



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:18 PM GMT

PDB ID : 3AX9  
Title : Bovine xanthine oxidase, protease cleaved form  
Authors : Ishikita, H.; Eger, B.T.; Pai, E.F.; Okamoto, K.; Nishino, T.  
Deposited on : 2011-03-31  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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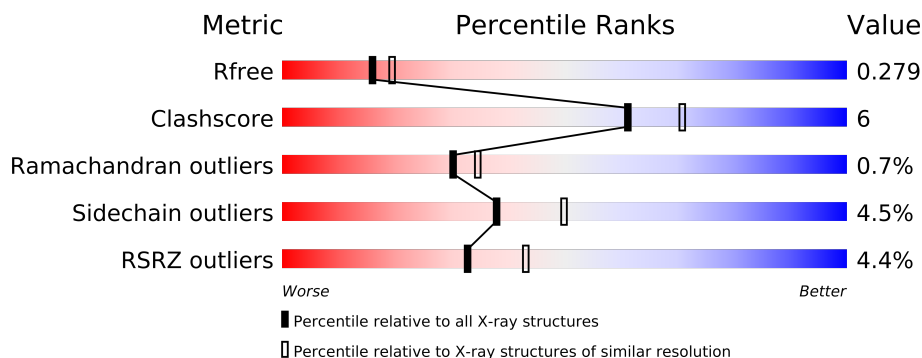
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1332	
1	B	1332	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	GOL	A	1338	-	X
7	GOL	B	1338	-	X
8	SAL	A	1341	-	X
8	SAL	B	1340	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19797 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

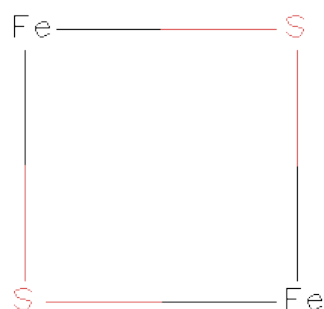
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1225	Total	C	N	O	S	0	0	0
			9476	6013	1632	1771	60			
1	B	1218	Total	C	N	O	S	0	0	0
			9433	5988	1623	1763	59			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	HIS	ASP	CONFLICT	UNP P80457
B	552	HIS	ASP	CONFLICT	UNP P80457

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



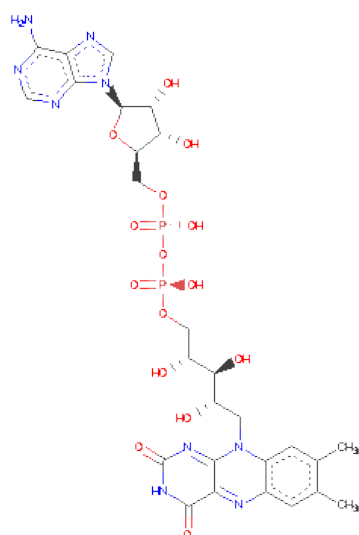
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		

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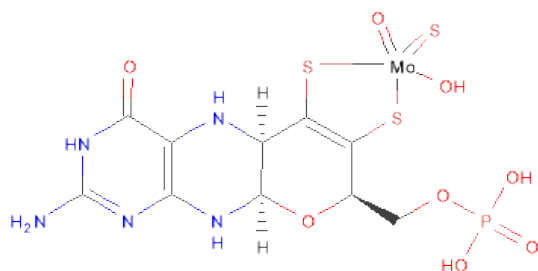
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 4 is {[ (5AR,8R,9AR)-2-AMINO-4-OXO-6,7-DI(SULFANYL-KAPPAS)-3,5,5A,8,9A,10-HEXAHYDRO-4H-PYRANO[3,2-G]PTERIDIN-8-YL]METHYLDIHYDROGENATO(2-) PHOSPHATE}(HYDROXY)OXO(THIOXO)MOLYBDENUM (three-letter code: XAX) (formula:  $C_{10}H_{13}MoN_5O_8PS_3$ ).

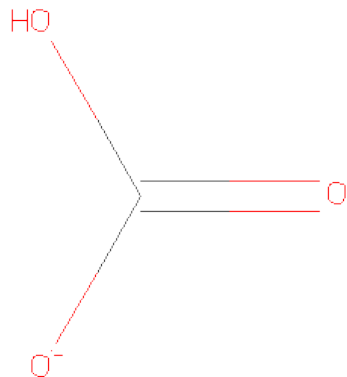


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
4	B	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



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

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



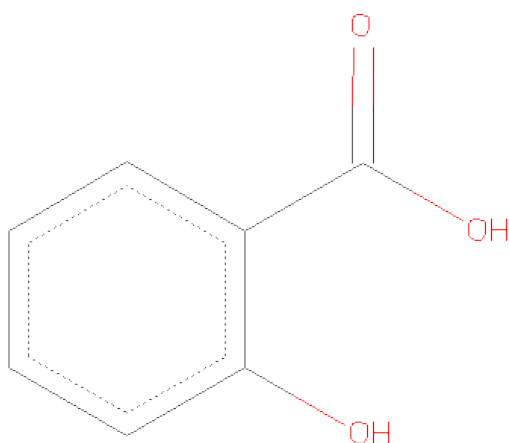
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 8 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
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 water.

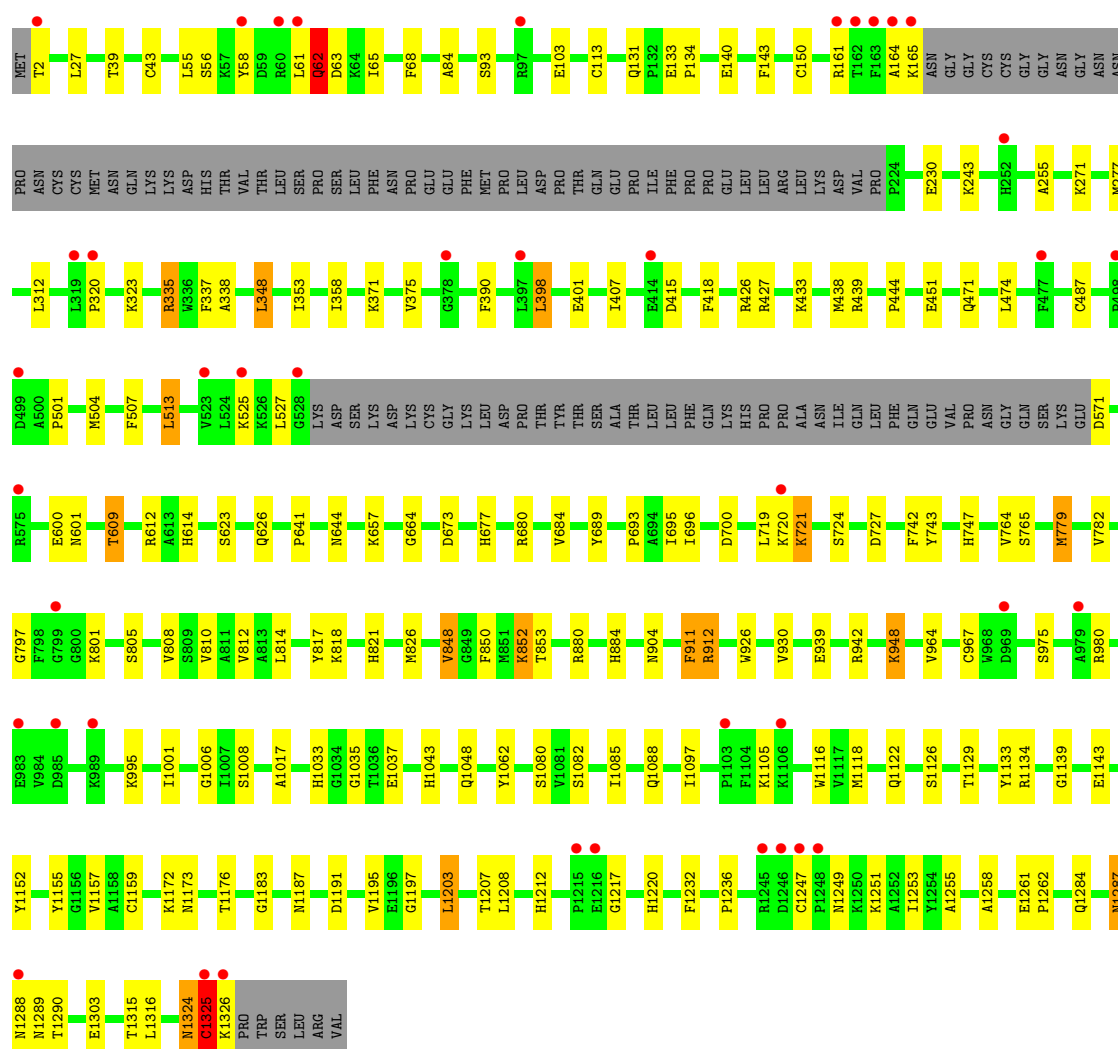
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	367	Total	O	0	0
			367	367		
9	B	283	Total	O	0	0
			283	283		

### 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 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: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.20Å 72.97Å 142.26Å 90.00° 98.84° 90.00°	Depositor
Resolution (Å)	38.13 – 2.30 38.14 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.13-2.30) 99.3 (38.14-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.59 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.215 , 0.279 0.217 , 0.279	Depositor DCC
$R_{free}$ test set	5953 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 26.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 118829 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	19797	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAX, GOL, SAL, CA, FES, BCT, FAD

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	0.71	0/9675	0.75	3/13085 (0.0%)
1	B	0.67	0/9631	0.73	6/13026 (0.0%)
All	All	0.69	0/19306	0.74	9/26111 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	839	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	B	839	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	513	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	398	LEU	CA-CB-CG	5.65	128.29	115.30
1	B	1203	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	398	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	942	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	1325	CYS	N-CA-C	5.05	124.63	111.00
1	A	942	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9476	0	9483	112	0
1	B	9433	0	9440	113	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	53	0	31	1	0
3	B	53	0	31	2	0
4	A	28	0	10	1	0
4	B	28	0	10	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	18	0	24	1	0
7	B	12	0	16	0	0
8	A	10	0	5	0	0
8	B	10	0	4	1	0
9	A	367	0	0	5	0
9	B	283	0	0	5	0
All	All	19797	0	19054	222	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (222) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:884:HIS:HE1	1:A:1006:GLY:H	1.17	0.92
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	1.68	0.92
1:A:995:LYS:HZ1	1:A:1284:GLN:HE21	1.20	0.89
1:A:131:GLN:HE21	1:A:133:GLU:H	1.18	0.89
1:A:695:ILE:H	1:A:904:ASN:HD22	1.21	0.88
1:B:884:HIS:HE1	1:B:1006:GLY:H	1.25	0.84
1:B:720:LYS:O	1:B:721:LYS:HB2	1.77	0.84
1:B:764:VAL:HG22	1:B:766:THR:HG22	1.66	0.76
1:B:764:VAL:CG2	1:B:766:THR:HG22	2.16	0.76
1:A:995:LYS:HZ1	1:A:1284:GLN:NE2	1.84	0.74
1:A:131:GLN:NE2	1:A:133:GLU:H	1.83	0.74
1:B:36:LEU:HD22	1:B:89:GLU:HG3	1.69	0.74
1:A:571:ASP:N	9:A:1440:HOH:O	2.20	0.73
1:B:884:HIS:CE1	1:B:1006:GLY:H	2.05	0.73
1:A:131:GLN:HE21	1:A:133:GLU:N	1.88	0.71
1:A:673:ASP:OD2	1:A:677:HIS:HD2	1.74	0.71
1:B:695:ILE:H	1:B:904:ASN:HD22	1.39	0.71
1:A:601:ASN:O	1:A:821:HIS:HD2	1.74	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:939:GLU:HG2	1:B:977:TYR:CE2	2.27	0.70
1:B:609:THR:HG22	9:B:1398:HOH:O	1.92	0.69
1:A:427:ARG:O	1:A:427:ARG:HG2	1.94	0.68
1:A:1143:GLU:H	1:A:1143:GLU:CD	1.96	0.68
1:A:1033:HIS:CD2	1:A:1035:GLY:H	2.11	0.68
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.41	0.67
1:A:995:LYS:NZ	1:A:1284:GLN:NE2	2.41	0.66
1:A:1287:ASN:ND2	1:A:1289:ASN:H	1.94	0.65
1:B:853:THR:HG23	1:B:944:LYS:NZ	2.11	0.65
1:A:1324:ASN:ND2	1:A:1324:ASN:N	2.44	0.65
1:B:610:SER:O	1:B:663:VAL:O	2.14	0.64
1:B:60:ARG:HB3	1:B:60:ARG:HH11	1.63	0.64
1:B:1249:ASN:O	1:B:1255:ALA:HA	1.98	0.64
1:A:58:TYR:HD1	1:A:65:ILE:HG13	1.62	0.63
1:A:884:HIS:CE1	1:A:1006:GLY:H	2.08	0.62
1:B:427:ARG:O	1:B:427:ARG:HG2	1.97	0.62
1:A:880:ARG:O	1:A:884:HIS:HD2	1.80	0.62
1:B:640:ILE:HG12	1:B:779:MET:HE1	1.82	0.62
1:B:880:ARG:O	1:B:884:HIS:HD2	1.82	0.62
1:B:1048:GLN:HE22	1:B:1187:ASN:HD22	1.48	0.61
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.35	0.61
1:B:673:ASP:OD2	1:B:677:HIS:HD2	1.84	0.61
1:A:623:SER:HA	1:A:626:GLN:HE21	1.66	0.60
1:A:850:PHE:CD1	1:A:930:VAL:HG13	2.37	0.60
1:A:61:LEU:O	1:A:62:GLN:HB3	2.01	0.60
1:B:232:GLU:OE1	1:B:677:HIS:HE1	1.85	0.60
1:A:765:SER:O	1:A:801:LYS:HD3	2.02	0.60
1:A:1287:ASN:HD22	1:A:1287:ASN:C	2.05	0.59
1:A:1324:ASN:H	1:A:1324:ASN:HD22	1.49	0.59
1:A:439:ARG:NH2	1:A:451:GLU:OE1	2.35	0.59
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.38	0.58
1:A:695:ILE:H	1:A:904:ASN:ND2	1.96	0.58
1:B:488:ALA:HA	1:B:1319:THR:OG1	2.03	0.58
1:B:1185:SER:HA	9:B:1486:HOH:O	2.03	0.57
1:A:1207:THR:OG1	1:A:1208:LEU:HD13	2.03	0.57
1:A:1324:ASN:O	1:A:1325:CYS:HB3	2.02	0.57
1:A:1325:CYS:O	1:A:1326:LYS:C	2.42	0.57
1:B:572:THR:HA	1:B:575:ARG:HD3	1.85	0.57
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.40	0.56
1:B:264:ILE:O	1:B:268:MET:HG2	2.05	0.56
1:B:853:THR:HG23	1:B:944:LYS:HZ3	1.70	0.56
1:A:964:VAL:HG23	1:A:1155:TYR:CD2	2.41	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:826:MET:HB3	7:A:1338:GOL:H32	1.87	0.55
1:B:346:ALA:HB1	3:B:1335:FAD:H4'	1.87	0.55
1:A:1324:ASN:N	1:A:1324:ASN:HD22	2.02	0.55
1:B:579:HIS:HB3	1:B:582:ALA:HB2	1.88	0.54
1:B:614:HIS:HD2	1:B:693:PRO:O	1.90	0.54
1:B:848:VAL:HG21	1:B:926:TRP:HB2	1.89	0.54
1:A:1172:LYS:HG3	9:A:1696:HOH:O	2.08	0.53
1:B:655:PHE:CD2	1:B:668:GLY:HA2	2.43	0.53
1:B:721:LYS:HA	1:B:724:SER:HB2	1.89	0.53
1:A:1105:LYS:HE2	1:A:1116:TRP:CZ3	2.43	0.53
1:B:1315:THR:O	1:B:1316:LEU:HB2	2.08	0.53
1:A:601:ASN:O	1:A:821:HIS:CD2	2.58	0.53
1:A:58:TYR:CD1	1:A:65:ILE:HG13	2.44	0.53
1:A:720:LYS:O	1:A:721:LYS:HB2	2.10	0.52
1:B:764:VAL:CG2	1:B:766:THR:CG2	2.86	0.52
1:A:134:PRO:O	1:A:164:ALA:HA	2.09	0.52
1:A:1126:SER:HB2	1:B:1132:PHE:CD1	2.44	0.52
1:A:1203:LEU:C	1:A:1203:LEU:HD12	2.29	0.52
1:A:1159:CYS:O	1:A:1176:THR:HA	2.09	0.52
1:B:1033:HIS:HD2	1:B:1035:GLY:H	1.58	0.52
1:B:840:HIS:HE1	1:B:874:SER:OG	1.93	0.52
1:B:144:GLN:HB3	1:B:339:GLY:HA2	1.92	0.52
1:B:469:THR:HG23	1:B:489:GLY:HA3	1.92	0.51
1:A:644:ASN:HB2	9:A:1687:HOH:O	2.10	0.51
1:A:609:THR:HG23	1:A:664:GLY:HA2	1.92	0.51
1:A:779:MET:HG2	1:A:810:VAL:HG13	1.93	0.50
1:B:131:GLN:HE21	1:B:133:GLU:H	1.59	0.50
1:A:62:GLN:O	1:A:62:GLN:NE2	2.35	0.50
1:A:471:GLN:NE2	1:A:474:LEU:CD1	2.73	0.50
1:B:624:GLU:HB3	1:B:684:VAL:HG13	1.94	0.50
1:B:884:HIS:HE1	1:B:1006:GLY:N	2.02	0.50
1:B:911:PHE:HD2	1:B:912:ARG:N	2.09	0.50
1:B:1038:MET:HG3	4:B:3003:XAX:C4	2.41	0.50
1:A:1324:ASN:O	1:A:1325:CYS:CB	2.60	0.50
1:B:848:VAL:HG13	1:B:859:LEU:HD13	1.92	0.50
1:A:1287:ASN:HD22	1:A:1288:ASN:N	2.09	0.50
1:A:1088:GLN:CG	1:A:1133:TYR:CD1	2.95	0.50
1:B:149:ARG:HD3	1:B:1229:ILE:HD12	1.92	0.50
1:B:802:GLU:OE1	8:B:1340:SAL:H4	2.11	0.49
1:B:439:ARG:NH2	1:B:451:GLU:OE1	2.45	0.49
1:B:93:SER:HB2	1:B:589:GLU:OE1	2.13	0.49
1:A:848:VAL:HG21	1:A:926:TRP:HB2	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:696:ILE:HD12	1:B:1217:GLY:HA3	1.94	0.49
1:B:875:HIS:HD2	1:B:879:GLU:OE2	1.94	0.49
1:B:55:LEU:HD12	1:B:68:PHE:CE1	2.48	0.48
1:A:1048:GLN:HE22	1:A:1187:ASN:HD22	1.59	0.48
1:A:747:HIS:HD1	1:A:805:SER:HA	1.76	0.48
1:A:727:ASP:HB3	1:A:852:LYS:HD2	1.94	0.48
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.14	0.47
1:A:27:LEU:HD13	1:A:39:THR:HG22	1.95	0.47
1:A:1315:THR:O	1:A:1316:LEU:HB2	2.15	0.47
1:A:348:LEU:HD13	1:A:407:ILE:HD13	1.96	0.47
1:A:320:PRO:HG2	1:A:323:LYS:HG3	1.94	0.47
1:A:338:ALA:HB2	3:A:1335:FAD:C6	2.44	0.47
1:A:696:ILE:HD12	1:A:1217:GLY:HA3	1.96	0.47
1:A:1017:ALA:HB2	1:A:1085:ILE:HD12	1.96	0.47
1:B:1081:VAL:O	1:B:1084:ASP:HB2	2.13	0.47
1:B:39:THR:HG22	1:B:51:CYS:HA	1.97	0.47
1:A:1080:SER:HB3	1:A:1258:ALA:HB1	1.96	0.47
1:A:1326:LYS:CG	1:A:1326:LYS:O	2.63	0.47
1:A:353:ILE:HG22	1:A:353:ILE:O	2.15	0.47
1:A:612:ARG:HG3	1:A:689:TYR:CG	2.49	0.46
1:B:358:ILE:CD1	1:B:430:ASP:HA	2.45	0.46
1:A:1324:ASN:ND2	9:A:1632:HOH:O	2.48	0.46
1:B:1289:ASN:HB2	1:B:1292:GLU:HB2	1.97	0.46
1:B:419:SER:HB2	1:B:519:PHE:CD1	2.51	0.46
1:B:964:VAL:N	1:B:965:PRO:HD2	2.31	0.46
1:A:1191:ASP:O	1:A:1195:VAL:HG23	2.15	0.46
1:B:358:ILE:HD11	1:B:430:ASP:HA	1.98	0.46
1:B:641:PRO:HG3	1:B:817:TYR:CE2	2.51	0.45
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.51	0.45
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.52	0.45
1:A:808:VAL:O	1:A:812:VAL:HG23	2.17	0.45
1:B:912:ARG:NH2	1:B:1198:ALA:HB2	2.32	0.45
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.52	0.45
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.45
1:A:56:SER:HB2	1:A:84:ALA:HB3	1.99	0.45
1:B:320:PRO:HD2	1:B:323:LYS:HD3	1.99	0.45
1:A:2:THR:CG2	1:A:230:GLU:OE2	2.65	0.45
1:A:27:LEU:CD1	1:A:39:THR:HG22	2.47	0.44
1:B:1289:ASN:H	1:B:1289:ASN:HD22	1.65	0.44
1:A:487:CYS:HB3	1:A:513:LEU:HD13	1.99	0.44
1:B:81:HIS:CD2	1:B:227:LEU:HD11	2.52	0.44
1:A:255:ALA:CB	1:A:277:MET:HG2	2.46	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:640:ILE:HA	1:B:641:PRO:HD3	1.85	0.44
1:B:655:PHE:CE2	1:B:668:GLY:HA2	2.52	0.44
1:A:614:HIS:HD2	1:A:693:PRO:O	2.00	0.44
1:A:131:GLN:HE21	1:A:133:GLU:C	2.21	0.44
1:A:1097:ILE:CD1	1:A:1129:THR:HG22	2.47	0.44
1:A:967:CYS:HB3	1:A:1157:VAL:HG23	2.00	0.44
1:B:779:MET:HG2	1:B:810:VAL:HG13	2.00	0.44
1:A:471:GLN:NE2	1:A:474:LEU:HD12	2.33	0.44
1:B:1082:SER:HB2	4:B:3003:XAX:O3P	2.17	0.44
1:A:507:PHE:CD1	1:A:1303:GLU:HA	2.53	0.44
1:A:695:ILE:HG23	1:A:700:ASP:HB3	2.00	0.43
1:B:911:PHE:O	1:B:912:ARG:C	2.57	0.43
1:A:143:PHE:HB3	1:A:1232:PHE:CE1	2.53	0.43
1:A:427:ARG:HD3	1:A:1212:HIS:CD2	2.53	0.43
1:B:388:THR:O	1:B:397:LEU:HD13	2.18	0.43
1:B:1080:SER:O	1:B:1258:ALA:HB1	2.18	0.43
1:B:1007:ILE:HD12	1:B:1258:ALA:HB3	2.00	0.43
1:B:700:ASP:O	1:B:704:ASN:ND2	2.50	0.43
1:B:370:THR:HG23	1:B:408:GLU:O	2.19	0.42
1:A:150:CYS:O	1:A:1197:GLY:HA3	2.19	0.42
1:A:1152:TYR:HB3	1:A:1251:LYS:HG3	2.01	0.42
1:B:277:MET:HA	1:B:277:MET:HE3	2.01	0.42
1:B:104:ARG:HD2	1:B:104:ARG:HA	1.89	0.42
1:A:427:ARG:NH1	1:A:504:MET:HG3	2.35	0.42
1:B:912:ARG:CZ	1:B:1198:ALA:HB2	2.50	0.42
1:B:9:PHE:CE2	1:B:14:LYS:HB2	2.54	0.42
1:A:948:LYS:HB3	1:A:948:LYS:HE2	1.84	0.42
1:B:999:CYS:SG	1:B:1001:ILE:HD12	2.58	0.42
1:B:232:GLU:OE1	1:B:677:HIS:CE1	2.70	0.42
1:B:338:ALA:HB2	3:B:1335:FAD:C6	2.50	0.42
1:B:2:THR:O	1:B:228:ARG:HD3	2.20	0.42
1:B:672:ALA:HB3	1:B:678:ALA:HB2	2.01	0.42
1:B:683:HIS:HB2	9:B:1620:HOH:O	2.20	0.42
1:B:875:HIS:CD2	1:B:879:GLU:OE2	2.72	0.42
1:A:911:PHE:O	1:A:912:ARG:C	2.56	0.42
1:A:975:SER:HB2	1:A:980:ARG:HH21	1.84	0.42
1:B:880:ARG:O	1:B:884:HIS:CD2	2.69	0.42
1:A:1143:GLU:CD	1:A:1143:GLU:N	2.68	0.42
1:B:60:ARG:HB3	1:B:60:ARG:NH1	2.32	0.42
1:A:600:GLU:CD	1:B:598:ARG:HG2	2.41	0.42
1:B:721:LYS:CA	1:B:724:SER:HB2	2.50	0.41
1:A:721:LYS:O	1:A:724:SER:HB2	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:798:PHE:HA	4:B:3003:XAX:HN5	1.84	0.41
1:A:1082:SER:HB2	4:A:3003:XAX:O3P	2.21	0.41
1:B:1091:TYR:O	1:B:1095:GLN:HG2	2.19	0.41
1:B:525:LYS:HA	1:B:525:LYS:HD2	1.86	0.41
1:B:1289:ASN:H	1:B:1289:ASN:ND2	2.19	0.41
1:B:104:ARG:CZ	1:B:162:THR:HG21	2.51	0.41
1:A:779:MET:HE1	1:A:814:LEU:HD13	2.01	0.41
1:A:471:GLN:HE21	1:A:474:LEU:HD12	1.85	0.41
1:A:55:LEU:HD12	1:A:68:PHE:CE1	2.55	0.41
1:B:585:GLN:NE2	9:B:1412:HOH:O	2.53	0.41
1:A:641:PRO:HG3	1:A:817:TYR:CE2	2.56	0.41
1:A:1287:ASN:HD22	1:A:1289:ASN:H	1.65	0.41
1:B:853:THR:HG23	1:B:944:LYS:HZ2	1.81	0.41
1:B:644:ASN:O	1:B:653:THR:HA	2.21	0.41
1:B:102:GLN:HG2	1:B:586:ALA:O	2.21	0.41
1:A:1062:TYR:OH	1:B:759:GLU:OE2	2.28	0.41
1:B:968:TRP:HA	1:B:1157:VAL:HG11	2.03	0.41
1:A:1173:ASN:O	1:A:1236:PRO:HA	2.20	0.41
1:B:1199:PHE:CE1	1:B:1267:GLY:HA2	2.55	0.41
1:B:117:THR:O	1:B:121:VAL:HG23	2.21	0.41
1:A:1183:GLY:HA2	1:A:1247:CYS:O	2.21	0.41
1:B:708:TYR:CE2	1:B:902:LYS:HD2	2.56	0.41
1:B:754:LYS:HB2	1:B:759:GLU:HB2	2.02	0.40
1:B:1080:SER:HB3	1:B:1258:ALA:HB1	2.03	0.40
1:A:390:PHE:HB3	9:A:1630:HOH:O	2.21	0.40
1:B:99:HIS:CG	1:B:100:PRO:HD2	2.57	0.40
1:A:415:ASP:OD2	1:A:444:PRO:HA	2.20	0.40
1:A:418:PHE:HA	1:A:438:MET:O	2.21	0.40
1:B:1193:GLY:HA2	9:B:1505:HOH:O	2.20	0.40
1:A:1118:MET:O	1:A:1122:GLN:HG3	2.20	0.40
1:B:683:HIS:O	1:B:683:HIS:CG	2.74	0.40
1:B:742:PHE:HA	1:B:829:ARG:NH2	2.37	0.40
1:B:56:SER:HA	1:B:66:ILE:O	2.21	0.40
1:A:1287:ASN:C	1:A:1287:ASN:ND2	2.72	0.40
1:B:131:GLN:HE21	1:B:133:GLU:C	2.25	0.40
1:B:158:GLN:O	1:B:161:ARG:HB2	2.21	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	1219/1332 (92%)	1162 (95%)	46 (4%)	11 (1%)	25	26
1	B	1212/1332 (91%)	1147 (95%)	58 (5%)	7 (1%)	33	39
All	All	2431/2664 (91%)	2309 (95%)	104 (4%)	18 (1%)	30	34

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1325	CYS
1	A	335	ARG
1	A	721	LYS
1	A	912	ARG
1	A	1008	SER
1	B	721	LYS
1	B	1008	SER
1	A	527	LEU
1	A	797	GLY
1	B	912	ARG
1	B	1139	GLY
1	A	43	CYS
1	A	62	GLN
1	B	338	ALA
1	B	797	GLY
1	B	520	TYR
1	A	1139	GLY
1	A	1253	ILE

### 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	1030/1128 (91%)	982 (95%)	48 (5%)	36	47
1	B	1026/1128 (91%)	982 (96%)	44 (4%)	40	52
All	All	2056/2256 (91%)	1964 (96%)	92 (4%)	38	50

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	63	ASP
1	A	93	SER
1	A	103	GLU
1	A	113	CYS
1	A	140	GLU
1	A	161	ARG
1	A	165	LYS
1	A	243	LYS
1	A	271	LYS
1	A	312	LEU
1	A	335	ARG
1	A	337	PHE
1	A	348	LEU
1	A	358	ILE
1	A	371	LYS
1	A	375	VAL
1	A	398	LEU
1	A	401	GLU
1	A	426	ARG
1	A	433	LYS
1	A	501	PRO
1	A	513	LEU
1	A	525	LYS
1	A	609	THR
1	A	657	LYS
1	A	680	ARG
1	A	684	VAL
1	A	719	LEU
1	A	742	PHE
1	A	743	TYR
1	A	764	VAL
1	A	779	MET
1	A	782	VAL
1	A	818	LYS

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Mol	Chain	Res	Type
1	A	848	VAL
1	A	852	LYS
1	A	853	THR
1	A	911	PHE
1	A	939	GLU
1	A	948	LYS
1	A	1001	ILE
1	A	1134	ARG
1	A	1203	LEU
1	A	1220	HIS
1	A	1287	ASN
1	A	1290	THR
1	A	1324	ASN
1	B	61	LEU
1	B	82	HIS
1	B	129	ARG
1	B	140	GLU
1	B	161	ARG
1	B	162	THR
1	B	249	LYS
1	B	268	MET
1	B	277	MET
1	B	312	LEU
1	B	337	PHE
1	B	348	LEU
1	B	426	ARG
1	B	468	LYS
1	B	476	LYS
1	B	506	GLU
1	B	525	LYS
1	B	609	THR
1	B	648	LEU
1	B	684	VAL
1	B	703	LYS
1	B	719	LEU
1	B	731	SER
1	B	742	PHE
1	B	743	TYR
1	B	764	VAL
1	B	779	MET
1	B	782	VAL
1	B	848	VAL

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Mol	Chain	Res	Type
1	B	852	LYS
1	B	895	ARG
1	B	899	ARG
1	B	911	PHE
1	B	948	LYS
1	B	969	ASP
1	B	1001	ILE
1	B	1134	ARG
1	B	1203	LEU
1	B	1208	LEU
1	B	1242	SER
1	B	1253	ILE
1	B	1287	ASN
1	B	1289	ASN
1	B	1319	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	146	ASN
1	A	471	GLN
1	A	614	HIS
1	A	626	GLN
1	A	677	HIS
1	A	821	HIS
1	A	840	HIS
1	A	884	HIS
1	A	904	ASN
1	A	1016	GLN
1	A	1033	HIS
1	A	1048	GLN
1	A	1137	ASN
1	A	1212	HIS
1	A	1284	GLN
1	A	1287	ASN
1	A	1324	ASN
1	B	131	GLN
1	B	144	GLN
1	B	146	ASN
1	B	473	GLN
1	B	614	HIS

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Mol	Chain	Res	Type
1	B	677	HIS
1	B	705	ASN
1	B	821	HIS
1	B	840	HIS
1	B	875	HIS
1	B	884	HIS
1	B	904	ASN
1	B	1033	HIS
1	B	1048	GLN
1	B	1088	GLN
1	B	1108	ASN
1	B	1284	GLN
1	B	1289	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FES	A	1334	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FAD	A	1335	-	58,58,58	1.09	4 (6%)	85,89,89	1.83	15 (17%)
6	BCT	A	1337	-	0,3,3	0.00	-	0,3,3	0.00	-
7	GOL	A	1338	-	5,5,5	0.46	0	5,5,5	0.70	0
7	GOL	A	1339	-	5,5,5	0.46	0	5,5,5	0.70	0
7	GOL	A	1340	-	5,5,5	0.21	0	5,5,5	0.91	0
8	SAL	A	1341	-	10,10,10	1.95	1 (10%)	13,13,13	1.39	1 (7%)
4	XAX	A	3003	-	29,31,31	6.94	11 (37%)	37,52,52	2.26	14 (37%)
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	FAD	B	1335	-	58,58,58	1.06	2 (3%)	85,89,89	1.92	16 (18%)
6	BCT	B	1337	-	0,3,3	0.00	-	0,3,3	0.00	-
7	GOL	B	1338	-	5,5,5	0.37	0	5,5,5	0.42	0
7	GOL	B	1339	-	5,5,5	0.21	0	5,5,5	0.29	0
8	SAL	B	1340	-	10,10,10	1.76	1 (10%)	13,13,13	1.30	1 (7%)
4	XAX	B	3003	-	29,31,31	7.27	8 (27%)	37,52,52	2.22	10 (27%)

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	0/0/1/1
2	FES	A	1334	1	-	0/0/4/4	0/0/1/1
3	FAD	A	1335	-	-	0/34/50/50	0/1/6/6
6	BCT	A	1337	-	-	0/0/0/0	0/0/0/0
7	GOL	A	1338	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1339	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1340	-	-	0/4/4/4	0/0/0/0
8	SAL	A	1341	-	-	0/4/4/4	0/1/1/1
4	XAX	A	3003	-	-	0/6/46/46	0/0/4/4
2	FES	B	1333	1	-	0/0/4/4	0/0/1/1
2	FES	B	1334	1	-	0/0/4/4	0/0/1/1
3	FAD	B	1335	-	-	0/34/50/50	0/1/6/6
6	BCT	B	1337	-	-	0/0/0/0	0/0/0/0
7	GOL	B	1338	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1339	-	-	0/4/4/4	0/0/0/0
8	SAL	B	1340	-	-	0/4/4/4	0/1/1/1
4	XAX	B	3003	-	-	0/6/46/46	0/0/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3003	XAX	O1-MO	37.21	2.05	1.70
4	A	3003	XAX	O1-MO	34.87	2.03	1.70
4	A	3003	XAX	O4-C4	6.42	1.37	1.24
8	A	1341	SAL	C1-C2	5.86	1.50	1.40
4	B	3003	XAX	O4-C4	5.83	1.35	1.24
4	A	3003	XAX	C9-C10	5.74	1.49	1.41
8	B	1340	SAL	C1-C2	5.12	1.49	1.40
4	A	3003	XAX	C4-C9	5.10	1.50	1.41
4	B	3003	XAX	C1'-S1'	-4.88	1.66	1.77
4	B	3003	XAX	C9-C10	4.85	1.48	1.41
4	A	3003	XAX	C1'-S1'	-4.66	1.67	1.77
4	B	3003	XAX	C2'-S2'	-4.48	1.67	1.77
4	B	3003	XAX	C4-C9	4.38	1.49	1.41
3	B	1335	FAD	C2A-N3A	3.98	1.40	1.32
4	A	3003	XAX	C2'-S2'	-3.65	1.69	1.77
3	A	1335	FAD	C1'-N10	3.32	1.51	1.48
3	A	1335	FAD	C1'-C2'	3.00	1.54	1.51
4	A	3003	XAX	C9-N5	2.91	1.48	1.38
4	B	3003	XAX	MO-S1'	-2.86	2.34	2.44
3	B	1335	FAD	C2A-N1A	2.81	1.39	1.33
3	A	1335	FAD	C2A-N3A	2.66	1.37	1.32
4	B	3003	XAX	C9-N5	2.66	1.47	1.38
4	A	3003	XAX	MO-S1'	-2.63	2.35	2.44
3	A	1335	FAD	C2A-N1A	2.50	1.38	1.33
4	A	3003	XAX	C2-N1	2.47	1.36	1.33
4	A	3003	XAX	C2-N2	2.47	1.36	1.32
4	A	3003	XAX	MO-S2'	-2.43	2.35	2.44

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1335	FAD	N3A-C2A-N1A	-10.01	120.34	128.71
3	A	1335	FAD	N3A-C2A-N1A	-9.50	120.76	128.71
4	B	3003	XAX	C6-C1'-S1'	-7.75	117.53	124.27
4	A	3003	XAX	C6-C1'-S1'	-6.23	118.85	124.27
3	B	1335	FAD	C2-N1-C10	6.05	121.08	114.98
3	A	1335	FAD	C1'-N10-C9A	5.11	123.85	118.87
3	B	1335	FAD	C1'-N10-C9A	4.74	123.48	118.87
4	B	3003	XAX	C7-C6-N5	4.22	113.81	108.44
3	A	1335	FAD	C2-N1-C10	4.18	119.19	114.98
4	A	3003	XAX	C7-C6-N5	4.08	113.63	108.44
3	B	1335	FAD	N3A-C4A-N9A	4.00	132.66	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3003	XAX	C4-C9-C10	-3.96	110.89	114.56
4	B	3003	XAX	C2-N1-C10	3.88	123.13	117.61
8	A	1341	SAL	C2-C1-C1'	3.76	124.26	120.03
4	A	3003	XAX	C10-C9-N5	-3.65	113.49	118.50
4	A	3003	XAX	O3P-P-O2P	3.64	122.35	110.44
4	A	3003	XAX	C2'-C1'-S1'	-3.62	118.09	120.15
3	A	1335	FAD	O4B-C1B-N9A	-3.59	105.10	108.44
3	A	1335	FAD	C9A-N10-C10	-3.41	118.42	121.77
3	A	1335	FAD	N3A-C4A-N9A	3.40	131.56	125.43
4	A	3003	XAX	C4-C9-N5	3.32	123.92	119.10
3	A	1335	FAD	C5X-C9A-N10	3.30	120.06	116.80
3	B	1335	FAD	C4X-N5-C5X	3.20	120.28	116.69
4	B	3003	XAX	C9-C4-N3	3.14	122.12	114.06
3	B	1335	FAD	C4X-C10-N1	-3.08	119.66	122.73
3	B	1335	FAD	C4-N3-C2	-3.03	119.18	125.39
4	B	3003	XAX	O1P-P-O2P	2.92	119.97	110.44
4	A	3003	XAX	C1'-C2'-S2'	-2.90	118.51	120.15
3	A	1335	FAD	C4-N3-C2	-2.88	119.47	125.39
3	A	1335	FAD	C4X-N5-C5X	2.83	119.87	116.69
4	A	3003	XAX	O3P-P-O4'	-2.79	98.96	106.65
4	A	3003	XAX	C3'-C2'-C1'	-2.75	119.59	124.32
4	A	3003	XAX	O4'-P-O2P	-2.68	98.85	106.71
4	A	3003	XAX	N8-C10-N1	2.65	120.67	116.51
4	B	3003	XAX	N8-C10-N1	2.60	120.59	116.51
4	B	3003	XAX	O4'-P-O2P	-2.59	99.11	106.71
3	A	1335	FAD	C4X-C10-N1	-2.53	120.20	122.73
4	B	3003	XAX	C1'-C2'-S2'	-2.53	118.71	120.15
3	B	1335	FAD	C5A-C4A-N3A	-2.52	120.20	125.70
3	B	1335	FAD	C9A-N10-C10	-2.52	119.30	121.77
3	B	1335	FAD	C5X-C9A-N10	2.51	119.27	116.80
3	A	1335	FAD	C4X-C10-N10	2.46	121.73	120.51
8	B	1340	SAL	C4-C3-C2	-2.35	116.92	120.05
3	B	1335	FAD	C4B-O4B-C1B	2.30	112.25	109.75
3	B	1335	FAD	C4A-C5A-N7A	-2.30	107.55	109.52
3	A	1335	FAD	C4A-C5A-N7A	-2.26	107.58	109.52
3	B	1335	FAD	C2'-C1'-N10	-2.25	109.46	112.45
4	A	3003	XAX	C9-C4-N3	2.21	119.74	114.06
4	A	3003	XAX	C2-N1-C10	2.19	120.72	117.61
3	B	1335	FAD	N7A-C8A-N9A	-2.19	108.16	114.36
3	A	1335	FAD	C5A-C4A-N3A	-2.17	120.98	125.70
3	B	1335	FAD	C2A-N3A-C4A	2.06	119.88	114.01
4	B	3003	XAX	N2-C2-N3	2.04	120.10	117.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1335	FAD	O4B-C1B-C2B	-2.03	103.66	106.77
3	A	1335	FAD	O2A-PA-O3P	2.02	114.74	105.14
4	A	3003	XAX	N2-C2-N1	-2.01	117.59	120.31
3	B	1335	FAD	O4'-C4'-C3'	2.00	114.04	109.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	1225/1332 (91%)	0.26	41 (3%)	44	54	12, 25, 39, 60	0
1	B	1218/1332 (91%)	0.45	67 (5%)	24	33	17, 29, 45, 63	0
All	All	2443/2664 (91%)	0.36	108 (4%)	33	43	12, 27, 42, 63	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1287	ASN	7.8
1	A	164	ALA	7.1
1	B	2	THR	6.0
1	B	165	LYS	6.0
1	B	1144	THR	4.7
1	A	162	THR	4.7
1	B	477	PHE	4.6
1	B	164	ALA	4.6
1	A	58	TYR	4.3
1	A	720	LYS	4.3
1	B	1288	ASN	4.3
1	A	163	PHE	4.0
1	B	162	THR	3.9
1	A	378	GLY	3.7
1	B	1290	THR	3.7
1	A	165	LYS	3.6
1	B	161	ARG	3.6
1	A	2	THR	3.5
1	A	498	PRO	3.5
1	A	499	ASP	3.4
1	B	97	ARG	3.4
1	B	982	SER	3.3
1	B	1143	GLU	3.2
1	B	136	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	397	LEU	3.2
1	A	1245	ARG	3.2
1	A	477	PHE	3.2
1	B	1264	LEU	3.1
1	B	471	GLN	3.1
1	A	61	LEU	3.1
1	B	163	PHE	3.1
1	A	1246	ASP	3.0
1	B	948	LYS	3.0
1	B	1317	CYS	3.0
1	B	1286	THR	3.0
1	A	1247	CYS	2.9
1	A	525	LYS	2.9
1	B	499	ASP	2.9
1	B	1248	PRO	2.8
1	B	336	TRP	2.8
1	B	3	ALA	2.8
1	B	133	GLU	2.8
1	B	718	ASP	2.7
1	A	161	ARG	2.7
1	B	445	GLY	2.7
1	B	917	PRO	2.7
1	A	1215	PRO	2.7
1	B	61	LEU	2.6
1	A	983	GLU	2.6
1	A	985	ASP	2.6
1	B	1107	LYS	2.6
1	B	294	PRO	2.6
1	A	575	ARG	2.5
1	A	528	GLY	2.5
1	B	725	GLU	2.5
1	B	921	PHE	2.5
1	B	272	ASN	2.5
1	A	979	ALA	2.5
1	B	528	GLY	2.4
1	B	316	VAL	2.4
1	A	989	LYS	2.4
1	A	1326	LYS	2.4
1	B	448	GLN	2.4
1	B	724	SER	2.4
1	B	973	LYS	2.3
1	B	976	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1215	PRO	2.3
1	A	252	HIS	2.3
1	B	321	THR	2.3
1	B	137	GLU	2.3
1	B	620	ILE	2.3
1	A	60	ARG	2.3
1	B	985	ASP	2.2
1	B	1115	ASP	2.2
1	B	720	LYS	2.2
1	B	1263	PRO	2.2
1	B	377	ARG	2.2
1	A	1288	ASN	2.2
1	B	461	ASP	2.1
1	B	1289	ASN	2.1
1	B	1216	GLU	2.1
1	A	799	GLY	2.1
1	B	475	SER	2.1
1	B	1141	SER	2.1
1	B	658	ASP	2.1
1	B	657	LYS	2.1
1	A	969	ASP	2.1
1	A	1106	LYS	2.1
1	A	319	LEU	2.1
1	A	523	VAL	2.1
1	A	320	PRO	2.1
1	A	1248	PRO	2.1
1	B	693	PRO	2.1
1	B	852	LYS	2.1
1	B	378	GLY	2.0
1	A	1325	CYS	2.0
1	A	1216	GLU	2.0
1	A	414	GLU	2.0
1	B	16	VAL	2.0
1	B	984	VAL	2.0
1	A	97	ARG	2.0
1	B	254	GLU	2.0
1	B	860	GLU	2.0
1	A	1103	PRO	2.0
1	B	60	ARG	2.0
1	B	1099	LYS	2.0
1	B	1146	SER	2.0
1	B	1250	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

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<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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	A	1338	6/6	0.20	4.60	22,26,27,28	0
8	SAL	B	1340	10/10	0.22	3.20	37,39,41,44	0
8	SAL	A	1341	10/10	0.23	3.12	22,25,28,29	0
7	GOL	B	1338	6/6	0.18	2.02	20,24,25,26	0
7	GOL	A	1340	6/6	0.19	1.27	33,35,38,39	0
7	GOL	A	1339	6/6	0.15	0.90	27,28,29,30	0
4	XAX	B	3003	28/28	0.17	0.11	20,22,26,33	0
6	BCT	A	1337	4/4	0.16	-0.11	14,14,15,17	0
7	GOL	B	1339	6/6	0.12	-0.41	21,25,27,30	0
6	BCT	B	1337	4/4	0.15	-0.56	24,24,24,24	0
3	FAD	A	1335	53/53	0.14	-0.72	14,19,25,28	0
2	FES	B	1333	4/4	0.11	-0.86	20,20,21,22	0
3	FAD	B	1335	53/53	0.12	-1.00	19,27,31,33	0
4	XAX	A	3003	28/28	0.12	-1.17	16,20,26,33	0
2	FES	A	1333	4/4	0.08	-1.58	18,20,21,21	0
2	FES	A	1334	4/4	0.09	-1.68	18,18,18,19	0
5	CA	A	1336	1/1	0.09	-2.08	26,26,26,26	0
2	FES	B	1334	4/4	0.10	-2.17	18,21,21,22	0
5	CA	B	1336	1/1	0.06	-4.99	22,22,22,22	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.