N272	Q273
MET	THR	A3	D4	E5	K18	R32	R37	D59	D63	K64	I65	H81	H82	I91	H99	P100	R104	C113	T117	P118	Q131	P132	E133	P134	T135	E138	D141	Q144	C150	T151	G152	Y153	R154	P155	A164	LYS	ASN	GLY	GLY	CYS	CYS	GLY			

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	2211 reflections (1.56%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21491	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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(°)	Ideal(°)
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 [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	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
4:B:1336:MOS:MO	4:B:1336:MOS:O2	1.68	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:GLU:HA	1:B:271:LYS:HG2	1.80	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:A:1249:ASN:O	1:A:1255:ALA:HA	1.97	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: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:100:PRO:O	1:A:104:ARG:HG3	2.05	0.56
1:A:149:ARG:HG3	1:A:742:PHE:O	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:1282:ARG:O	1:A:1286:THR:HB	2.09	0.53
1:A:1082:SER:HB2	3:A:1335:MTE:O3P	2.08	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:247:ASP:HB3	1:A:251:GLN:NE2	2.24	0.52
1:A:739:GLN:HG2	1:A:911:PHE:CE1	2.44	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: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:863:HIS:O	1:B:898:GLY:HA2	2.11	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:A:948:LYS:HG2	1:A:951:ASP:OD2	2.10	0.51
1:B:443:GLN:HB2	1:B:446:SER:OG	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:814:LEU:C	1:A:814:LEU:HD13	2.32	0.50
1:A:911:PHE:O	1:A:912:ARG:C	2.49	0.50
1:B:1279:ARG:NH2	1:B:1290:THR:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LEU:HB2	1:B:331:LEU:HD21	1.93	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:1007:ILE:O	1:A:1008:SER:CB	2.60	0.50
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.75	0.50
1:A:390:PHE:HB3	11:A:1552:HOH:O	2.10	0.50
1:A:719:LEU:HD11	1:A:895:ARG:HB3	1.93	0.50
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.47	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:197:ASN:ND2	1:B:200:GLU:HG3	2.27	0.49
1:B:711:GLU:HA	1:B:899:ARG:CD	2.42	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:1017:ALA:HB1	1:A:1086:TYR:CD2	2.48	0.49
1:A:544:SER:HA	1:A:547:LEU:HD12	1.93	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: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:1007:ILE:HG22	1:B:1081:VAL:HG12	1.95	0.48
1:A:430:ASP:CG	1:A:1228:LYS:HE2	2.34	0.48
1:B:1082:SER:HB2	3:B:1335:MTE:O3P	2.14	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:A:721:LYS:NZ	1:A:721:LYS:HB3	2.29	0.47
1:B:506:GLU:H	1:B:506:GLU:CD	2.17	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: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:670:VAL:HG11	1:B:681:ALA:HB3	1.95	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:B:646:THR:O	1:B:650:ASN:HA	2.14	0.47
1:A:154:ARG:N	1:A:155:PRO:HD2	2.30	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: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: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:955:PHE:HA	1:B:1145:ASN:ND2	2.12	0.47
1:B:1279:ARG:NH1	1:B:1279:ARG:HG3	2.28	0.47
1:B:335:ARG:HH21	1:B:551:LYS:NZ	2.13	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:A:416:GLU:OE1	1:A:439:ARG:HD2	2.16	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:B:660:VAL:HA	1:B:665:HIS:ND1	2.31	0.46
1:B:949:GLU:OE2	1:B:960:GLU:HA	2.16	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:255:ALA:HB1	1:B:279:ILE:HG13	1.97	0.45
1:B:700:ASP:HA	1:B:703:LYS:NZ	2.32	0.45
1:A:242:LEU:O	1:A:246:LEU:HG	2.16	0.45
1:A:885:MET:SD	1:A:896:GLY:HA3	2.56	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:A:342:VAL:HG23	11:A:1746:HOH:O	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:B:135:THR:OG1	1:B:138:GLU:HG3	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:144:GLN:HB2	1:B:339:GLY:HA2	1.99	0.45
1:B:403:ILE:C	1:B:403:ILE:HD13	2.37	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: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:195:LEU:HD22	1:B:1189:ALA:HA	1.99	0.45
1:A:1312:LYS:HE3	1:A:1313:PHE:CZ	2.52	0.44
1:A:725:GLU:HG2	1:A:725:GLU:O	2.16	0.44
1:B:1045:LYS:O	1:B:1049:VAL:HG23	2.17	0.44
1:B:141:ASP:O	1:B:144:GLN:HG3	2.17	0.44
1:A:312:LEU:O	1:A:316:VAL:HG23	2.17	0.44
1:A:997:GLY:HA3	1:A:1273:ALA:O	2.17	0.44
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.65	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:376:SER:HB3	1:A:402:GLU:HG2	1.99	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: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:A:1108:ASN:N	1:A:1109:PRO:HD3	2.33	0.44
1:B:154:ARG:N	1:B:155:PRO:HD2	2.33	0.44
1:A:496:LEU:HB2	1:A:505:ILE:HG23	1.99	0.44
1:A:736:ILE:HG23	1:A:736:ILE:O	2.18	0.44
1:B:315:ALA:HA	1:B:318:LYS:NZ	2.31	0.44
1:B:657:LYS:O	1:B:658:ASP:HB2	2.18	0.44
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.32	0.44
1:A:1000:ILE:O	1:A:1000:ILE:HG23	2.17	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:B:519:PHE:O	1:B:523:VAL:HG23	2.18	0.43
1:A:1281:ALA:O	1:A:1284:GLN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:C	1:A:154:ARG:HD2	2.38	0.43
1:A:779:MET:HG3	1:A:810:VAL:CG1	2.48	0.43
1:A:736:ILE:CG2	1:A:842:PHE:HB2	2.48	0.43
1:B:721:LYS:HD2	1:B:721:LYS:O	2.18	0.43
1:A:117:THR:CG2	1:A:586:ALA:HA	2.48	0.43
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.00	0.43
1:A:772:THR:O	1:A:776:VAL:HG23	2.19	0.43
1:A:226:GLN:HB2	1:A:244:GLU:OE1	2.18	0.43
1:A:383:VAL:HA	1:A:384:PRO:HD3	1.91	0.43
1:B:844:ALA:HB2	1:B:922:ILE:HD13	2.01	0.43
1:A:254:GLU:H	1:A:254:GLU:CD	2.21	0.43
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.84	0.43
1:A:616:LYS:O	1:A:689:TYR:HA	2.18	0.43
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.54	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:228:ARG:HG3	1:B:237:ILE:CD1	2.49	0.43
1:A:267:GLU:HA	1:A:271:LYS:HB2	1.99	0.43
1:B:1008:SER:HA	1:B:1081:VAL:HG11	2.01	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:152:GLY:CA	1:A:1200:VAL:HG21	2.47	0.43
1:A:284:ILE:HA	1:A:285:PRO:HD3	1.88	0.43
1:A:522:THR:HG22	1:A:526:LYS:HE3	2.00	0.43
1:A:752:ILE:HD13	1:A:822:PRO:HB3	2.00	0.43
1:A:844:ALA:CB	1:A:922:ILE:HD13	2.47	0.43
1:B:1017:ALA:HB1	1:B:1086:TYR:CE2	2.54	0.43
1:B:731:SER:OG	1:B:847:LYS:HG3	2.19	0.43
1:B:1113:TRP:O	1:B:1117:VAL:HG23	2.19	0.43
1:B:802:GLU:HG2	1:B:803:THR:HG23	2.01	0.43
1:B:217:LEU:O	1:B:220:LYS:HG2	2.19	0.42
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: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:37:ARG:HD2	1:A:595:ASP:O	2.19	0.42
1:A:868:GLY:HA3	1:A:907:SER:HA	2.02	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:1259:VAL:O	1:B:1259:VAL:HG22	2.18	0.42
1:B:850:PHE:CD2	1:B:850:PHE:N	2.87	0.42
1:B:1012:PRO:HB2	11:B:1817:HOH:O	2.18	0.42
1:B:331:LEU:O	1:B:335:ARG:HG3	2.20	0.42
1:A:1132:PHE:CD1	1:B:1126:SER:HB2	2.55	0.42
1:A:878:MET:O	1:A:881:ALA:HB3	2.19	0.42
1:B:747:HIS:ND1	1:B:805:SER:HA	2.35	0.42
1:A:1007:ILE:HD12	1:A:1258:ALA:HB3	2.01	0.42
1:A:102:GLN:NE2	1:A:587:SER:HA	2.35	0.42
1:A:909:THR:OG1	1:A:910:ALA:N	2.51	0.42
1:B:1031:VAL:HB	1:B:1063:ILE:HG12	2.01	0.42
1:B:117:THR:HB	1:B:118:PRO:HD3	2.01	0.42
1:B:905:LEU:O	1:B:906:SER:C	2.56	0.42
1:A:1173:ASN:O	1:A:1236:PRO:HA	2.19	0.42
1:A:912:ARG:N	4:A:1336:MOS:S	2.93	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: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:712:LEU:HD21	1:B:879:GLU:HG3	2.02	0.41
1:B:952:LEU:HD23	1:B:958:ARG:HA	2.01	0.41
1:A:105:ILE:HA	11:A:1766:HOH:O	2.20	0.41
1:A:1199:PHE:CE1	1:A:1267:GLY:HA2	2.55	0.41
1:A:891:ILE:HA	1:A:892:PRO:HD2	1.87	0.41
1:B:748:CYS:HB2	1:B:826:MET:HG3	2.02	0.41
1:B:926:TRP:O	1:B:930:VAL:HG23	2.20	0.41
1:A:1328:TRP:CE3	1:A:1329:SER:HB3	2.55	0.41
1:A:403:ILE:HD12	1:A:403:ILE:C	2.39	0.41
1:A:721:LYS:HD2	1:A:721:LYS:O	2.21	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:802:GLU:OE1	9:A:1344:SAL:H3	2.20	0.41
1:A:866:ASN:C	1:A:866:ASN:HD22	2.23	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:B:91:ILE:O	1:B:99:HIS:HB2	2.20	0.41
1:A:598:ARG:HG3	1:B:600:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:SER:HA	1:A:626:GLN:HE21	1.86	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:152:GLY:HA2	1:B:1200:VAL:HG21	2.03	0.41
1:B:5:GLU:OE2	1:B:18:LYS:HE2	2.21	0.41
1:A:632:VAL:HB	1:A:671:VAL:O	2.21	0.41
1:B:1326:LYS:CG	1:B:1327:PRO:HD2	2.50	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:A:468:LYS:HB2	1:A:493:GLU:OE2	2.21	0.41
1:A:899:ARG:HA	1:A:899:ARG:HD2	1.91	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:A:471:GLN:NE2	1:A:471:GLN:HA	2.36	0.40
1:B:100:PRO:O	1:B:104:ARG:HG3	2.22	0.40
1:B:1286:THR:CG2	1:B:1287:ASN:N	2.78	0.40
1:A:887:ASN:OD1	1:A:1003:THR:HA	2.21	0.40
1:A:428:GLU:O	1:A:429:ASP:C	2.60	0.40
1:B:81:HIS:O	1:B:82:HIS:HB2	2.21	0.40
1:A:1259:VAL:O	1:A:1259:VAL:HG22	2.20	0.40
1:A:433:LYS:HA	1:A:433:LYS:HD3	1.91	0.40
1:A:570:GLU:OE2	1:A:1057:PRO:HG3	2.21	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:B:64:LYS:CB	1:B:64:LYS:NZ	2.84	0.40
1:A:350:GLY:C	5:A:1337:FAD:H5'1	2.42	0.40
1:A:925:ASN:O	1:A:929:GLU:HG3	2.21	0.40
1:B:271:LYS:HB2	1:B:273:GLN:HG2	2.02	0.40
1:B:32:ARG:NH2	1:B:676:GLU:OE2	2.54	0.40
1:B:1021:ILE:HD12	1:B:1093:ALA:HB3	2.03	0.40
1:B:152:GLY:O	1:B:1235:ILE:HG21	2.22	0.40
1:B:912:ARG:N	4:B:1336:MOS:S	2.95	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%)	32	34
1	B	1280/1332 (96%)	1228 (96%)	46 (4%)	6 (0%)	32	34
All	All	2561/2664 (96%)	2457 (96%)	92 (4%)	12 (0%)	32	34

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%)	75	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1092/1128 (97%)	1080 (99%)	12 (1%)	78	88
All	All	2184/2256 (97%)	2159 (99%)	25 (1%)	78	88

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

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	21,26,26	2.47	7 (33%)	19,40,40	2.72	7 (36%)
4	MOS	A	1336	3	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	A	1337	-	51,58,58	3.02	19 (37%)	54,89,89	2.93	16 (29%)
6	NAI	A	1338	-	40,48,48	1.18	3 (7%)	41,73,73	1.85	3 (7%)
7	GOL	A	1339	-	5,5,5	0.39	0	5,5,5	0.33	0
7	GOL	A	1340	-	5,5,5	0.20	0	5,5,5	0.16	0
7	GOL	A	1341	-	5,5,5	0.35	0	5,5,5	0.36	0
7	GOL	A	1342	-	5,5,5	0.41	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	1.78	3 (42%)	9,13,13	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	21,26,26	2.48	7 (33%)	19,40,40	2.74	8 (42%)
4	MOS	B	1336	3	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	B	1337	-	51,58,58	2.98	19 (37%)	54,89,89	2.95	15 (27%)
6	NAI	B	1338	-	40,48,48	1.19	2 (5%)	41,73,73	1.85	3 (7%)
7	GOL	B	1339	-	5,5,5	0.29	0	5,5,5	0.22	0
7	GOL	B	1340	-	5,5,5	0.40	0	5,5,5	0.35	0
7	GOL	B	1341	-	5,5,5	0.28	0	5,5,5	0.31	0
7	GOL	B	1342	-	5,5,5	0.33	0	5,5,5	0.29	0
7	GOL	B	1343	-	5,5,5	0.33	0	5,5,5	0.32	0
8	CO3	B	1344	-	0,3,3	0.00	-	0,3,3	0.00	-
9	SAL	B	1345	-	7,10,10	1.93	3 (42%)	9,13,13	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	-	-	0/28/50/50	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	-	-	0/28/50/50	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	-3.74	1.41	1.49
6	B	1338	NAI	C4N-C5N	-3.56	1.41	1.49
5	A	1337	FAD	C2B-C1B	-2.41	1.49	1.53
5	B	1337	FAD	C2B-C1B	-2.00	1.50	1.53
9	A	1344	SAL	C3-C2	2.13	1.43	1.39
3	A	1335	MTE	C7-C6	2.14	1.55	1.53
6	A	1338	NAI	O4B-C1B	2.20	1.44	1.41
9	A	1344	SAL	C6-C1	2.27	1.43	1.39
9	B	1345	SAL	C3-C2	2.41	1.43	1.39
9	B	1345	SAL	C6-C1	2.45	1.43	1.39
3	A	1335	MTE	C4-N3	2.79	1.38	1.33
5	B	1337	FAD	C5A-C4A	2.86	1.47	1.40
5	A	1337	FAD	C6-C5X	2.87	1.46	1.41
5	A	1337	FAD	C5A-C4A	2.87	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1335	MTE	C9-C10	2.97	1.47	1.41
3	B	1335	MTE	C4-N3	2.99	1.38	1.33
9	A	1344	SAL	C5-C6	3.00	1.44	1.38
3	B	1335	MTE	C9-C10	3.00	1.47	1.41
3	B	1335	MTE	C7-C6	3.00	1.55	1.53
5	A	1337	FAD	C9-C9A	3.07	1.47	1.40
9	B	1345	SAL	C5-C6	3.14	1.44	1.38
5	B	1337	FAD	C6-C5X	3.19	1.46	1.41
5	B	1337	FAD	C9-C9A	3.40	1.48	1.40
5	A	1337	FAD	C9A-C5X	3.49	1.49	1.42
5	B	1337	FAD	O4B-C4B	3.49	1.52	1.45
5	B	1337	FAD	C4X-N5	3.57	1.38	1.33
5	B	1337	FAD	C9A-C5X	3.60	1.50	1.42
5	B	1337	FAD	C2-N3	3.65	1.45	1.38
5	A	1337	FAD	C4X-N5	3.68	1.38	1.33
5	B	1337	FAD	C4-C4X	3.73	1.48	1.41
5	A	1337	FAD	C8-C7	3.74	1.50	1.41
5	A	1337	FAD	C2-N3	3.80	1.45	1.38
5	B	1337	FAD	C8-C7	3.83	1.50	1.41
3	B	1335	MTE	O3'-C7	3.85	1.49	1.43
6	A	1338	NAI	C6N-C5N	3.95	1.40	1.33
5	A	1337	FAD	O4B-C4B	3.99	1.54	1.45
5	A	1337	FAD	C4-C4X	4.02	1.49	1.41
5	B	1337	FAD	C2A-N1A	4.10	1.41	1.33
3	A	1335	MTE	O3'-C7	4.12	1.49	1.43
3	A	1335	MTE	O4-C4	4.15	1.35	1.24
3	B	1335	MTE	O4-C4	4.18	1.35	1.24
5	A	1337	FAD	C2A-N1A	4.21	1.41	1.33
6	B	1338	NAI	C6N-C5N	4.29	1.41	1.33
5	B	1337	FAD	C2A-N3A	4.41	1.39	1.32
5	A	1337	FAD	C5X-N5	4.47	1.42	1.35
5	A	1337	FAD	C2A-N3A	4.55	1.39	1.32
5	B	1337	FAD	C4-N3	4.68	1.41	1.33
5	A	1337	FAD	C4-N3	4.70	1.41	1.33
5	B	1337	FAD	C4A-N3A	4.87	1.42	1.35
5	B	1337	FAD	C5X-N5	4.99	1.43	1.35
3	B	1335	MTE	C9-N5	5.01	1.49	1.37
5	A	1337	FAD	C4A-N3A	5.03	1.43	1.35
3	A	1335	MTE	C9-N5	5.19	1.49	1.37
5	A	1337	FAD	C10-N1	5.34	1.40	1.33
5	B	1337	FAD	C10-N1	5.37	1.40	1.33
5	A	1337	FAD	C4X-C10	5.61	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1337	FAD	C4X-C10	5.66	1.51	1.41
3	B	1335	MTE	O3'-C3'	5.75	1.51	1.43
3	A	1335	MTE	O3'-C3'	5.96	1.52	1.43
5	B	1337	FAD	O4B-C1B	7.47	1.51	1.41
5	A	1337	FAD	O4B-C1B	7.91	1.52	1.41
5	B	1337	FAD	C9A-N10	9.61	1.51	1.38
5	A	1337	FAD	C9A-N10	9.85	1.51	1.38

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1338	NAI	N3A-C2A-N1A	-9.48	120.60	128.86
6	A	1338	NAI	N3A-C2A-N1A	-9.34	120.72	128.86
5	A	1337	FAD	N3A-C2A-N1A	-8.50	121.45	128.86
5	B	1337	FAD	N3A-C2A-N1A	-8.36	121.58	128.86
5	B	1337	FAD	C5X-C9A-N10	-7.86	111.82	117.66
5	A	1337	FAD	C5X-C9A-N10	-7.58	112.03	117.66
5	B	1337	FAD	C4-C4X-C10	-6.14	115.00	119.96
5	A	1337	FAD	C4-C4X-C10	-5.95	115.14	119.96
3	B	1335	MTE	N3-C2-N1	-5.41	116.69	125.45
3	A	1335	MTE	N3-C2-N1	-5.32	116.82	125.45
5	A	1337	FAD	C4X-C10-N10	-5.07	117.00	120.52
5	B	1337	FAD	C4X-C10-N10	-4.89	117.12	120.52
6	B	1338	NAI	O4D-C1D-N1N	-4.54	98.92	108.07
6	A	1338	NAI	O4D-C1D-N1N	-4.42	99.16	108.07
3	A	1335	MTE	O3'-C7-C6	-3.83	106.41	108.96
3	B	1335	MTE	O3'-C7-C6	-3.70	106.50	108.96
5	A	1337	FAD	C4X-C4-N3	-3.39	118.65	123.48
5	B	1337	FAD	C4X-C4-N3	-3.35	118.72	123.48
5	B	1337	FAD	C1'-N10-C9A	-2.61	115.95	118.35
5	B	1337	FAD	C8M-C8-C9	-2.60	113.81	120.34
6	A	1338	NAI	C3N-C2N-N1N	-2.60	119.31	123.08
5	B	1337	FAD	O3B-C3B-C4B	-2.54	103.67	111.09
5	A	1337	FAD	C8M-C8-C9	-2.53	113.99	120.34
5	A	1337	FAD	C4B-O4B-C1B	-2.45	107.17	109.77
6	B	1338	NAI	C3N-C2N-N1N	-2.43	119.55	123.08
5	A	1337	FAD	C1'-N10-C9A	-2.43	116.12	118.35
5	A	1337	FAD	O3B-C3B-C4B	-2.41	104.05	111.09
5	B	1337	FAD	O4B-C4B-C5B	-2.10	102.31	109.40
5	A	1337	FAD	C4'-C3'-C2'	-2.01	109.08	113.41
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1337	FAD	O3'-C3'-C4'	2.34	114.62	108.82
3	B	1335	MTE	P-O4'-C4'	2.36	124.80	118.30
5	B	1337	FAD	C4A-C5A-N7A	2.37	111.70	109.41
5	A	1337	FAD	C4A-C5A-N7A	2.42	111.75	109.41
5	A	1337	FAD	O3'-C3'-C4'	2.47	114.94	108.82
5	A	1337	FAD	C8M-C8-C7	3.51	128.08	120.72
3	A	1335	MTE	N8-C10-N1	3.55	123.77	116.90
5	B	1337	FAD	C8M-C8-C7	3.59	128.25	120.72
3	B	1335	MTE	N8-C10-N1	3.70	124.07	116.90
3	B	1335	MTE	C4-N3-C2	4.66	122.77	116.06
3	A	1335	MTE	C4-N3-C2	4.70	122.82	116.06
3	B	1335	MTE	N2-C2-N3	4.80	124.92	117.24
5	B	1337	FAD	C4X-N5-C5X	4.81	121.84	116.76
3	B	1335	MTE	C2-N1-C10	4.87	125.48	114.51
3	A	1335	MTE	N2-C2-N3	4.92	125.10	117.24
3	A	1335	MTE	C2-N1-C10	4.92	125.60	114.51
5	A	1337	FAD	C4X-N5-C5X	5.06	122.10	116.76
5	A	1337	FAD	C4-C4X-N5	5.68	124.91	118.68
5	B	1337	FAD	C4-C4X-N5	5.82	125.06	118.68
5	A	1337	FAD	C4-N3-C2	10.52	124.36	115.16
5	B	1337	FAD	C4-N3-C2	10.83	124.63	115.16

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1289/1332 (96%)	-0.28	24 (1%) 67 65	7, 22, 40, 65	0
1	B	1288/1332 (96%)	-0.27	23 (1%) 69 66	7, 23, 39, 65	0
All	All	2577/2664 (96%)	-0.27	47 (1%) 69 66	7, 22, 40, 65	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1288	ASN	7.5
1	A	1288	ASN	6.6
1	A	565	ASN	5.4
1	A	1286	THR	4.7
1	B	223	PRO	4.5
1	A	1320	GLY	4.4
1	B	1287	ASN	4.4
1	B	1286	THR	4.3
1	A	1290	THR	4.0
1	A	1318	VAL	3.8
1	A	1321	ALA	3.6
1	A	221	ASP	3.4
1	A	272	ASN	3.3
1	B	1290	THR	3.3
1	B	1318	VAL	3.1
1	A	1319	THR	3.0
1	A	223	PRO	3.0
1	A	378	GLY	2.9
1	B	1319	THR	2.8
1	B	566	GLY	2.7
1	A	553	PRO	2.6
1	B	852	LYS	2.6
1	B	553	PRO	2.5
1	A	222	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1320	GLY	2.5
1	A	551	LYS	2.5
1	A	540	PRO	2.4
1	B	221	ASP	2.4
1	A	564	PRO	2.4
1	A	566	GLY	2.4
1	B	222	VAL	2.4
1	B	272	ASN	2.4
1	B	271	LYS	2.3
1	A	1289	ASN	2.3
1	B	64	LYS	2.3
1	B	565	ASN	2.2
1	A	1287	ASN	2.2
1	A	721	LYS	2.1
1	A	703	LYS	2.1
1	B	550	GLN	2.1
1	B	551	LYS	2.1
1	B	1289	ASN	2.1
1	A	64	LYS	2.1
1	B	63	ASP	2.1
1	A	528	GLY	2.1
1	B	703	LYS	2.0
1	B	724	SER	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<sup>th</sup> 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( $\text{\AA}^2$ )	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
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
7	GOL	B	1343	6/6	0.94	0.13	-0.11	30,33,35,38	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 [i](#)

There are no such residues in this entry.