



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:50 AM GMT

PDB ID : 2HQM  
Title : Crystal Structure of Glutathione Reductase Glr1 from the Yeast *Saccharomyces cerevisiae*  
Authors : Yu, J.; Zhou, C.Z.  
Deposited on : 2006-07-19  
Resolution : 2.40 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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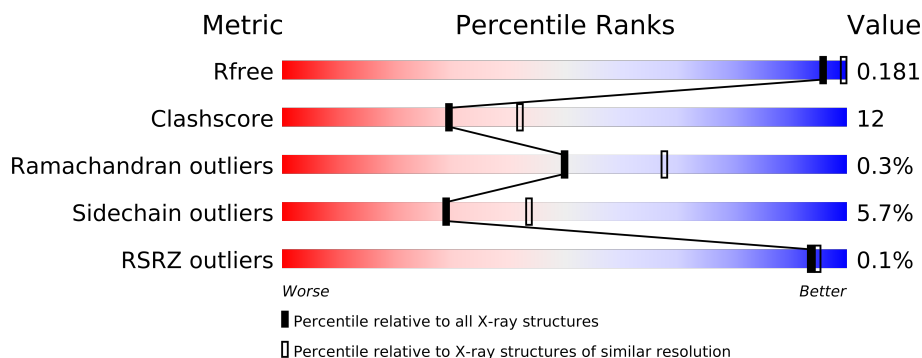
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	479	
1	B	479	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	PO4	B	5002	-	X
5	GSH	A	3001	-	X
5	GSH	B	4001	-	X
6	GOL	A	6001	X	X
6	GOL	A	6005	-	X
6	GOL	A	6006	X	-

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Mol	Type	Chain	Res	Geometry	Electron density
6	GOL	A	6008	-	X
6	GOL	A	6011	-	X
6	GOL	B	6002	-	X
6	GOL	B	6003	X	X
6	GOL	B	6004	X	X
6	GOL	B	6007	-	X
6	GOL	B	6009	X	X
6	GOL	B	6010	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8152 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.

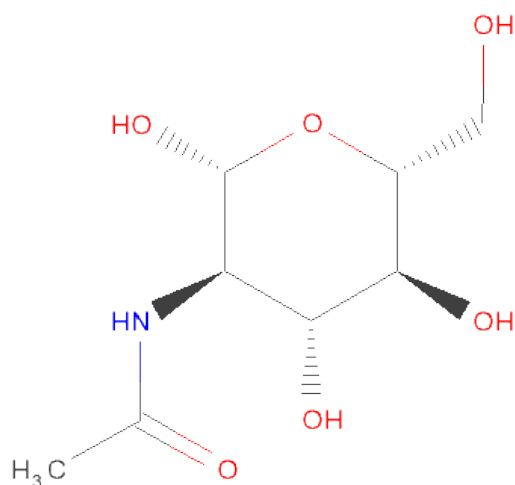
- Molecule 1 is a protein called Glutathione reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3588	2277	620	679	12			
1	B	461	Total	C	N	O	S	0	0	0
			3588	2277	620	679	12			

There are 24 discrepancies between the modelled and reference sequences:

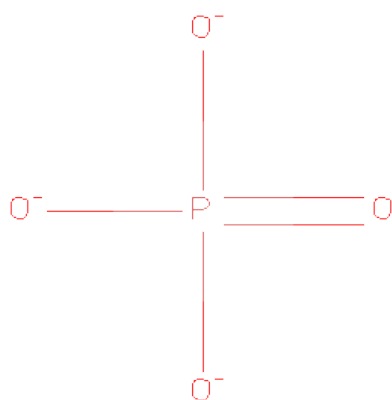
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	TYR	-	CLONING ARTIFACT	UNP P41921
A	14	VAL	-	CLONING ARTIFACT	UNP P41921
A	15	GLU	-	CLONING ARTIFACT	UNP P41921
A	16	PHE	-	CLONING ARTIFACT	UNP P41921
A	484	GLY	-	CLONING ARTIFACT	UNP P41921
A	485	SER	-	CLONING ARTIFACT	UNP P41921
A	486	HIS	-	CLONING ARTIFACT	UNP P41921
A	487	HIS	-	CLONING ARTIFACT	UNP P41921
A	488	HIS	-	CLONING ARTIFACT	UNP P41921
A	489	HIS	-	CLONING ARTIFACT	UNP P41921
A	490	HIS	-	CLONING ARTIFACT	UNP P41921
A	491	HIS	-	CLONING ARTIFACT	UNP P41921
B	13	TYR	-	CLONING ARTIFACT	UNP P41921
B	14	VAL	-	CLONING ARTIFACT	UNP P41921
B	15	GLU	-	CLONING ARTIFACT	UNP P41921
B	16	PHE	-	CLONING ARTIFACT	UNP P41921
B	484	GLY	-	CLONING ARTIFACT	UNP P41921
B	485	SER	-	CLONING ARTIFACT	UNP P41921
B	486	HIS	-	CLONING ARTIFACT	UNP P41921
B	487	HIS	-	CLONING ARTIFACT	UNP P41921
B	488	HIS	-	CLONING ARTIFACT	UNP P41921
B	489	HIS	-	CLONING ARTIFACT	UNP P41921
B	490	HIS	-	CLONING ARTIFACT	UNP P41921
B	491	HIS	-	CLONING ARTIFACT	UNP P41921

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



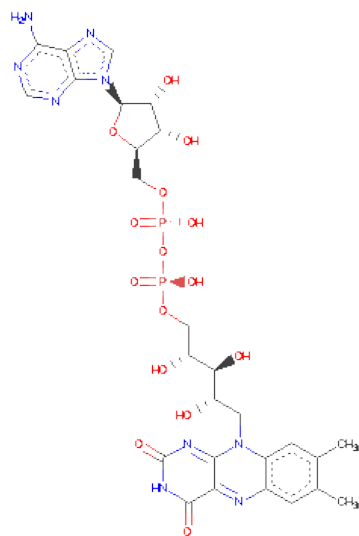
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



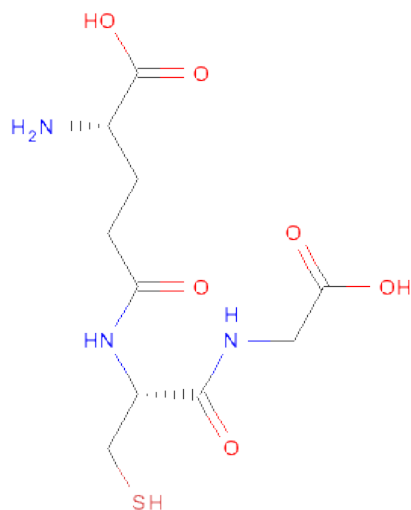
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



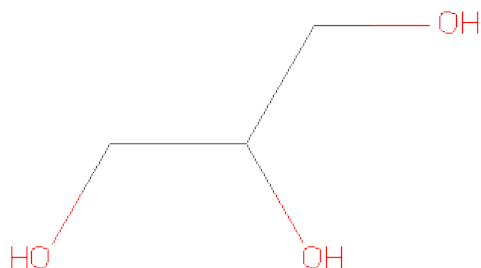
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is GLUTATHIONE (three-letter code: GSH) (formula:  $C_{10}H_{17}N_3O_6S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
5	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	377	Total	O	0	0
			377	377		
7	B	349	Total	O	0	0
			349	349		

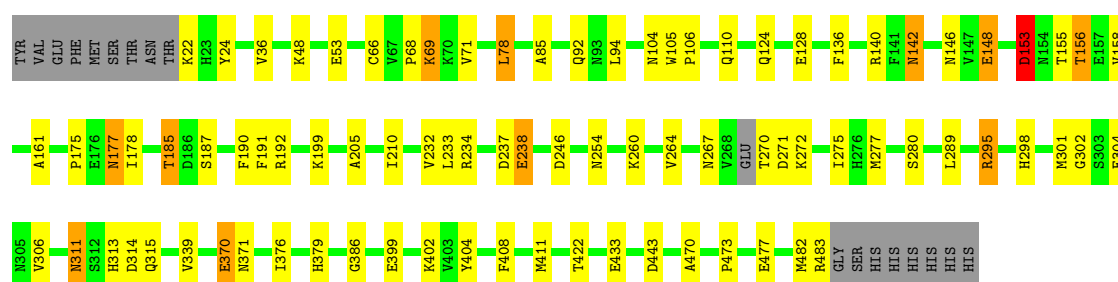


### 3 Residue-property plots

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.

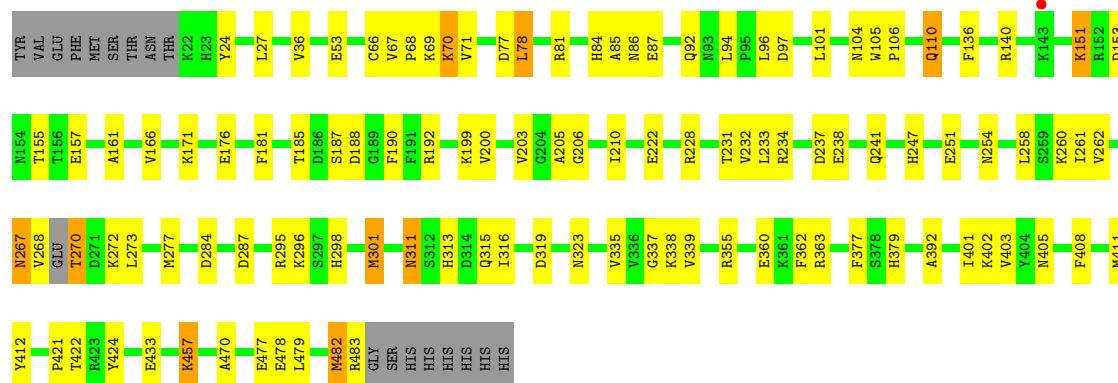
#### • Molecule 1: Glutathione reductase

Chain A:



#### • Molecule 1: Glutathione reductase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.97Å 116.97Å 85.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.05 – 2.40 21.05 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.8 (21.05-2.40) 92.9 (21.05-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.202 , 0.205 0.181 , 0.181	Depositor DCC
$R_{free}$ test set	2118 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 35.3	EDS
Estimated twinning fraction	0.487 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 41845 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: GOL, PO4, NAG, FAD, GSH

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	0.55	0/3658	0.75	5/4939 (0.1%)
1	B	0.57	2/3658 (0.1%)	0.74	3/4939 (0.1%)
All	All	0.56	2/7316 (0.0%)	0.74	8/9878 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	482	MET	C-N	5.33	1.46	1.34
1	B	87	GLU	CA-CB	-5.20	1.42	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ASP	N-CA-C	-5.85	95.20	111.00
1	B	237	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	97	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	148	GLU	CA-CB-CG	5.40	125.27	113.40
1	A	271	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	237	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	87	GLU	CB-CG-CD	-5.18	100.21	114.20
1	A	295	ARG	NE-CZ-NH2	-5.05	117.78	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	3588	0	3579	78	0
1	B	3588	0	3579	95	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
4	A	53	0	31	2	0
4	B	53	0	31	0	0
5	A	20	0	14	8	0
5	B	20	0	14	8	0
6	A	30	0	40	15	0
6	B	36	0	44	20	0
7	A	377	0	0	16	0
7	B	349	0	0	11	0
All	All	8152	0	7358	181	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 12.

All (181) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:B:6009:GOL:C2	6:B:6009:GOL:O2	1.63	1.46
6:A:6001:GOL:C2	6:A:6001:GOL:O2	1.64	1.43
6:A:6006:GOL:O2	6:A:6006:GOL:C2	1.67	1.40
6:B:6004:GOL:O2	6:B:6004:GOL:C2	1.73	1.37
1:B:110:GLN:HE21	1:B:110:GLN:HA	1.23	1.03
1:A:270:THR:HG22	1:A:272:LYS:H	1.32	0.93
1:A:205:ALA:HB3	7:A:6384:HOH:O	1.71	0.89
1:A:470:ALA:HB1	1:A:477:GLU:HG3	1.56	0.88
1:B:470:ALA:HB1	1:B:477:GLU:HG3	1.56	0.86
1:A:370:GLU:HG3	7:A:6323:HOH:O	1.75	0.84
1:A:104:ASN:HD22	1:B:92:GLN:HE22	1.26	0.84
6:B:6004:GOL:O2	6:B:6004:GOL:C1	2.26	0.83
1:A:473:PRO:HG2	1:B:70:LYS:HG3	1.61	0.82
1:A:36:VAL:HG12	3:A:5001:PO4:O3	1.81	0.80
6:B:6004:GOL:O2	6:B:6004:GOL:C3	2.31	0.79
1:B:337:GLY:C	6:B:6010:GOL:O1	2.21	0.79
1:B:238:GLU:HG3	5:B:4001:GSH:HA1	1.63	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:A:6001:GOL:O2	6:A:6001:GOL:C1	2.32	0.78
1:A:402:LYS:HD3	1:A:433:GLU:OE2	1.84	0.78
1:A:177:ASN:H	1:A:177:ASN:HD22	1.31	0.78
1:A:411:MET:CE	1:B:70:LYS:HB3	2.14	0.77
1:A:379:HIS:HD2	7:A:6234:HOH:O	1.68	0.75
1:A:142:ASN:C	1:A:142:ASN:HD22	1.91	0.73
1:A:238:GLU:CB	5:A:3001:GSH:HA1	2.19	0.73
6:A:6006:GOL:O2	6:A:6006:GOL:C1	2.37	0.72
1:B:36:VAL:HG12	3:B:5002:PO4:O2	1.90	0.72
6:A:6001:GOL:O2	6:A:6001:GOL:C3	2.37	0.72
1:A:411:MET:HE2	1:B:70:LYS:HB3	1.71	0.71
1:B:295:ARG:NE	7:B:6347:HOH:O	2.22	0.71
6:B:6009:GOL:C1	6:B:6009:GOL:O2	2.37	0.71
6:A:6006:GOL:O2	6:A:6006:GOL:C3	2.37	0.71
1:A:238:GLU:HB3	5:A:3001:GSH:HA1	1.72	0.71
1:B:110:GLN:HE21	1:B:110:GLN:CA	2.02	0.71
1:B:110:GLN:NE2	1:B:110:GLN:HA	2.01	0.70
1:A:148:GLU:HB3	1:A:158:VAL:HG22	1.72	0.70
1:A:92:GLN:HE22	1:B:104:ASN:HD22	1.39	0.69
1:A:311:ASN:ND2	1:A:315:GLN:H	1.91	0.69
1:A:175:PRO:HB2	1:A:178:ILE:HD12	1.74	0.68
1:A:233:LEU:HD13	1:A:376:ILE:HD13	1.76	0.67
1:A:275:ILE:HD11	1:A:289:LEU:HD22	1.77	0.67
1:B:238:GLU:CB	5:B:4001:GSH:HA1	2.25	0.67
1:B:238:GLU:CG	5:B:4001:GSH:HA1	2.25	0.66
1:B:360:GLU:O	1:B:363:ARG:HG3	1.95	0.66
5:A:3001:GSH:HB13	7:A:6247:HOH:O	1.96	0.66
1:B:205:ALA:HB3	7:B:6257:HOH:O	1.97	0.65
6:B:6009:GOL:C3	6:B:6009:GOL:O2	2.44	0.65
1:A:295:ARG:NH2	7:A:6380:HOH:O	2.30	0.64
1:B:268:VAL:HG12	1:B:268:VAL:O	1.97	0.64
1:A:155:THR:HG22	1:A:156:THR:N	2.11	0.64
1:B:479:LEU:HD23	1:B:482:MET:HE1	1.79	0.64
1:B:311:ASN:ND2	1:B:315:GLN:H	1.97	0.62
1:A:238:GLU:CG	5:A:3001:GSH:HA1	2.30	0.62
1:A:185:THR:HG22	7:A:6330:HOH:O	1.99	0.61
1:B:251:GLU:OE1	1:B:379:HIS:HD2	1.84	0.61
1:B:379:HIS:HB2	7:B:6205:HOH:O	2.01	0.60
1:A:178:ILE:HD11	6:A:6005:GOL:H11	1.84	0.59
1:B:402:LYS:HD3	1:B:433:GLU:OE1	2.03	0.59
6:B:6009:GOL:C2	6:B:6009:GOL:HO2	2.07	0.59
1:B:171:LYS:HE3	1:B:296:LYS:HE3	1.85	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:A:6001:GOL:HO2	6:A:6001:GOL:C2	2.08	0.58
1:A:192:ARG:NH2	6:A:6011:GOL:O3	2.36	0.58
1:B:151:LYS:HE3	1:B:157:GLU:HB2	1.84	0.58
1:B:228:ARG:HG2	6:B:6003:GOL:H12	1.84	0.58
1:B:295:ARG:NH2	7:B:6347:HOH:O	2.37	0.57
1:B:86:ASN:HD21	1:B:96:LEU:H	1.53	0.57
1:A:443:ASP:CG	7:A:6293:HOH:O	2.42	0.57
1:B:238:GLU:HB2	5:B:4001:GSH:HA1	1.87	0.57
6:A:6006:GOL:HO2	6:A:6006:GOL:C2	2.11	0.56
1:B:166:VAL:HG11	1:B:301:MET:CE	2.35	0.56
1:A:205:ALA:CB	6:A:6001:GOL:H2	2.36	0.56
1:B:254:ASN:HB3	7:B:6248:HOH:O	2.05	0.56
1:B:231:THR:HG21	1:B:241:GLN:OE1	2.06	0.56
1:A:205:ALA:HB3	6:A:6001:GOL:H2	1.88	0.55
1:B:205:ALA:HB3	6:B:6003:GOL:O2	2.06	0.55
1:B:166:VAL:HG11	1:B:301:MET:HE3	1.89	0.55
1:A:443:ASP:CB	7:A:6293:HOH:O	2.55	0.54
1:B:295:ARG:CZ	7:B:6347:HOH:O	2.56	0.54
1:B:408:PHE:CE1	1:B:478:GLU:HG3	2.42	0.54
1:A:254:ASN:HB3	7:A:6163:HOH:O	2.08	0.53
1:A:177:ASN:H	1:A:177:ASN:ND2	2.04	0.53
1:B:479:LEU:HD23	1:B:482:MET:CE	2.38	0.53
1:B:311:ASN:ND2	1:B:313:HIS:H	2.07	0.53
1:A:275:ILE:CD1	1:A:289:LEU:HD22	2.39	0.53
1:B:247:HIS:HA	6:B:6007:GOL:H32	1.91	0.53
1:B:392:ALA:HB1	1:B:401:ILE:HD12	1.90	0.53
1:B:338:LYS:N	6:B:6010:GOL:O1	2.42	0.53
1:A:311:ASN:HD21	1:A:315:GLN:H	1.54	0.53
1:B:192:ARG:NH2	6:B:6009:GOL:O1	2.42	0.52
1:A:411:MET:HE1	1:B:70:LYS:HB3	1.89	0.52
1:A:205:ALA:HB3	6:A:6001:GOL:C2	2.39	0.52
1:A:238:GLU:HG3	5:A:3001:GSH:HA1	1.91	0.52
1:A:379:HIS:CD2	7:A:6234:HOH:O	2.53	0.52
1:B:323:ASN:ND2	6:B:6002:GOL:O3	2.39	0.52
1:B:206:GLY:O	1:B:210:ILE:HD13	2.10	0.51
1:B:228:ARG:CG	6:B:6003:GOL:H12	2.40	0.51
1:A:199:LYS:NZ	7:A:6314:HOH:O	2.24	0.51
1:B:234:ARG:HG2	7:B:6257:HOH:O	2.10	0.51
1:A:71:VAL:HG23	1:B:411:MET:HE3	1.92	0.51
6:B:6004:GOL:H31	7:B:6106:HOH:O	2.11	0.51
1:A:142:ASN:HD21	1:A:146:ASN:H	1.58	0.50
1:B:267:ASN:ND2	1:B:268:VAL:H	2.08	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:267:ASN:HB3	1:A:270:THR:HG21	1.94	0.50
1:A:192:ARG:NH1	7:A:6286:HOH:O	2.44	0.50
1:B:238:GLU:HB2	5:B:4001:GSH:CA1	2.42	0.50
1:B:405:ASN:ND2	5:B:4001:GSH:O2	2.44	0.50
1:A:443:ASP:HB2	7:A:6293:HOH:O	2.12	0.50
1:B:24:TYR:O	1:B:161:ALA:HA	2.13	0.49
1:B:421:PRO:HG3	6:B:6007:GOL:H12	1.94	0.49
1:B:203:VAL:HG21	1:B:261:ILE:HD12	1.94	0.49
1:A:153:ASP:HB3	1:A:155:THR:OG1	2.13	0.48
1:A:238:GLU:HB3	5:A:3001:GSH:CB1	2.43	0.48
1:A:205:ALA:CB	7:A:6384:HOH:O	2.44	0.48
1:A:78:LEU:HD13	1:B:85:ALA:HA	1.95	0.48
1:A:371:ASN:ND2	1:A:386:GLY:HA2	2.28	0.48
1:A:142:ASN:C	1:A:142:ASN:ND2	2.65	0.48
1:B:77:ASP:O	1:B:81:ARG:HG3	2.13	0.48
1:B:424:TYR:HB3	1:B:482:MET:HE1	1.96	0.48
1:A:105:TRP:HB3	1:A:106:PRO:HD3	1.95	0.48
1:A:238:GLU:HB3	5:A:3001:GSH:CA1	2.44	0.47
1:B:153:ASP:OD2	1:B:155:THR:HG23	2.15	0.47
1:B:176:GLU:HG2	1:B:181:PHE:CZ	2.49	0.47
1:B:27:LEU:C	1:B:27:LEU:HD23	2.35	0.47
1:A:238:GLU:HB3	5:A:3001:GSH:HB12	1.96	0.47
1:A:205:ALA:HB1	1:A:232:VAL:HA	1.95	0.47
1:B:392:ALA:HB1	1:B:401:ILE:CD1	2.45	0.47
1:B:105:TRP:HB3	1:B:106:PRO:HD3	1.97	0.47
1:A:71:VAL:CG2	1:B:411:MET:HE3	2.45	0.46
1:A:124:GLN:O	1:A:128:GLU:HG2	2.15	0.46
1:A:399:GLU:H	1:A:399:GLU:CD	2.19	0.46
1:A:411:MET:HE3	1:B:71:VAL:HG23	1.97	0.45
1:A:246:ASP:OD2	7:A:6108:HOH:O	2.21	0.45
1:A:311:ASN:HD22	1:A:311:ASN:C	2.19	0.45
1:A:311:ASN:ND2	1:A:313:HIS:H	2.14	0.45
1:B:166:VAL:CG1	1:B:301:MET:HE3	2.46	0.45
6:B:6007:GOL:O2	7:B:6120:HOH:O	2.21	0.45
1:B:228:ARG:O	1:B:258:LEU:HA	2.16	0.45
5:B:4001:GSH:HG12	7:B:6252:HOH:O	2.16	0.45
1:B:153:ASP:C	1:B:153:ASP:OD2	2.55	0.45
1:B:270:THR:HG22	1:B:272:LYS:H	1.81	0.45
1:B:234:ARG:HG3	1:B:234:ARG:HH11	1.82	0.45
1:B:110:GLN:NE2	1:B:110:GLN:CA	2.69	0.44
1:B:311:ASN:HD22	1:B:311:ASN:C	2.20	0.44
1:A:85:ALA:HA	1:B:78:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:311:ASN:HD21	1:B:315:GLN:H	1.66	0.44
1:B:238:GLU:HB2	5:B:4001:GSH:CB1	2.48	0.44
1:B:408:PHE:CZ	1:B:422:THR:HG21	2.53	0.43
1:B:53:GLU:O	1:B:136:PHE:HA	2.18	0.43
1:A:404:TYR:HD1	1:A:483:ARG:HB3	1.83	0.43
1:B:272:LYS:HE2	1:B:287:ASP:OD1	2.17	0.43
1:B:268:VAL:CG1	1:B:268:VAL:O	2.64	0.43
1:B:319:ASP:OD2	1:B:323:ASN:HB2	2.18	0.43
1:B:84:HIS:HD2	1:B:412:TYR:OH	2.02	0.43
1:B:171:LYS:CE	1:B:296:LYS:HE3	2.48	0.43
1:A:408:PHE:CZ	1:A:422:THR:HG21	2.53	0.42
1:B:233:LEU:HA	7:B:6063:HOH:O	2.18	0.42
1:A:24:TYR:O	1:A:161:ALA:HA	2.19	0.42
1:A:264:VAL:HG22	1:A:275:ILE:HD13	2.00	0.42
1:B:70:LYS:HE3	1:B:377:PHE:CZ	2.55	0.42
1:B:457:LYS:HD2	1:B:457:LYS:HA	1.84	0.42
1:A:140:ARG:HG3	1:A:302:GLY:N	2.33	0.42
1:A:199:LYS:CE	7:A:6314:HOH:O	2.68	0.42
1:B:403:VAL:O	1:B:483:ARG:CZ	2.68	0.42
1:A:260:LYS:HA	6:A:6005:GOL:O3	2.20	0.42
1:A:68:PRO:HB2	1:A:191:PHE:CE1	2.54	0.42
1:A:53:GLU:O	1:A:136:PHE:HA	2.20	0.41
1:B:188:ASP:HB2	6:B:6009:GOL:H2	2.01	0.41
1:A:234:ARG:NH2	6:A:6001:GOL:O1	2.48	0.41
1:B:355:ARG:HA	1:B:362:PHE:O	2.21	0.41
1:B:187:SER:O	1:B:190:PHE:HB3	2.21	0.41
1:A:24:TYR:CD2	1:A:48:LYS:HG2	2.56	0.41
1:A:187:SER:O	1:A:190:PHE:HB3	2.21	0.41
1:B:232:VAL:O	1:B:241:GLN:HG2	2.21	0.41
1:B:247:HIS:CA	6:B:6007:GOL:H32	2.50	0.41
4:A:1001:FAD:H1'1	4:A:1001:FAD:H9	1.85	0.41
1:B:199:LYS:HE3	1:B:222:GLU:OE2	2.21	0.40
1:B:316:ILE:HD12	1:B:335:VAL:CG2	2.52	0.40
1:B:67:VAL:HB	1:B:68:PRO:CD	2.51	0.40
1:A:233:LEU:CD1	1:A:376:ILE:HD13	2.50	0.40
1:A:411:MET:HE1	1:B:70:LYS:CB	2.52	0.40
1:A:69:LYS:NZ	4:A:1001:FAD:N5	2.69	0.40
1:B:231:THR:CG2	1:B:241:GLN:OE1	2.69	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	457/479 (95%)	438 (96%)	17 (4%)	2 (0%)	43	61
1	B	457/479 (95%)	438 (96%)	18 (4%)	1 (0%)	56	74
All	All	914/958 (95%)	876 (96%)	35 (4%)	3 (0%)	50	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	THR
1	A	339	VAL
1	B	339	VAL

### 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	386/403 (96%)	364 (94%)	22 (6%)	29	44
1	B	386/403 (96%)	364 (94%)	22 (6%)	29	44
All	All	772/806 (96%)	728 (94%)	44 (6%)	29	44

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	66	CYS
1	A	69	LYS
1	A	78	LEU
1	A	94	LEU
1	A	110	GLN

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Mol	Chain	Res	Type
1	A	142	ASN
1	A	153	ASP
1	A	177	ASN
1	A	185	THR
1	A	210	ILE
1	A	238	GLU
1	A	277	MET
1	A	280	SER
1	A	298	HIS
1	A	301	MET
1	A	304	GLU
1	A	306	VAL
1	A	311	ASN
1	A	314	ASP
1	A	370	GLU
1	A	482	MET
1	B	66	CYS
1	B	69	LYS
1	B	70	LYS
1	B	78	LEU
1	B	94	LEU
1	B	101	LEU
1	B	110	GLN
1	B	140	ARG
1	B	151	LYS
1	B	185	THR
1	B	200	VAL
1	B	260	LYS
1	B	262	VAL
1	B	267	ASN
1	B	270	THR
1	B	273	LEU
1	B	277	MET
1	B	284	ASP
1	B	298	HIS
1	B	301	MET
1	B	311	ASN
1	B	457	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	93	ASN
1	A	117	HIS
1	A	126	ASN
1	A	142	ASN
1	A	146	ASN
1	A	177	ASN
1	A	242	ASN
1	A	276	HIS
1	A	298	HIS
1	A	311	ASN
1	A	323	ASN
1	A	371	ASN
1	A	432	ASN
1	B	84	HIS
1	B	86	ASN
1	B	92	GLN
1	B	110	GLN
1	B	267	ASN
1	B	298	HIS
1	B	311	ASN
1	B	371	ASN
1	B	405	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 ⓘ

19 ligands are modelled in this entry.

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
4	FAD	A	1001	-	58,58,58	1.19	4 (6%)	85,89,89	1.66	12 (14%)
2	NAG	A	1301	1	12,14,15	0.64	0	15,19,21	0.97	1 (6%)
5	GSH	A	3001	1	19,19,19	1.43	4 (21%)	24,24,24	1.49	3 (12%)
3	PO4	A	5001	-	4,4,4	0.69	0	6,6,6	0.31	0
6	GOL	A	6001	-	5,5,5	3.41	3 (60%)	5,5,5	3.68	5 (100%)
6	GOL	A	6005	-	5,5,5	0.33	0	5,5,5	0.97	0
6	GOL	A	6006	-	5,5,5	4.22	3 (60%)	5,5,5	3.72	5 (100%)
6	GOL	A	6008	-	5,5,5	1.21	1 (20%)	5,5,5	1.54	1 (20%)
6	GOL	A	6011	-	5,5,5	1.61	1 (20%)	5,5,5	1.60	1 (20%)
2	NAG	B	1303	1	12,14,15	0.47	0	15,19,21	0.89	0
4	FAD	B	2001	-	58,58,58	1.20	4 (6%)	85,89,89	1.61	11 (12%)
5	GSH	B	4001	1	19,19,19	1.44	3 (15%)	24,24,24	2.24	10 (41%)
3	PO4	B	5002	-	4,4,4	0.78	0	6,6,6	0.31	0
6	GOL	B	6002	-	5,5,5	0.91	0	5,5,5	1.01	0
6	GOL	B	6003	-	5,5,5	4.73	3 (60%)	5,5,5	5.36	5 (100%)
6	GOL	B	6004	-	5,5,5	4.53	3 (60%)	5,5,5	3.61	4 (80%)
6	GOL	B	6007	-	5,5,5	1.93	2 (40%)	5,5,5	3.04	3 (60%)
6	GOL	B	6009	-	5,5,5	3.39	3 (60%)	5,5,5	2.93	4 (80%)
6	GOL	B	6010	-	5,5,5	2.24	1 (20%)	5,5,5	2.46	4 (80%)

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
4	FAD	A	1001	-	-	0/34/50/50	0/1/6/6
2	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	GSH	A	3001	1	-	0/24/24/24	0/0/0/0
3	PO4	A	5001	-	-	0/0/0/0	0/0/0/0
6	GOL	A	6001	-	-	0/4/4/4	0/0/0/0
6	GOL	A	6005	-	-	0/4/4/4	0/0/0/0
6	GOL	A	6006	-	-	0/4/4/4	0/0/0/0
6	GOL	A	6008	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	6011	-	-	0/4/4/4	0/0/0/0
2	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
4	FAD	B	2001	-	-	0/34/50/50	0/1/6/6
5	GSH	B	4001	1	-	0/24/24/24	0/0/0/0
3	PO4	B	5002	-	-	0/0/0/0	0/0/0/0
6	GOL	B	6002	-	-	0/4/4/4	0/0/0/0
6	GOL	B	6003	-	-	0/4/4/4	0/0/0/0
6	GOL	B	6004	-	-	0/4/4/4	0/0/0/0
6	GOL	B	6007	-	-	0/4/4/4	0/0/0/0
6	GOL	B	6009	-	-	0/4/4/4	0/0/0/0
6	GOL	B	6010	-	-	0/4/4/4	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	6004	GOL	O2-C2	9.49	1.73	1.43
6	B	6003	GOL	O2-C2	-8.51	1.17	1.43
6	A	6006	GOL	O2-C2	7.68	1.67	1.43
6	A	6001	GOL	O2-C2	6.66	1.64	1.43
6	B	6009	GOL	O2-C2	6.40	1.63	1.43
6	B	6010	GOL	O2-C2	4.51	1.57	1.43
6	B	6003	GOL	O3-C3	4.44	1.61	1.42
6	B	6003	GOL	O1-C1	3.72	1.58	1.42
6	A	6006	GOL	O1-C1	3.58	1.57	1.42
6	A	6006	GOL	O3-C3	3.56	1.57	1.42
4	B	2001	FAD	C5X-N5	3.35	1.40	1.35
6	A	6011	GOL	O2-C2	3.33	1.54	1.43
6	B	6007	GOL	O2-C2	-3.22	1.33	1.43
4	A	1001	FAD	C5X-N5	3.22	1.40	1.35
5	B	4001	GSH	O12-C1	-2.96	1.19	1.30
4	B	2001	FAD	C4A-N9A	-2.90	1.33	1.37
4	A	1001	FAD	C4A-N9A	-2.81	1.33	1.37
4	B	2001	FAD	C10-N1	2.79	1.40	1.35
4	A	1001	FAD	C10-N1	2.79	1.40	1.35
6	A	6001	GOL	O1-C1	2.79	1.54	1.42
6	B	6009	GOL	O3-C3	2.72	1.54	1.42
6	A	6008	GOL	O2-C2	2.56	1.51	1.43
6	B	6009	GOL	O1-C1	2.56	1.53	1.42
5	A	3001	GSH	O12-C1	-2.54	1.21	1.30
5	A	3001	GSH	O2-C2	2.50	1.28	1.23
6	B	6007	GOL	O1-C1	-2.43	1.31	1.42
6	A	6001	GOL	O3-C3	2.40	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4001	GSH	O2-C2	2.35	1.28	1.23
5	B	4001	GSH	OE1-CD1	2.29	1.28	1.23
5	A	3001	GSH	CB1-CA1	-2.25	1.47	1.54
6	B	6004	GOL	O1-C1	2.24	1.52	1.42
4	B	2001	FAD	C6-C5X	-2.22	1.39	1.41
4	A	1001	FAD	C8A-N9A	-2.08	1.33	1.36
6	B	6004	GOL	C1-C2	2.03	1.60	1.52
5	A	3001	GSH	OE1-CD1	2.01	1.27	1.23

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	FAD	N3A-C2A-N1A	-8.69	121.45	128.71
4	B	2001	FAD	N3A-C2A-N1A	-8.26	121.80	128.71
6	B	6003	GOL	O2-C2-C1	6.35	137.15	108.22
6	B	6003	GOL	O2-C2-C3	5.66	134.01	108.22
6	B	6007	GOL	C3-C2-C1	-5.23	88.18	111.26
6	B	6003	GOL	C3-C2-C1	-5.15	88.54	111.26
6	B	6004	GOL	O2-C2-C1	-5.00	85.47	108.22
4	A	1001	FAD	N3A-C4A-N9A	4.92	134.32	125.43
4	B	2001	FAD	N3A-C4A-N9A	4.77	134.05	125.43
6	B	6003	GOL	O3-C3-C2	-4.74	86.60	109.71
6	B	6003	GOL	O1-C1-C2	-4.72	86.67	109.71
6	A	6006	GOL	C3-C2-C1	-4.67	90.62	111.26
5	B	4001	GSH	CB1-CA1-N1	-4.57	98.95	110.14
5	B	4001	GSH	CG1-CD1-N2	4.49	124.36	115.83
6	B	6004	GOL	O2-C2-C3	-4.47	87.85	108.22
6	A	6001	GOL	O1-C1-C2	-4.47	87.90	109.71
6	A	6001	GOL	C3-C2-C1	-4.15	92.94	111.26
5	B	4001	GSH	OE1-CD1-CG1	-4.07	113.82	121.92
6	A	6006	GOL	O1-C1-C2	-3.79	91.20	109.71
6	A	6001	GOL	O3-C3-C2	-3.78	91.25	109.71
6	B	6009	GOL	C3-C2-C1	-3.70	94.92	111.26
6	B	6004	GOL	C3-C2-C1	-3.69	94.96	111.26
4	B	2001	FAD	C2-N1-C10	3.61	118.61	114.98
4	B	2001	FAD	C4B-O4B-C1B	-3.59	105.85	109.75
5	B	4001	GSH	C1-CA1-N1	3.58	115.30	109.36
4	A	1001	FAD	O4B-C1B-C2B	-3.53	101.35	106.77
6	A	6006	GOL	O3-C3-C2	-3.50	92.65	109.71
4	A	1001	FAD	C2-N1-C10	3.42	118.43	114.98
4	A	1001	FAD	C4B-O4B-C1B	-3.42	106.04	109.75
6	B	6009	GOL	O1-C1-C2	-3.42	93.05	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	6006	GOL	O2-C2-C1	-3.33	93.05	108.22
4	A	1001	FAD	C5A-C4A-N3A	-3.28	118.57	125.70
4	A	1001	FAD	C4X-N5-C5X	3.20	120.29	116.69
6	A	6001	GOL	O2-C2-C1	-3.16	93.83	108.22
5	B	4001	GSH	O12-C1-CA1	-3.12	109.89	116.88
6	A	6006	GOL	O2-C2-C3	-3.10	94.10	108.22
4	B	2001	FAD	C5A-C4A-N3A	-3.03	119.09	125.70
6	B	6010	GOL	C3-C2-C1	-3.03	97.87	111.26
4	B	2001	FAD	O4B-C1B-N9A	-3.02	105.63	108.44
6	A	6011	GOL	C3-C2-C1	-2.97	98.15	111.26
6	B	6010	GOL	O1-C1-C2	-2.96	95.29	109.71
5	A	3001	GSH	CA3-N3-C2	-2.88	114.91	121.29
6	B	6007	GOL	O2-C2-C1	2.88	121.33	108.22
6	B	6007	GOL	O2-C2-C3	2.87	121.30	108.22
5	A	3001	GSH	C3-CA3-N3	-2.84	106.03	112.83
2	A	1301	NAG	C3-C2-N2	-2.78	107.53	111.76
5	A	3001	GSH	CB1-CA1-N1	2.75	116.86	110.14
4	B	2001	FAD	O4B-C1B-C2B	-2.72	102.61	106.77
4	B	2001	FAD	C4X-N5-C5X	2.67	119.69	116.69
6	B	6009	GOL	O2-C2-C1	-2.66	96.11	108.22
4	A	1001	FAD	C2A-N3A-C4A	2.62	121.47	114.01
6	B	6009	GOL	O3-C3-C2	-2.58	97.14	109.71
6	B	6004	GOL	O1-C1-C2	-2.53	97.35	109.71
4	A	1001	FAD	P-O3P-PA	-2.50	124.35	131.68
6	A	6001	GOL	O2-C2-C3	-2.50	96.84	108.22
6	A	6008	GOL	C3-C2-C1	-2.49	100.27	111.26
4	A	1001	FAD	C5X-C9A-N10	2.45	119.22	116.80
4	A	1001	FAD	C4-N3-C2	-2.44	120.38	125.39
5	B	4001	GSH	CA3-N3-C2	-2.44	115.89	121.29
5	B	4001	GSH	O11-C1-CA1	-2.43	111.35	118.36
4	B	2001	FAD	C4-N3-C2	-2.38	120.51	125.39
4	B	2001	FAD	C2A-N3A-C4A	2.34	120.68	114.01
4	B	2001	FAD	P-O3P-PA	-2.30	124.93	131.68
5	B	4001	GSH	C3-CA3-N3	-2.26	107.43	112.83
6	B	6010	GOL	O2-C2-C1	-2.23	98.08	108.22
5	B	4001	GSH	CB2-CA2-C2	-2.21	104.88	109.70
5	B	4001	GSH	O12-C1-O11	2.19	129.03	124.07
4	A	1001	FAD	C4A-C5A-N7A	-2.17	107.66	109.52
6	B	6010	GOL	O3-C3-C2	-2.11	99.44	109.71

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	461/479 (96%)	-0.54	0 100 100	12, 22, 48, 73	0
1	B	461/479 (96%)	-0.52	1 (0%) 93 94	13, 22, 47, 68	0
All	All	922/958 (96%)	-0.53	1 (0%) 93 95	12, 22, 48, 73	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	143	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
6	GOL	B	6010	6/6	0.32	20.98	46,47,48,48	6
6	GOL	A	6001	6/6	0.33	19.52	33,36,39,42	6

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	A	6008	6/6	0.28	14.18	41,46,47,49	6
6	GOL	B	6003	6/6	0.42	12.25	28,30,33,35	6
6	GOL	A	6005	6/6	0.25	4.67	32,33,33,34	6
6	GOL	B	6007	6/6	0.19	4.30	29,30,32,33	6
6	GOL	B	6009	6/6	0.18	3.90	40,42,43,43	6
5	GSH	A	3001	20/20	0.33	3.84	27,43,54,54	20
3	PO4	B	5002	5/5	0.19	3.67	40,40,41,41	5
6	GOL	B	6002	6/6	0.27	3.25	39,43,44,45	6
6	GOL	B	6004	6/6	0.19	2.92	25,30,31,35	6
5	GSH	B	4001	20/20	0.31	2.90	23,40,49,49	20
6	GOL	A	6011	6/6	0.19	2.75	39,41,42,44	6
3	PO4	A	5001	5/5	0.16	1.43	41,42,43,44	5
6	GOL	A	6006	6/6	0.24	1.30	38,38,39,41	6
2	NAG	B	1303	14/15	0.14	0.15	31,35,38,40	0
4	FAD	A	1001	53/53	0.11	0.08	10,17,24,26	0
2	NAG	A	1301	14/15	0.13	-0.18	30,33,36,36	0
4	FAD	B	2001	53/53	0.11	-0.22	12,16,22,24	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.