



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:13 am GMT

PDB ID : 3BDJ  
Title : Crystal Structure of Bovine Milk Xanthine Dehydrogenase with a Covalently Bound Oxipurinol Inhibitor  
Authors : Eger, B.T.; Okamoto, K.; Nishino, T.; Pai, E.F.; Nishino, T.  
Deposited on : 2007-11-14  
Resolution : 2.00 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

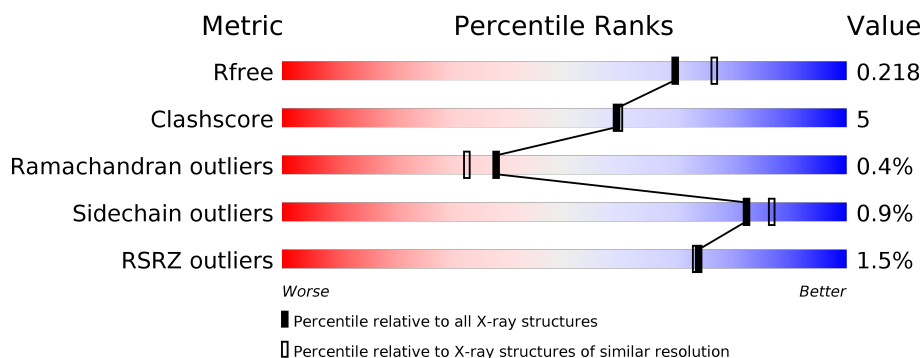
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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>%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>••</div> </div> </div>
1	B	1332	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</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
3	FES	B	4002	-	-	X	-
8	GOL	B	5002	-	-	-	X
8	GOL	B	5004	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21626 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	0	0
			9991	6354	1712	1865	60			
1	B	1286	Total	C	N	O	S	0	0	0
			9991	6354	1712	1865	60			

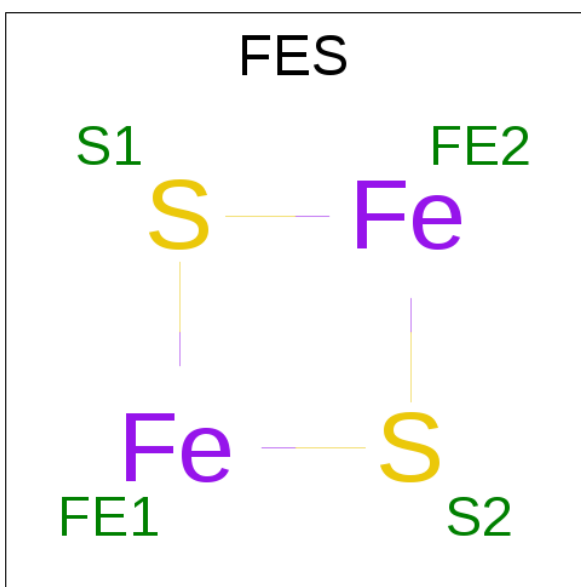
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	HIS	ASP	SEE REMARK 999	UNP P80457
B	552	HIS	ASP	SEE REMARK 999	UNP P80457

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

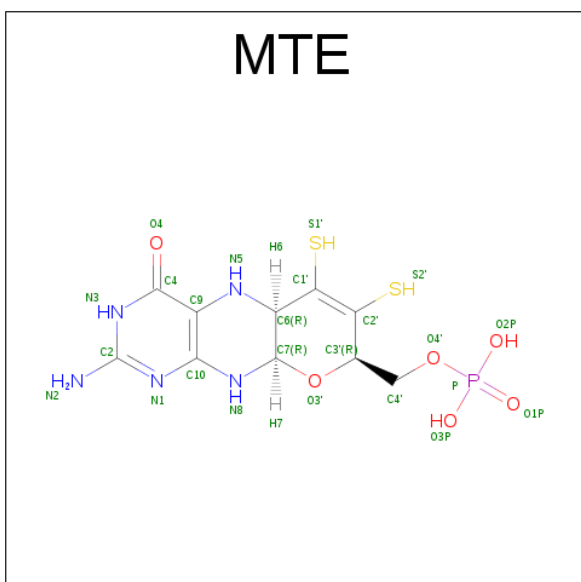
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



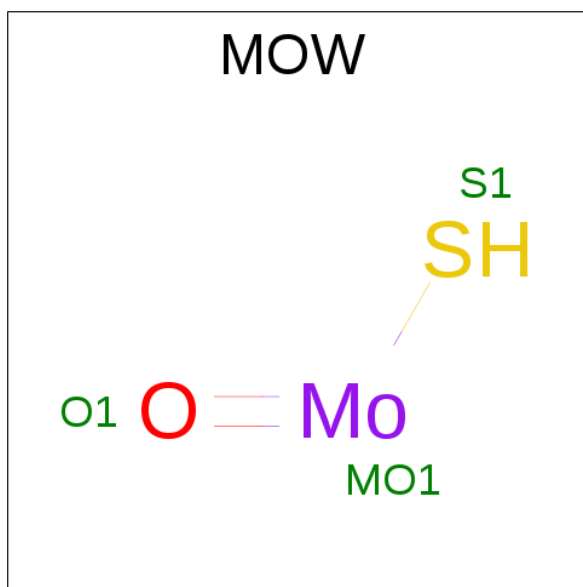
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 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:  $C_{10}H_{14}N_5O_6PS_2$ ).



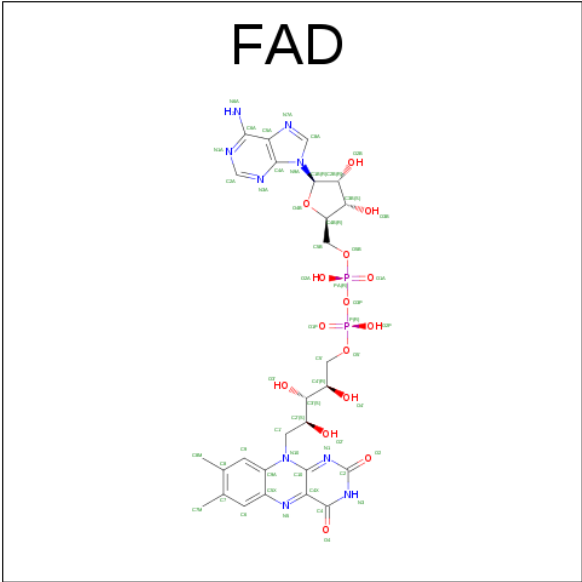
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
4	B	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	

- Molecule 5 is OXO(SULFANYL)MOLYBDENUM(IV) ION (three-letter code: MOW) (formula: HMoOS).



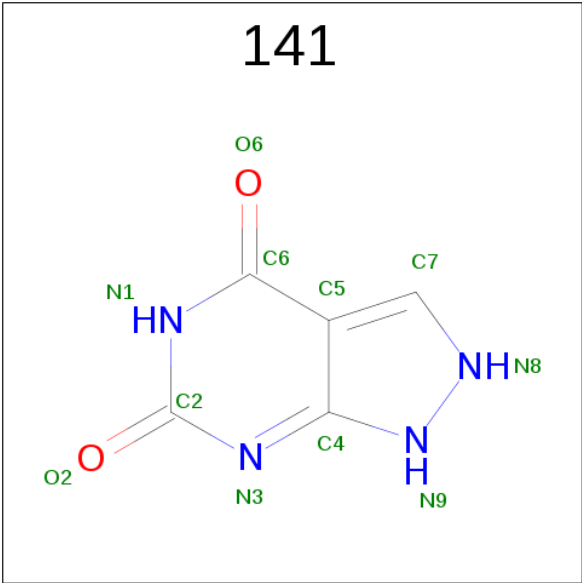
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Mo	O	S		
			3	1	1	1		
5	B	1	Total	Mo	O	S		
			3	1	1	1		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



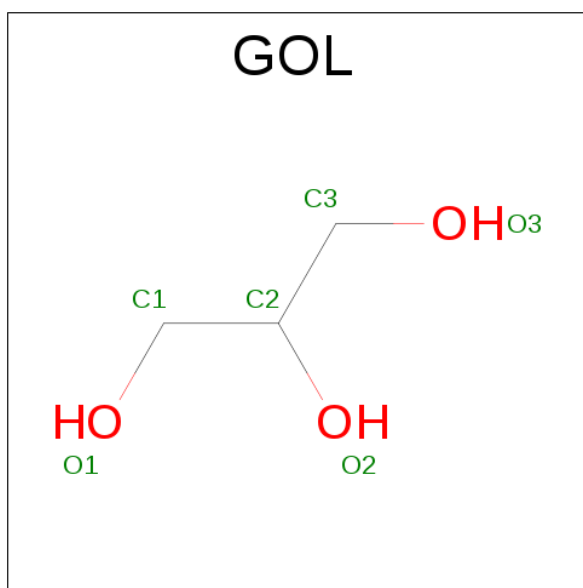
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
6	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 7 is OXYPURINOL (three-letter code: 141) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			11	5	4	2		
7	B	1	Total	C	N	O	0	0
			11	5	4	2		

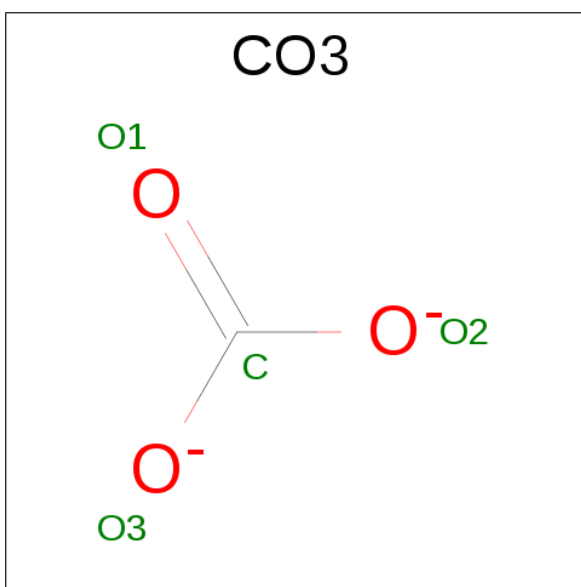
- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 9 is CARBONATE ION (three-letter code: CO3) (formula:  $CO_3$ ).





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

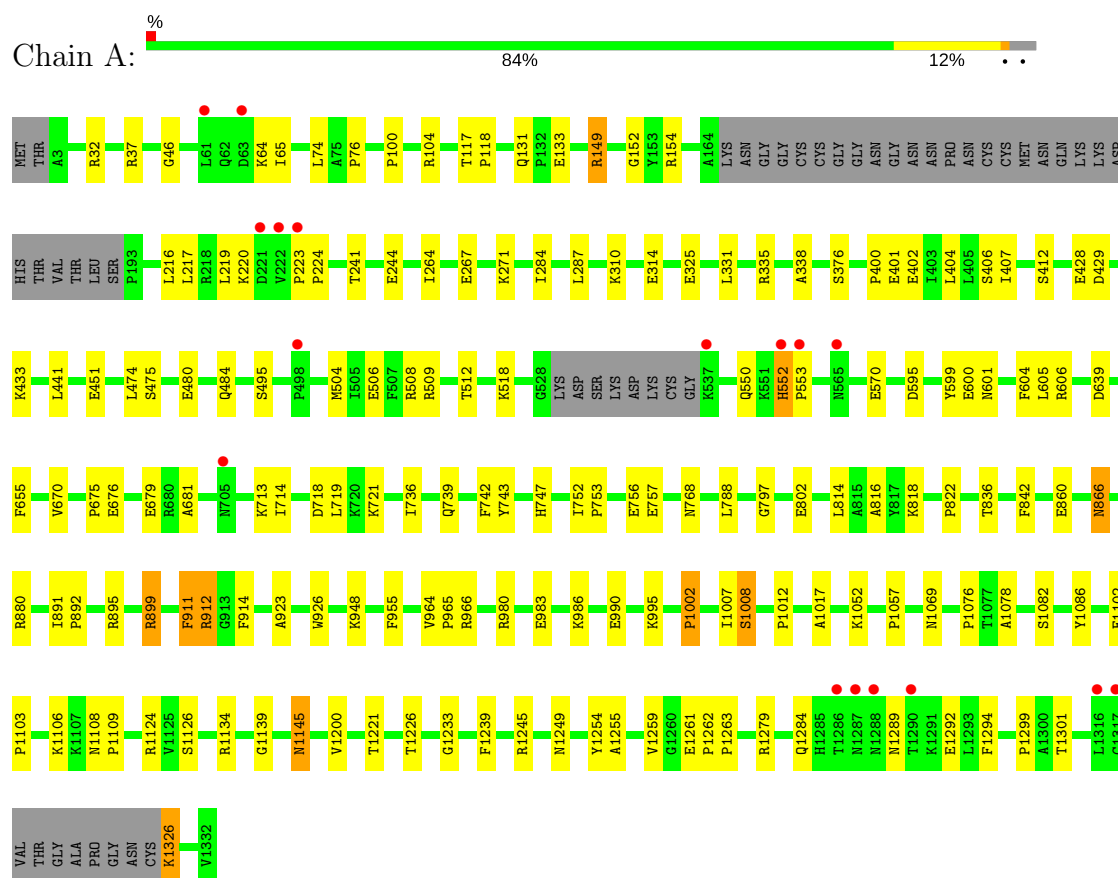
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	706	Total	O	0	0
			706	706		
10	B	688	Total	O	0	0
			688	688		

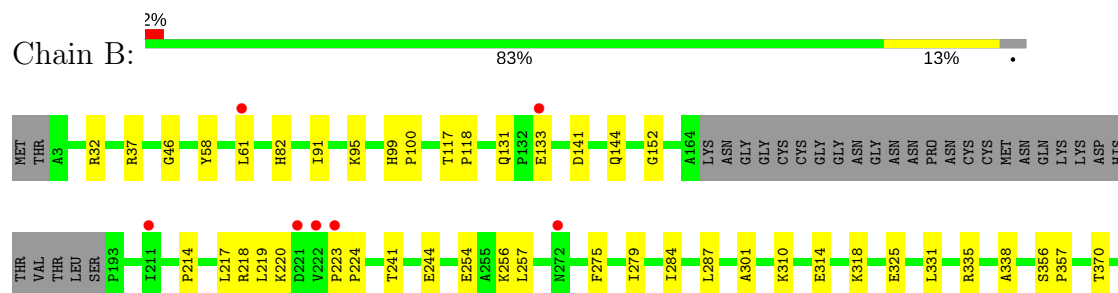
### 3 Residue-property plots

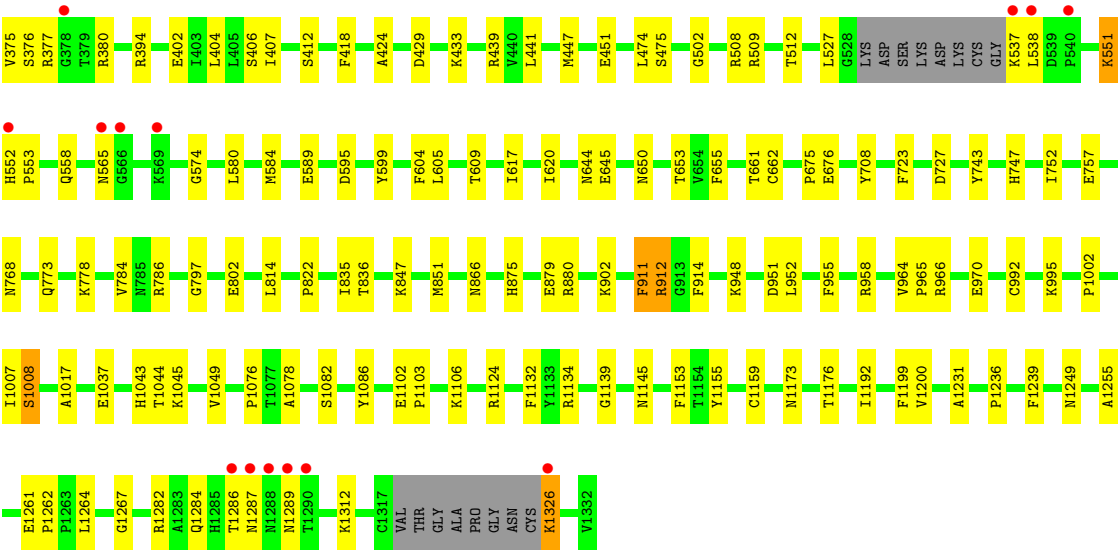
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.52Å 124.07Å 148.80Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	19.96 – 2.00 19.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.6 (19.96-2.00) 89.2 (19.96-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 1.99Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.191 , 0.224 0.184 , 0.218	Depositor DCC
$R_{free}$ test set	2299 reflections (1.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 59.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21626	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CO3, 141, CA, MOW, 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	0.33	0/10210	0.60	0/13818
1	B	0.32	0/10210	0.60	0/13818
All	All	0.33	0/20420	0.60	0/27636

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	9991	0	9991	106	0
1	B	9991	0	9991	117	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	0	1	0
3	B	8	0	0	2	0
4	A	24	0	10	1	0
4	B	24	0	10	1	0
5	A	3	0	0	1	0
5	B	3	0	0	1	0
6	A	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	53	0	31	0	0
7	A	11	0	3	2	0
7	B	11	0	3	2	0
8	A	18	0	24	0	0
8	B	24	0	32	1	0
9	A	4	0	0	0	0
9	B	4	0	0	0	0
10	A	706	0	0	4	0
10	B	688	0	0	4	0
All	All	21626	0	20126	216	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 5.

All (216) 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:757:GLU:H	1:B:584:MET:HE3	1.21	1.01
1:B:551:LYS:HD2	1:B:551:LYS:H	1.33	0.92
1:B:1326:LYS:HZ2	1:B:1326:LYS:N	1.68	0.91
1:B:131:GLN:HE21	1:B:133:GLU:H	1.18	0.90
1:B:404:LEU:HD21	1:B:407:ILE:HD11	1.53	0.88
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.39	0.86
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.39	0.84
1:A:756:GLU:HA	1:B:584:MET:HE1	1.60	0.83
1:B:948:LYS:HG2	1:B:951:ASP:OD2	1.85	0.76
1:A:131:GLN:HE21	1:A:133:GLU:H	1.31	0.76
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.51	0.75
1:A:719:LEU:HD11	1:A:895:ARG:CB	2.18	0.74
1:A:757:GLU:N	1:B:584:MET:HE3	2.02	0.72
1:A:719:LEU:HD11	1:A:895:ARG:HB3	1.71	0.71
1:B:314:GLU:O	1:B:318:LYS:HG2	1.92	0.70
1:B:1287:ASN:ND2	1:B:1289:ASN:HB3	2.06	0.70
1:B:404:LEU:CD2	1:B:407:ILE:HD11	2.24	0.66
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.77	0.65
1:A:570:GLU:OE2	1:A:1057:PRO:HG3	1.98	0.64
5:A:3004:MOW:MO1	5:A:3004:MOW:O1	1.68	0.64
5:B:4004:MOW:O1	5:B:4004:MOW:MO1	1.67	0.64
1:B:1078:ALA:HB1	7:B:5102:141:C7	2.30	0.62
1:A:719:LEU:HD13	1:A:860:GLU:OE2	2.01	0.61
1:B:406:SER:C	1:B:407:ILE:HD12	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:O	1:A:220:LYS:HG2	2.00	0.60
1:A:639:ASP:HB3	1:A:818:LYS:HD2	1.84	0.60
1:A:406:SER:C	1:A:407:ILE:HD12	2.22	0.60
1:B:474:LEU:O	1:B:475:SER:HB2	2.01	0.60
1:B:37:ARG:HD3	1:B:595:ASP:O	2.01	0.60
1:B:551:LYS:CD	1:B:551:LYS:H	2.11	0.60
1:A:1078:ALA:HB1	7:A:5101:141:C7	2.32	0.59
1:B:375:VAL:HG12	1:B:380:ARG:HG3	1.85	0.59
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.68	0.58
1:B:131:GLN:NE2	1:B:133:GLU:H	1.96	0.58
1:B:552:HIS:CG	1:B:553:PRO:HD2	2.39	0.58
1:A:64:LYS:HG2	1:A:65:ILE:N	2.20	0.57
1:A:1221:THR:HG22	1:A:1226:THR:HB	1.86	0.57
1:A:719:LEU:HD11	1:A:895:ARG:HB2	1.85	0.57
1:A:37:ARG:HD3	1:A:595:ASP:O	2.04	0.57
1:A:216:LEU:HD23	1:A:219:LEU:HD12	1.87	0.56
1:A:757:GLU:H	1:B:584:MET:CE	2.07	0.55
1:A:604:PHE:CD2	1:A:675:PRO:HG3	2.42	0.55
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.88	0.55
1:B:310:LYS:O	1:B:314:GLU:HG3	2.07	0.55
1:B:46:GLY:HA2	3:B:4002:FES:S1	2.47	0.54
1:A:428:GLU:OE2	1:A:1233:GLY:HA3	2.07	0.54
1:B:241:THR:OG1	1:B:244:GLU:HG3	2.06	0.54
1:B:131:GLN:HE21	1:B:133:GLU:N	1.96	0.54
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.08	0.54
1:B:1287:ASN:HD22	1:B:1289:ASN:HB3	1.72	0.53
1:B:32:ARG:HH12	1:B:676:GLU:CD	2.10	0.53
1:A:433:LYS:HE2	1:A:504:MET:SD	2.48	0.53
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.74	0.52
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.90	0.52
1:A:100:PRO:O	1:A:104:ARG:HG3	2.10	0.52
1:A:264:ILE:HD11	6:A:3005:FAD:H3B	1.91	0.52
1:A:1326:LYS:HD2	1:A:1326:LYS:N	2.25	0.52
1:B:256:LYS:HE3	1:B:275:PHE:CE2	2.45	0.51
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.92	0.51
1:A:1082:SER:HB2	4:A:3003:MTE:O3P	2.10	0.51
1:A:948:LYS:HB2	1:A:948:LYS:NZ	2.25	0.51
1:B:727:ASP:HB2	1:B:851:MET:HA	1.92	0.51
1:B:377:ARG:HB3	1:B:377:ARG:NH1	2.25	0.51
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.75	0.51
1:A:719:LEU:HD13	1:A:860:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:GLU:HB3	1:B:786:ARG:HE	1.75	0.50
1:A:713:LYS:HG2	1:A:714:ILE:N	2.26	0.50
1:B:370:THR:CG2	1:B:407:ILE:HG23	2.41	0.50
1:A:756:GLU:HA	1:B:584:MET:CE	2.36	0.50
1:B:723:PHE:CE2	1:B:847:LYS:HE2	2.46	0.50
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.11	0.50
1:A:911:PHE:O	1:A:912:ARG:C	2.50	0.50
1:A:474:LEU:O	1:A:475:SER:HB2	2.11	0.50
1:A:1126:SER:HB2	1:B:1132:PHE:CD1	2.47	0.50
1:B:217:LEU:O	1:B:220:LYS:HG2	2.12	0.50
1:B:376:SER:HB3	1:B:402:GLU:HG2	1.93	0.50
1:B:509:ARG:HG2	1:B:509:ARG:HH11	1.77	0.49
1:A:752:ILE:CD1	1:A:822:PRO:HB3	2.42	0.49
1:A:508:ARG:O	1:A:512:THR:HG23	2.11	0.49
1:B:551:LYS:HD2	1:B:551:LYS:N	2.14	0.49
1:B:257:LEU:HA	1:B:279:ILE:O	2.13	0.49
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.13	0.49
1:B:82:HIS:NE2	1:B:219:LEU:HD13	2.28	0.49
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.48	0.48
1:A:966:ARG:HG3	10:A:5839:HOH:O	2.13	0.48
1:B:152:GLY:HA2	1:B:1200:VAL:HG21	1.94	0.48
1:B:644:ASN:O	1:B:653:THR:HA	2.13	0.48
1:A:284:ILE:CG2	1:A:287:LEU:HD23	2.43	0.48
1:B:1326:LYS:N	1:B:1326:LYS:NZ	2.51	0.48
1:A:752:ILE:HD13	1:A:822:PRO:HB3	1.95	0.48
1:B:1282:ARG:O	1:B:1286:THR:HB	2.14	0.48
1:B:604:PHE:CD2	1:B:675:PRO:HG3	2.49	0.48
1:A:407:ILE:N	1:A:407:ILE:HD12	2.28	0.48
1:A:404:LEU:HD21	1:A:407:ILE:HD11	1.96	0.48
1:A:599:TYR:HA	1:B:599:TYR:HA	1.96	0.48
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.49	0.48
1:B:537:LYS:HG2	1:B:537:LYS:O	2.15	0.47
1:A:149:ARG:HG3	1:A:742:PHE:O	2.13	0.47
1:B:911:PHE:O	1:B:912:ARG:C	2.53	0.47
1:A:400:PRO:HG2	1:A:401:GLU:OE1	2.15	0.47
1:B:1102:GLU:HB3	1:B:1103:PRO:HD3	1.97	0.47
1:B:1007:ILE:O	1:B:1008:SER:CB	2.61	0.47
1:B:1102:GLU:OE2	1:B:1106:LYS:HE3	2.14	0.47
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.97	0.47
1:A:495:SER:HA	1:A:509:ARG:NH1	2.30	0.47
1:B:605:LEU:HD23	1:B:605:LEU:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:ASN:N	1:A:1109:PRO:HD3	2.30	0.46
1:A:46:GLY:HA2	3:A:3002:FES:S1	2.56	0.46
1:A:310:LYS:O	1:A:314:GLU:HG3	2.16	0.46
1:A:899:ARG:HA	1:A:899:ARG:HD2	1.78	0.46
1:A:152:GLY:HA2	1:A:1200:VAL:HG21	1.97	0.46
1:A:739:GLN:HG2	1:A:911:PHE:CE1	2.50	0.46
1:A:1245:ARG:HG2	10:A:5542:HOH:O	2.16	0.46
1:B:424:ALA:HA	1:B:433:LYS:HG2	1.97	0.46
1:B:574:GLY:CA	8:B:5003:GOL:H12	2.46	0.46
1:A:1102:GLU:OE2	1:A:1106:LYS:HE3	2.16	0.45
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.79	0.45
1:B:61:LEU:HD12	1:B:61:LEU:N	2.31	0.45
1:A:325:GLU:HB2	1:A:412:SER:CB	2.46	0.45
1:A:338:ALA:HA	1:A:429:ASP:OD1	2.17	0.45
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.80	0.45
1:A:1052:LYS:HD3	1:A:1254:TYR:CE1	2.51	0.45
1:A:284:ILE:HG21	1:A:287:LEU:HD23	1.98	0.45
1:A:518:LYS:HE3	10:A:5595:HOH:O	2.15	0.45
1:A:718:ASP:HB3	1:A:721:LYS:HE3	1.98	0.45
1:A:655:PHE:CE1	1:A:814:LEU:HD23	2.51	0.45
1:B:287:LEU:HD12	1:B:301:ALA:HB3	1.98	0.45
1:B:992:CYS:HA	1:B:1284:GLN:NE2	2.32	0.45
1:B:394:ARG:HD2	10:B:5750:HOH:O	2.16	0.45
1:B:768:ASN:ND2	1:B:1076:PRO:HB3	2.32	0.45
1:A:1007:ILE:O	1:A:1008:SER:CB	2.64	0.45
1:A:325:GLU:HB2	1:A:412:SER:HB3	1.99	0.45
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.52	0.44
1:B:1312:LYS:HG2	10:B:5915:HOH:O	2.18	0.44
1:B:325:GLU:HB2	1:B:412:SER:HB3	1.99	0.44
1:A:441:LEU:HD23	1:A:451:GLU:HG3	1.98	0.44
1:A:980:ARG:HA	1:A:983:GLU:OE1	2.18	0.44
1:B:1264:LEU:HD23	1:B:1264:LEU:C	2.37	0.44
1:B:802:GLU:OE2	7:B:5102:141:H1	2.18	0.44
1:B:46:GLY:CA	3:B:4002:FES:S1	3.06	0.44
1:B:95:LYS:HG3	1:B:589:GLU:OE2	2.17	0.44
1:B:708:TYR:CE2	1:B:902:LYS:HD3	2.53	0.44
1:B:966:ARG:O	1:B:970:GLU:HG3	2.18	0.44
1:B:331:LEU:O	1:B:335:ARG:HG3	2.18	0.43
1:B:1199:PHE:CE1	1:B:1267:GLY:HA2	2.53	0.43
1:B:1082:SER:HB2	4:B:4003:MTE:O3P	2.18	0.43
1:B:661:THR:O	1:B:662:CYS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:LEU:C	1:A:605:LEU:HD23	2.38	0.43
1:A:1134:ARG:CD	1:B:1124:ARG:HB2	2.49	0.43
1:B:508:ARG:O	1:B:512:THR:HG23	2.18	0.43
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.93	0.43
1:B:1173:ASN:O	1:B:1236:PRO:HA	2.18	0.43
1:A:376:SER:HB3	1:A:402:GLU:HG2	2.01	0.43
1:A:986:LYS:O	1:A:990:GLU:HG3	2.19	0.43
1:A:964:VAL:HB	1:A:965:PRO:HD3	2.00	0.42
1:A:552:HIS:CG	1:A:553:PRO:HD2	2.54	0.42
1:B:433:LYS:HA	1:B:433:LYS:HE2	2.00	0.42
1:A:1017:ALA:HB1	1:A:1086:TYR:CD2	2.55	0.42
1:A:480:GLU:HG3	1:A:484:GLN:HE21	1.84	0.42
1:B:1153:PHE:HB2	1:B:1155:TYR:CZ	2.54	0.42
1:B:141:ASP:O	1:B:144:GLN:HG3	2.20	0.42
1:A:117:THR:HB	1:A:118:PRO:HD3	2.01	0.42
1:B:1159:CYS:O	1:B:1176:THR:HA	2.19	0.42
1:B:875:HIS:O	1:B:879:GLU:HG3	2.20	0.42
1:A:1289:ASN:ND2	1:A:1292:GLU:HB2	2.34	0.42
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.55	0.42
1:B:214:PRO:O	1:B:218:ARG:HG3	2.20	0.42
1:B:773:GLN:HG2	1:B:784:VAL:HG13	2.02	0.42
1:B:609:THR:HG21	1:B:835:ILE:HD11	2.00	0.42
1:A:154:ARG:C	1:A:154:ARG:HD2	2.40	0.42
1:B:338:ALA:HA	1:B:429:ASP:OD1	2.20	0.42
1:B:447:MET:HG2	1:B:527:LEU:HD13	2.02	0.42
1:A:1102:GLU:HB3	1:A:1103:PRO:HD3	2.02	0.42
1:A:506:GLU:CD	1:A:506:GLU:H	2.23	0.41
1:A:1124:ARG:CB	1:B:1134:ARG:HD3	2.50	0.41
1:B:58:TYR:CZ	1:B:220:LYS:HD2	2.55	0.41
1:B:418:PHE:CD1	1:B:439:ARG:HB2	2.55	0.41
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.93	0.41
1:B:752:ILE:CD1	1:B:822:PRO:HB3	2.50	0.41
1:A:1279:ARG:HG2	1:A:1294:PHE:HE2	1.86	0.41
1:A:802:GLU:OE2	7:A:5101:141:H1	2.21	0.41
1:A:866:ASN:HD22	1:A:866:ASN:C	2.23	0.41
1:B:1231:ALA:HB1	10:B:5694:HOH:O	2.20	0.41
1:A:788:LEU:HD13	1:A:1069:ASN:HB3	2.03	0.41
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	2.18	0.41
1:B:1287:ASN:HD22	1:B:1289:ASN:H	1.67	0.41
1:B:580:LEU:HG	1:B:1044:THR:HG23	2.01	0.41
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1299:PRO:HG2	1:A:1301:THR:HG23	2.02	0.41
1:B:502:GLY:HA3	10:B:5831:HOH:O	2.20	0.41
1:B:723:PHE:CE2	1:B:847:LYS:HG2	2.55	0.41
1:A:267:GLU:HA	1:A:271:LYS:HG2	2.02	0.41
1:A:736:ILE:CG2	1:A:842:PHE:HB2	2.50	0.41
1:A:1259:VAL:O	1:A:1259:VAL:HG22	2.21	0.41
1:A:1012:PRO:HB2	10:A:5821:HOH:O	2.21	0.41
1:A:331:LEU:O	1:A:335:ARG:HG3	2.21	0.41
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	2.03	0.41
1:A:32:ARG:NH1	1:A:676:GLU:OE2	2.42	0.41
1:B:952:LEU:HD23	1:B:958:ARG:HA	2.02	0.41
1:A:600:GLU:HG3	1:A:601:ASN:N	2.36	0.41
1:A:606:ARG:CZ	1:A:679:GLU:HG3	2.51	0.41
1:A:891:ILE:HA	1:A:892:PRO:HD2	1.92	0.41
1:B:117:THR:HB	1:B:118:PRO:HD3	2.03	0.41
1:B:254:GLU:OE2	1:B:254:GLU:N	2.36	0.41
1:B:617:ILE:CG2	1:B:620:ILE:HD11	2.51	0.41
1:B:91:ILE:O	1:B:99:HIS:HB2	2.21	0.40
1:B:1045:LYS:O	1:B:1049:VAL:HG23	2.21	0.40
1:A:768:ASN:ND2	1:A:1076:PRO:HB3	2.36	0.40
1:A:74:LEU:O	1:A:76:PRO:HD3	2.22	0.40
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.37	0.40
1:B:284:ILE:CG2	1:B:287:LEU:HD23	2.52	0.40
1:B:356:SER:HA	1:B:357:PRO:HD3	1.95	0.40
1:B:325:GLU:HB2	1:B:412:SER:CB	2.52	0.40
1:A:1262:PRO:HB2	1:A:1263:PRO:HD3	2.02	0.40
1:A:433:LYS:HA	1:A:433:LYS:HD3	1.91	0.40
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1278/1332 (96%)	1238 (97%)	35 (3%)	5 (0%)	38	33
1	B	1278/1332 (96%)	1232 (96%)	41 (3%)	5 (0%)	38	33
All	All	2556/2664 (96%)	2470 (97%)	76 (3%)	10 (0%)	38	33

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	A	912	ARG
1	B	1139	GLY
1	A	1139	GLY
1	B	912	ARG
1	A	797	GLY
1	B	797	GLY
1	B	538	LEU
1	A	1002	PRO

### 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	1091/1128 (97%)	1080 (99%)	11 (1%)	80	84
1	B	1091/1128 (97%)	1082 (99%)	9 (1%)	85	88
All	All	2182/2256 (97%)	2162 (99%)	20 (1%)	82	87

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ARG
1	A	550	GLN
1	A	552	HIS
1	A	743	TYR
1	A	866	ASN
1	A	899	ARG

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Mol	Chain	Res	Type
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	551	LYS
1	B	565	ASN
1	B	743	TYR
1	B	866	ASN
1	B	911	PHE
1	B	1002	PRO
1	B	1239	PHE
1	B	1326	LYS

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

Mol	Chain	Res	Type
1	A	131	GLN
1	A	272	ASN
1	A	351	ASN
1	A	471	GLN
1	A	473	GLN
1	A	484	GLN
1	A	626	GLN
1	A	683	HIS
1	A	866	ASN
1	A	1088	GLN
1	A	1145	ASN
1	A	1284	GLN
1	B	130	ASN
1	B	131	GLN
1	B	351	ASN
1	B	471	GLN
1	B	473	GLN
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	866	ASN
1	B	1088	GLN
1	B	1122	GLN
1	B	1145	ASN

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Mol	Chain	Res	Type
1	B	1284	GLN
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 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	$\# Z  > 2$
3	FES	A	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	A	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	MTE	A	3003	5	21,26,26	2.53	8 (38%)	19,40,40	2.84	8 (42%)
5	MOW	A	3004	4	0,2,2	0.00	-	0,1,1	0.00	-
6	FAD	A	3005	-	51,58,58	2.96	19 (37%)	54,89,89	2.97	16 (29%)
8	GOL	A	5005	-	5,5,5	0.65	0	5,5,5	0.40	0
8	GOL	A	5006	-	5,5,5	0.62	0	5,5,5	0.30	0
8	GOL	A	5007	-	5,5,5	0.65	0	5,5,5	0.25	0
7	141	A	5101	-	10,12,12	1.87	2 (20%)	4,17,17	11.84	4 (100%)
9	CO3	A	5201	-	0,3,3	0.00	-	0,3,3	0.00	-
3	FES	B	4001	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
3	FES	B	4002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	MTE	B	4003	5	21,26,26	2.52	8 (38%)	19,40,40	2.79	7 (36%)
5	MOW	B	4004	4	0,2,2	0.00	-	0,1,1	0.00	-
6	FAD	B	4005	-	51,58,58	2.97	19 (37%)	54,89,89	2.96	16 (29%)
8	GOL	B	5001	-	5,5,5	0.62	0	5,5,5	0.29	0
8	GOL	B	5002	-	5,5,5	0.60	0	5,5,5	0.42	0
8	GOL	B	5003	-	5,5,5	0.59	0	5,5,5	0.33	0
8	GOL	B	5004	-	5,5,5	0.61	0	5,5,5	0.34	0
7	141	B	5102	-	10,12,12	1.84	2 (20%)	4,17,17	11.89	4 (100%)
9	CO3	B	5202	-	0,3,3	0.00	-	0,3,3	0.00	-

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
3	FES	A	3001	1	-	0/0/4/4	0/1/1/1
3	FES	A	3002	1	-	0/0/4/4	0/1/1/1
4	MTE	A	3003	5	-	0/6/34/34	0/3/3/3
5	MOW	A	3004	4	-	0/0/0/0	0/0/0/0
6	FAD	A	3005	-	-	0/28/50/50	0/6/6/6
8	GOL	A	5005	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5006	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5007	-	-	0/4/4/4	0/0/0/0
7	141	A	5101	-	-	0/0/0/0	0/2/2/2
9	CO3	A	5201	-	-	0/0/0/0	0/0/0/0
3	FES	B	4001	1	-	0/0/4/4	0/1/1/1
3	FES	B	4002	1	-	0/0/4/4	0/1/1/1
4	MTE	B	4003	5	-	0/6/34/34	0/3/3/3
5	MOW	B	4004	4	-	0/0/0/0	0/0/0/0
6	FAD	B	4005	-	-	0/28/50/50	0/6/6/6
8	GOL	B	5001	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5002	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5003	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5004	-	-	0/4/4/4	0/0/0/0
7	141	B	5102	-	-	0/0/0/0	0/2/2/2
9	CO3	B	5202	-	-	0/0/0/0	0/0/0/0

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	4005	FAD	C2B-C1B	-2.71	1.49	1.53
6	A	3005	FAD	C2B-C1B	-2.30	1.50	1.53
4	B	4003	MTE	C2-N1	2.30	1.39	1.35
7	B	5102	141	C4-N9	2.33	1.38	1.34
7	A	5101	141	C4-N9	2.41	1.38	1.34
4	A	3003	MTE	C2-N1	2.71	1.40	1.35
6	B	4005	FAD	C5A-C4A	2.74	1.46	1.40
6	A	3005	FAD	C4-C4X	2.76	1.46	1.41
4	A	3003	MTE	C7-C6	2.77	1.55	1.53
6	A	3005	FAD	C5A-C4A	2.78	1.46	1.40
6	A	3005	FAD	C6-C5X	3.09	1.46	1.41
6	B	4005	FAD	C9-C9A	3.11	1.47	1.40
6	A	3005	FAD	C4X-N5	3.11	1.37	1.33
6	B	4005	FAD	C6-C5X	3.14	1.46	1.41
6	B	4005	FAD	C4-C4X	3.17	1.47	1.41
4	B	4003	MTE	C7-C6	3.18	1.55	1.53
4	B	4003	MTE	C9-C10	3.21	1.47	1.41
4	B	4003	MTE	C4-N3	3.32	1.39	1.33
4	A	3003	MTE	C4-N3	3.38	1.39	1.33
6	A	3005	FAD	C9-C9A	3.43	1.48	1.40
4	A	3003	MTE	C9-C10	3.45	1.48	1.41
6	B	4005	FAD	C4X-N5	3.52	1.38	1.33
6	B	4005	FAD	O4B-C4B	3.67	1.53	1.45
6	A	3005	FAD	C9A-C5X	3.70	1.50	1.42
6	A	3005	FAD	O4B-C4B	3.71	1.53	1.45
4	A	3003	MTE	O3'-C7	3.72	1.49	1.43
4	B	4003	MTE	O3'-C7	3.75	1.49	1.43
6	A	3005	FAD	C8-C7	3.79	1.50	1.41
4	B	4003	MTE	O4-C4	3.83	1.34	1.24
6	B	4005	FAD	C2A-N1A	3.88	1.41	1.33
6	A	3005	FAD	C2-N3	3.89	1.45	1.38
6	B	4005	FAD	C8-C7	3.91	1.50	1.41
6	B	4005	FAD	C2-N3	4.00	1.46	1.38
6	B	4005	FAD	C9A-C5X	4.05	1.50	1.42
7	B	5102	141	C6-N1	4.14	1.40	1.33
6	A	3005	FAD	C2A-N1A	4.18	1.41	1.33
7	A	5101	141	C6-N1	4.20	1.40	1.33
4	A	3003	MTE	O4-C4	4.24	1.35	1.24
6	A	3005	FAD	C5X-N5	4.34	1.42	1.35
6	B	4005	FAD	C2A-N3A	4.43	1.39	1.32
6	B	4005	FAD	C10-N1	4.51	1.39	1.33
6	A	3005	FAD	C2A-N3A	4.54	1.39	1.32
6	B	4005	FAD	C5X-N5	4.60	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3005	FAD	C4A-N3A	4.72	1.42	1.35
6	B	4005	FAD	C4A-N3A	4.78	1.42	1.35
4	A	3003	MTE	O3'-C3'	5.08	1.50	1.43
6	A	3005	FAD	C4-N3	5.08	1.42	1.33
6	B	4005	FAD	C4-N3	5.08	1.42	1.33
4	B	4003	MTE	C9-N5	5.12	1.49	1.37
6	A	3005	FAD	C10-N1	5.13	1.40	1.33
4	A	3003	MTE	C9-N5	5.31	1.49	1.37
4	B	4003	MTE	O3'-C3'	5.52	1.51	1.43
6	A	3005	FAD	C4X-C10	5.69	1.51	1.41
6	B	4005	FAD	C4X-C10	5.76	1.51	1.41
6	A	3005	FAD	O4B-C1B	7.49	1.51	1.41
6	B	4005	FAD	O4B-C1B	7.60	1.51	1.41
6	B	4005	FAD	C9A-N10	9.50	1.51	1.38
6	A	3005	FAD	C9A-N10	9.74	1.51	1.38

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	5102	141	C5-C6-N1	-18.57	111.35	124.45
7	A	5101	141	C5-C6-N1	-18.43	111.45	124.45
6	A	3005	FAD	N3A-C2A-N1A	-8.52	121.44	128.86
6	B	4005	FAD	N3A-C2A-N1A	-8.28	121.65	128.86
6	B	4005	FAD	C5X-C9A-N10	-8.16	111.60	117.66
6	A	3005	FAD	C5X-C9A-N10	-8.15	111.61	117.66
6	B	4005	FAD	C4-C4X-C10	-6.11	115.02	119.96
6	A	3005	FAD	C4-C4X-C10	-5.98	115.12	119.96
4	A	3003	MTE	N3-C2-N1	-5.41	116.68	125.45
4	B	4003	MTE	N3-C2-N1	-5.27	116.91	125.45
6	A	3005	FAD	C4X-C10-N10	-5.21	116.91	120.52
4	A	3003	MTE	O3'-C7-C6	-5.06	105.59	108.96
6	B	4005	FAD	C4X-C10-N10	-4.80	117.19	120.52
4	B	4003	MTE	O3'-C7-C6	-4.78	105.78	108.96
6	B	4005	FAD	C4X-C4-N3	-3.53	118.45	123.48
6	A	3005	FAD	C4X-C4-N3	-3.43	118.59	123.48
7	A	5101	141	C5-C7-N8	-2.90	104.65	110.70
7	B	5102	141	C5-C7-N8	-2.80	104.86	110.70
6	B	4005	FAD	C4'-C3'-C2'	-2.74	107.51	113.41
6	B	4005	FAD	C4B-O4B-C1B	-2.72	106.87	109.77
6	A	3005	FAD	O3B-C3B-C4B	-2.67	103.29	111.09
6	B	4005	FAD	O3B-C3B-C4B	-2.65	103.35	111.09
6	A	3005	FAD	C4'-C3'-C2'	-2.50	108.04	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	4005	FAD	C8M-C8-C9	-2.46	114.17	120.34
6	A	3005	FAD	C8M-C8-C9	-2.42	114.27	120.34
6	A	3005	FAD	C1'-N10-C9A	-2.21	116.32	118.35
6	A	3005	FAD	C4B-O4B-C1B	-2.16	107.47	109.77
6	B	4005	FAD	C1'-N10-C9A	-2.01	116.50	118.35
4	A	3003	MTE	C4-C9-C10	2.24	116.60	114.56
4	A	3003	MTE	P-O4'-C4'	2.32	124.69	118.30
6	B	4005	FAD	C4A-C5A-N7A	2.37	111.70	109.41
6	A	3005	FAD	O3'-C3'-C4'	2.39	114.72	108.82
6	B	4005	FAD	O3'-C3'-C4'	2.39	114.73	108.82
6	A	3005	FAD	C4A-C5A-N7A	2.44	111.76	109.41
4	B	4003	MTE	P-O4'-C4'	2.50	125.19	118.30
6	A	3005	FAD	C8M-C8-C7	3.28	127.60	120.72
6	B	4005	FAD	C8M-C8-C7	3.31	127.66	120.72
4	A	3003	MTE	N8-C10-N1	3.59	123.84	116.90
4	B	4003	MTE	N8-C10-N1	3.73	124.12	116.90
7	B	5102	141	C7-C5-C4	4.51	109.36	105.20
4	B	4003	MTE	C4-N3-C2	4.57	122.64	116.06
4	B	4003	MTE	N2-C2-N3	4.62	124.63	117.24
7	A	5101	141	C7-C5-C4	4.64	109.49	105.20
4	A	3003	MTE	C4-N3-C2	4.68	122.79	116.06
4	A	3003	MTE	C2-N1-C10	4.80	125.33	114.51
4	A	3003	MTE	N2-C2-N3	4.83	124.97	117.24
4	B	4003	MTE	C2-N1-C10	4.97	125.69	114.51
6	B	4005	FAD	C4X-N5-C5X	4.99	122.03	116.76
6	A	3005	FAD	C4X-N5-C5X	5.09	122.14	116.76
6	A	3005	FAD	C4-C4X-N5	5.58	124.79	118.68
6	B	4005	FAD	C4-C4X-N5	5.84	125.09	118.68
6	B	4005	FAD	C4-N3-C2	10.50	124.34	115.16
6	A	3005	FAD	C4-N3-C2	10.66	124.48	115.16
7	A	5101	141	C6-N1-C2	13.83	127.25	115.16
7	B	5102	141	C6-N1-C2	13.88	127.30	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3002	FES	1	0
4	A	3003	MTE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3004	MOW	1	0
6	A	3005	FAD	1	0
7	A	5101	141	2	0
3	B	4002	FES	2	0
4	B	4003	MTE	1	0
5	B	4004	MOW	1	0
8	B	5003	GOL	1	0
7	B	5102	141	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	1286/1332 (96%)	-0.31	17 (1%) 77 77	10, 19, 34, 57	0
1	B	1286/1332 (96%)	-0.29	21 (1%) 72 71	8, 19, 34, 56	0
All	All	2572/2664 (96%)	-0.30	38 (1%) 74 73	8, 19, 34, 57	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	565	ASN	7.3
1	B	1288	ASN	6.5
1	B	537	LYS	5.5
1	A	1288	ASN	5.3
1	B	566	GLY	5.1
1	A	565	ASN	4.7
1	A	223	PRO	4.7
1	A	221	ASP	4.0
1	B	222	VAL	3.7
1	B	552	HIS	3.6
1	A	537	LYS	3.5
1	B	221	ASP	3.4
1	B	223	PRO	3.3
1	A	552	HIS	3.2
1	A	1290	THR	3.1
1	A	1286	THR	3.0
1	B	1287	ASN	2.7
1	B	61	LEU	2.6
1	A	553	PRO	2.5
1	B	272	ASN	2.5
1	B	538	LEU	2.5
1	B	1290	THR	2.4
1	A	1287	ASN	2.4
1	A	222	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	569	LYS	2.4
1	B	1286	THR	2.4
1	A	1317	CYS	2.3
1	A	498	PRO	2.3
1	A	1316	LEU	2.3
1	B	1326	LYS	2.2
1	B	540	PRO	2.2
1	A	61	LEU	2.1
1	A	63	ASP	2.1
1	B	133	GLU	2.1
1	B	378	GLY	2.1
1	B	1289	ASN	2.1
1	B	211	ILE	2.0
1	A	705	ASN	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(Å <sup>2</sup> )	Q<0.9
8	GOL	B	5002	6/6	0.92	0.15	5.20	20,23,25,25	0
8	GOL	B	5004	6/6	0.89	0.15	3.81	21,28,29,34	0
8	GOL	A	5005	6/6	0.93	0.12	1.70	18,19,19,20	0
8	GOL	A	5007	6/6	0.96	0.11	1.18	22,26,27,27	0
8	GOL	A	5006	6/6	0.93	0.13	0.81	28,28,29,31	0
8	GOL	B	5003	6/6	0.93	0.15	0.60	29,30,31,33	0
8	GOL	B	5001	6/6	0.93	0.12	0.48	24,26,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MTE	B	4003	24/24	0.98	0.09	-0.05	9,13,16,18	0
6	FAD	B	4005	53/53	0.97	0.08	-0.60	12,15,20,22	0
6	FAD	A	3005	53/53	0.98	0.08	-0.73	12,16,20,23	0
7	141	B	5102	11/11	0.98	0.07	-1.17	13,15,16,16	0
4	MTE	A	3003	24/24	0.98	0.07	-1.19	10,12,15,17	0
3	FES	A	3001	4/4	0.99	0.05	-1.47	11,11,13,13	0
7	141	A	5101	11/11	0.98	0.07	-1.67	12,14,15,16	0
9	CO3	B	5202	4/4	0.98	0.07	-1.86	14,15,15,17	0
9	CO3	A	5201	4/4	0.99	0.07	-1.89	12,13,13,15	0
3	FES	B	4001	4/4	1.00	0.04	-2.16	11,12,12,14	0
3	FES	B	4002	4/4	1.00	0.04	-2.50	11,12,12,12	0
2	CA	B	5302	1/1	0.99	0.03	-2.95	15,15,15,15	0
3	FES	A	3002	4/4	1.00	0.03	-3.26	11,11,11,12	0
2	CA	A	5301	1/1	1.00	0.04	-3.97	15,15,15,15	0
5	MOW	B	4004	3/3	1.00	0.03	-4.76	13,13,14,16	0
5	MOW	A	3004	3/3	1.00	0.03	-5.68	14,14,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.