



# Full wwPDB X-ray Structure Validation Report

Nov 6, 2014 – 11:02 PM EST

PDB ID : 3DB2  
Title : Crystal structure of a putative nadph-dependent oxidoreductase (dhaf\_2064)  
from desulfitobacterium hafniense dcb-2 at 1.70 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2008-05-30  
Resolution : 1.70 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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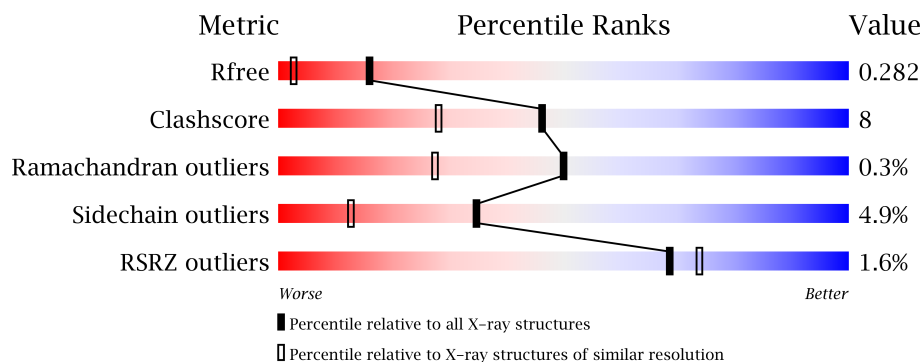
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24103  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24103

# 1 Overall quality at a glance

The reported resolution of this entry is 1.70 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	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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	354	
1	B	354	
1	C	354	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	C	355	-	X

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 8697 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.

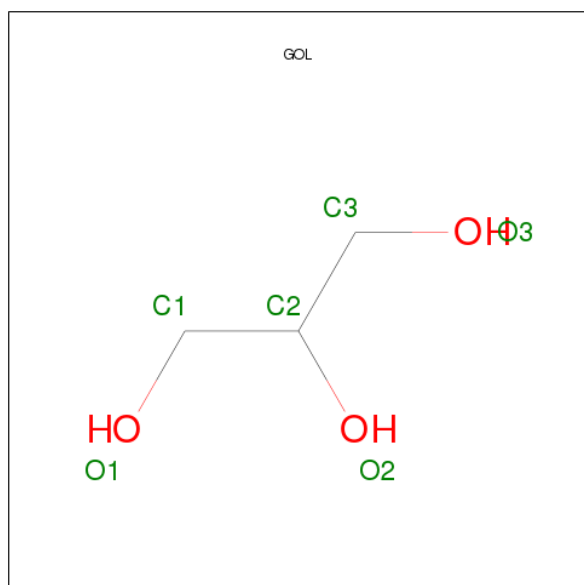
- Molecule 1 is a protein called putative NADPH-dependent oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	Se	0	5	0
			2685	1703	467	504	5	6			
1	B	343	Total	C	N	O	S	Se	0	5	0
			2666	1692	458	505	5	6			
1	C	346	Total	C	N	O	S	Se	0	8	0
			2736	1735	471	518	5	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP Q18XG3
B	0	GLY	-	leader sequence	UNP Q18XG3
C	0	GLY	-	leader sequence	UNP Q18XG3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 3 is water.

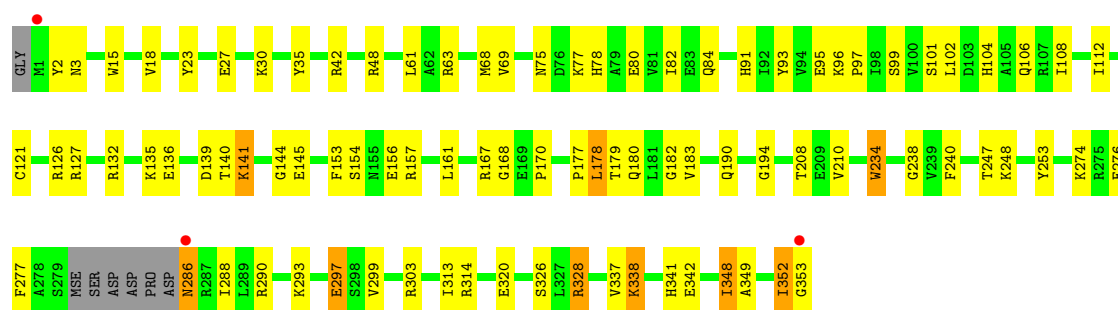
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	191	Total	O	0	0
			191	191		
3	B	154	Total	O	0	0
			154	154		
3	C	253	Total	O	0	0
			253	253		

### 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.

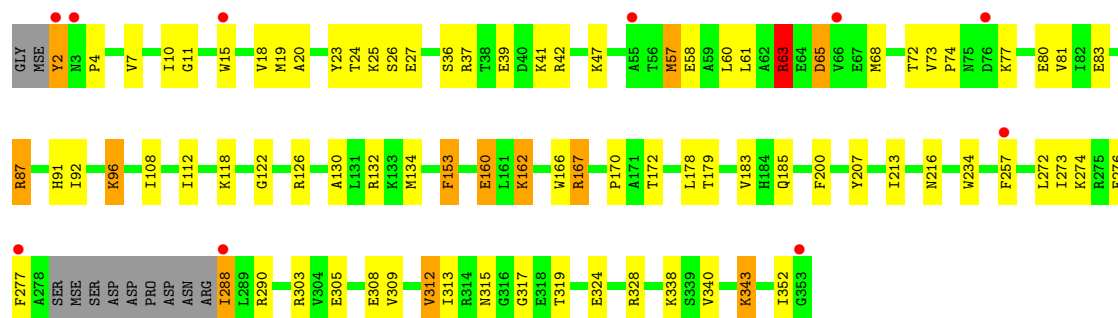
- Molecule 1: putative NADPH-dependent oxidoreductase

Chain A: 



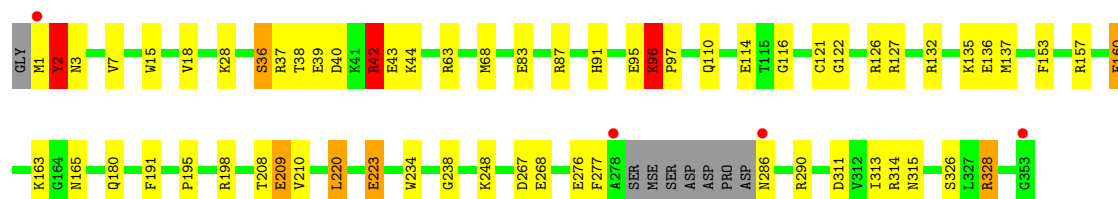
- Molecule 1: putative NADPH-dependent oxidoreductase

Chain B: 



- Molecule 1: putative NADPH-dependent oxidoreductase

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.62Å 104.62Å 173.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.75 – 1.70 29.46 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.75-1.70) 97.7 (29.46-1.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 1.70Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.142 , 0.174 0.265 , 0.282	Depositor DCC
$R_{free}$ test set	5942 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.9	EDS
Estimated twinning fraction	0.380 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 120815 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	8697	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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

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	0.45	0/2740	1.29	22/3697 (0.6%)
1	B	0.45	0/2720	1.27	19/3673 (0.5%)
1	C	0.49	0/2802	1.26	14/3779 (0.4%)
All	All	0.46	0/8262	1.28	55/11149 (0.5%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	198	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	B	63	ARG	NE-CZ-NH2	-10.23	115.19	120.30
1	C	314	ARG	NE-CZ-NH2	9.66	125.13	120.30
1	A	42	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	B	132	ARG	CD-NE-CZ	8.47	135.46	123.60
1	A	63	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	B	23	TYR	CB-CG-CD1	8.17	125.90	121.00
1	A	93	TYR	CB-CG-CD2	7.96	125.78	121.00
1	B	96	LYS	CA-C-N	7.64	138.48	117.10
1	A	96	LYS	CA-C-N	7.59	138.35	117.10
1	B	303	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	B	328	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	C	97	PRO	N-CA-C	-6.93	94.08	112.10
1	A	314	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	63	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	328	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	A	144	GLY	C-N-CA	6.56	138.11	121.70
1	A	48	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	C	2	TYR	CB-CG-CD1	6.39	124.84	121.00
1	A	126	ARG	CD-NE-CZ	6.35	132.49	123.60
1	A	96	LYS	O-C-N	-6.35	109.04	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	42[A]	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	42[B]	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	96	LYS	CA-C-N	6.23	134.55	117.10
1	B	26	SER	C-N-CA	6.20	137.21	121.70
1	C	127	ARG	CD-NE-CZ	6.19	132.27	123.60
1	B	96	LYS	O-C-N	-6.19	109.34	121.10
1	A	27	GLU	C-N-CA	6.19	137.16	121.70
1	B	126	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	2	TYR	CA-CB-CG	6.04	124.88	113.40
1	C	132	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	C	63	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	290	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	23	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	B	305	GLU	CA-CB-CG	5.78	126.11	113.40
1	A	240	PHE	CB-CG-CD1	5.72	124.80	120.80
1	B	87	ARG	CD-NE-CZ	5.71	131.60	123.60
1	A	253	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	B	200	PHE	CB-CG-CD2	5.55	124.69	120.80
1	A	314	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	352	ILE	C-N-CA	5.50	133.85	122.30
1	A	23	TYR	CA-CB-CG	5.46	123.78	113.40
1	A	35	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	B	207	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	C	126	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	B	27	GLU	C-N-CA	5.29	134.92	121.70
1	B	37	ARG	C-N-CA	5.27	134.87	121.70
1	C	132	ARG	CD-NE-CZ	5.15	130.81	123.60
1	B	290	ARG	CD-NE-CZ	5.10	130.73	123.60
1	A	253	TYR	CB-CG-CD1	5.04	124.02	121.00
1	C	96	LYS	CA-C-O	-5.03	109.53	120.10
1	A	297	GLU	CA-CB-CG	5.02	124.44	113.40
1	A	303	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	B	167	ARG	NE-CZ-NH2	-5.01	117.80	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	2685	0	2661	45	0
1	B	2666	0	2621	49	0
1	C	2736	0	2732	39	0
2	C	12	0	16	3	0
3	A	191	0	0	7	0
3	B	154	0	0	6	0
3	C	253	0	0	8	0
All	All	8697	0	8030	133	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 8.

All (133) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1:MSE:SE	1:C:28:LYS:HE3	1.98	1.13
1:C:1:MSE:SE	1:C:28:LYS:CE	2.73	0.85
1:B:308[B]:GLU:O	1:B:312:VAL:HG22	1.83	0.79
1:C:36:SER:O	1:C:42[A]:ARG:HD2	1.83	0.78
1:B:15:TRP:CZ2	1:B:19:MSE:SE	2.87	0.77
1:C:39:GLU:O	1:C:43:GLU:HG2	1.85	0.76
1:A:135:LYS:HE3	1:A:139:ASP:OD2	1.84	0.76
1:C:137:MSE:HE3	2:C:354:GOL:H12	1.68	0.75
1:B:80:GLU:HG2	3:B:415:HOH:O	1.85	0.75
1:B:160:GLU:HB2	3:B:482:HOH:O	1.88	0.74
1:B:309:VAL:O	1:B:313:ILE:HG13	1.89	0.73
1:C:38:THR:O	1:C:42[A]:ARG:HD3	1.88	0.72
1:A:248:LYS:HE3	3:A:475:HOH:O	1.90	0.72
1:B:308[A]:GLU:O	1:B:312:VAL:HG22	1.91	0.70
1:A:208:THR:OG1	1:A:210:VAL:HG22	1.93	0.69
1:C:160:GLU:O	1:C:160:GLU:HG3	1.95	0.67
1:B:160:GLU:O	1:B:162:LYS:HE3	1.96	0.66
1:A:102:LEU:O	1:A:106:GLN:HG3	1.96	0.66
1:C:83:GLU:O	1:C:87:ARG:HG3	1.97	0.65
1:A:190:GLN:OE1	1:A:328:ARG:HD3	1.96	0.65
1:B:77:LYS:O	1:B:81:VAL:HG23	1.97	0.64
1:A:157:ARG:O	1:A:161:LEU:HD13	1.98	0.64
1:C:267:ASP:O	2:C:355:GOL:H11	1.98	0.63
1:B:74:PRO:O	1:B:77:LYS:HB3	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:108:ILE:O	1:A:112:ILE:HG12	1.98	0.63
1:B:41:LYS:HE3	3:B:501:HOH:O	2.00	0.62
1:B:160:GLU:HA	1:B:160:GLU:OE1	2.00	0.62
1:B:170:PRO:HD2	3:B:458:HOH:O	2.00	0.61
1:C:3:ASN:HB2	3:C:537:HOH:O	2.02	0.60
1:A:80:GLU:HB3	3:A:446:HOH:O	2.01	0.60
1:B:83:GLU:O	1:B:87:ARG:HG3	2.02	0.60
1:B:108:ILE:O	1:B:112:ILE:HG12	2.02	0.59
1:C:163:LYS:HG2	1:C:209:GLU:O	2.01	0.59
1:A:328:ARG:NH2	1:A:348:ILE:HG21	2.18	0.58
1:B:36:SER:O	1:B:42:ARG:HD3	2.03	0.58
1:C:40:ASP:O	1:C:43:GLU:HB2	2.03	0.58
1:C:136:GLU:HG2	3:C:582:HOH:O	2.05	0.57
1:B:60:LEU:O	1:B:63:ARG:HB2	2.05	0.56
1:B:179:THR:O	1:B:183:VAL:HG23	2.06	0.56
1:B:15:TRP:CE2	1:B:19:MSE:SE	3.09	0.55
1:B:15:TRP:CZ3	1:B:18:VAL:HG11	2.42	0.55
1:B:324:GLU:HG3	3:B:356:HOH:O	2.05	0.55
1:A:157:ARG:HD2	1:A:167:ARG:CZ	2.37	0.54
1:B:7:VAL:HA	1:B:68:MSE:O	2.06	0.54
1:B:10:ILE:HD13	1:B:57:MSE:SE	2.58	0.54
1:C:39:GLU:HA	1:C:42[A]:ARG:NE	2.23	0.54
1:A:15:TRP:CZ3	1:A:18:VAL:HG11	2.43	0.54
1:B:308[A]:GLU:OE2	1:B:319:THR:HB	2.06	0.53
1:C:91:HIS:ND1	1:C:313:ILE:HG12	2.24	0.53
1:A:97:PRO:HB2	1:A:99:SER:O	2.08	0.53
1:B:63:ARG:HB3	1:B:65:ASP:OD1	2.09	0.52
1:C:208:THR:OG1	1:C:210:VAL:HG22	2.09	0.52
1:C:277:PHE:HB3	1:C:286:ASN:CB	2.38	0.52
1:A:91:HIS:ND1	1:A:313:ILE:HG12	2.24	0.52
1:A:328:ARG:CZ	1:A:348:ILE:HG21	2.40	0.52
1:B:340:VAL:O	1:B:343:LYS:HE2	2.10	0.51
1:B:130:ALA:O	1:B:134:MSE:HG3	2.11	0.51
1:A:177:PRO:HD3	1:A:234:TRP:CE3	2.46	0.51
1:A:61:LEU:CD1	1:A:84:GLN:HG2	2.41	0.50
1:C:43:GLU:HA	1:C:43:GLU:OE2	2.11	0.50
1:B:2:TYR:O	1:B:4:PRO:HD3	2.12	0.50
1:C:135:LYS:HE2	1:C:191:PHE:O	2.11	0.50
1:A:121:CYS:HB3	1:A:326:SER:OG	2.13	0.49
1:A:349:ALA:HB1	3:A:483:HOH:O	2.13	0.49
1:A:180:GLN:HB2	3:A:439:HOH:O	2.12	0.48
1:B:96:LYS:HB3	1:B:122:GLY:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:LYS:HE2	1:A:145:GLU:OE2	2.14	0.48
1:B:39:GLU:HA	1:B:42:ARG:NH1	2.28	0.48
1:A:145:GLU:O	1:A:247:THR:HG23	2.13	0.47
1:A:15:TRP:CD1	1:A:95:GLU:HG3	2.49	0.47
1:C:165:ASN:HA	3:C:572:HOH:O	2.13	0.47
1:C:15:TRP:CZ3	1:C:18:VAL:HG11	2.49	0.47
1:C:96:LYS:HG3	1:C:122:GLY:O	2.14	0.47
1:C:96:LYS:HD3	1:C:96:LYS:O	2.14	0.47
1:A:77:LYS:HD2	1:A:80:GLU:OE2	2.15	0.47
1:B:20:ALA:O	1:B:24:THR:HG23	2.15	0.47
1:A:78:HIS:O	1:A:82:ILE:HG13	2.16	0.46
1:A:75:ASN:ND2	1:A:97:PRO:HG2	2.31	0.46
1:B:118:LYS:HE3	1:B:317:GLY:O	2.15	0.46
1:C:268:GLU:HA	2:C:355:GOL:C1	2.45	0.46
1:B:213:ILE:HG21	1:B:216:ASN:OD1	2.16	0.46
1:B:272:LEU:O	1:B:273:ILE:HD13	2.15	0.46
1:A:168:GLY:HA3	3:A:499:HOH:O	2.16	0.46
1:C:44:LYS:NZ	3:C:487:HOH:O	2.50	0.45
1:B:57:MSE:O	1:B:61:LEU:HD12	2.16	0.45
1:A:104:HIS:O	1:A:108:ILE:HD12	2.16	0.45
1:B:65:ASP:N	1:B:65:ASP:OD1	2.50	0.45
1:C:110:GLN:NE2	1:C:114:GLU:OE2	2.50	0.44
1:C:121:CYS:HB3	1:C:326:SER:OG	2.17	0.44
1:A:277:PHE:CD1	1:A:286:ASN:HA	2.52	0.44
1:A:136:GLU:O	1:A:140:THR:HG23	2.18	0.44
1:A:337:VAL:HG13	1:A:341:HIS:NE2	2.33	0.43
1:C:328[A]:ARG:HG3	3:C:498:HOH:O	2.19	0.43
1:A:352:ILE:HG22	1:A:353:GLY:N	2.33	0.43
1:B:185:GLN:HA	1:B:185:GLN:OE1	2.18	0.43
1:B:11:GLY:O	1:B:72:THR:OG1	2.37	0.43
1:C:116:GLY:HA2	3:C:539:HOH:O	2.19	0.43
1:A:127:ARG:O	1:A:299:VAL:HG11	2.19	0.43
1:C:276:GLU:OE2	1:C:290:ARG:NE	2.51	0.43
1:C:315:ASN:ND2	3:C:552:HOH:O	2.50	0.43
1:C:28:LYS:HZ3	1:C:311:ASP:CG	2.22	0.43
1:A:274:LYS:HE2	1:A:276:GLU:OE1	2.18	0.43
1:B:25:LYS:NZ	3:B:385:HOH:O	2.49	0.43
1:B:274:LYS:HE3	1:B:276:GLU:CD	2.40	0.43
1:A:68:MSE:HG2	1:A:69:VAL:N	2.33	0.42
1:C:157:ARG:HB3	1:C:234:TRP:CD1	2.54	0.42
1:B:338:LYS:HG2	1:B:338:LYS:O	2.19	0.42
1:C:248[A]:LYS:HE3	3:C:538:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:91:HIS:CD2	1:B:313:ILE:HG12	2.55	0.42
1:A:328:ARG:HG2	1:A:328:ARG:O	2.20	0.42
1:A:338:LYS:HD2	1:A:342:GLU:OE2	2.19	0.42
1:A:170:PRO:HD2	3:A:489:HOH:O	2.19	0.41
1:B:153:PHE:HZ	1:B:257:PHE:CE1	2.38	0.41
1:B:277:PHE:HA	1:B:288:ILE:O	2.20	0.41
1:C:15:TRP:CD1	1:C:95:GLU:HG3	2.55	0.41
1:A:170:PRO:HB2	3:A:507:HOH:O	2.20	0.41
1:A:190:GLN:HG2	1:A:194:GLY:O	2.20	0.41
1:B:73:VAL:HG23	1:B:74:PRO:O	2.20	0.41
1:C:195:PRO:O	1:C:223:GLU:OE2	2.38	0.41
1:C:7:VAL:HG12	1:C:68:MSE:HB3	2.02	0.41
1:A:154:SER:O	1:A:238:GLY:HA2	2.20	0.41
1:B:274:LYS:HE3	1:B:276:GLU:OE1	2.20	0.41
1:A:179:THR:O	1:A:183:VAL:HG23	2.21	0.41
1:B:166:TRP:CE2	1:B:167:ARG:HG3	2.55	0.41
1:A:132[A]:ARG:HH22	1:A:320:GLU:CD	2.24	0.40
1:B:91:HIS:O	1:B:92:ILE:HD13	2.20	0.40
1:A:178:LEU:O	1:A:182:GLY:HA3	2.21	0.40
1:B:10:ILE:HD11	1:B:57:MSE:HE1	2.02	0.40
1:A:75:ASN:CG	1:A:97:PRO:HG2	2.42	0.40
1:B:7:VAL:HG12	1:B:68:MSE:HB3	2.03	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	348/354 (98%)	336 (97%)	12 (3%)	0	100	100
1	B	344/354 (97%)	324 (94%)	18 (5%)	2 (1%)	33	13
1	C	350/354 (99%)	341 (97%)	8 (2%)	1 (0%)	50	27
All	All	1042/1062 (98%)	1001 (96%)	38 (4%)	3 (0%)	50	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	ARG
1	C	2	TYR
1	B	352	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	279/291 (96%)	265 (95%)	14 (5%)	34	12
1	B	278/291 (96%)	263 (95%)	15 (5%)	31	11
1	C	292/291 (100%)	277 (95%)	15 (5%)	33	12
All	All	849/873 (97%)	805 (95%)	44 (5%)	35	11

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

Mol	Chain	Res	Type
1	A	2	TYR
1	A	3	ASN
1	A	30	LYS
1	A	101	SER
1	A	141	LYS
1	A	153	PHE
1	A	178	LEU
1	A	234	TRP
1	A	286	ASN
1	A	288	ILE
1	A	293	LYS
1	A	297	GLU
1	A	338	LYS
1	A	348	ILE
1	B	2	TYR
1	B	47	LYS
1	B	57	MSE
1	B	58	GLU
1	B	65	ASP
1	B	153	PHE

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Mol	Chain	Res	Type
1	B	160	GLU
1	B	162	LYS
1	B	172	THR
1	B	178	LEU
1	B	234	TRP
1	B	288	ILE
1	B	312	VAL
1	B	315	ASN
1	B	343	LYS
1	C	2	TYR
1	C	36	SER
1	C	37	ARG
1	C	42[A]	ARG
1	C	42[B]	ARG
1	C	96	LYS
1	C	153	PHE
1	C	160	GLU
1	C	180	GLN
1	C	209	GLU
1	C	220[A]	LEU
1	C	220[B]	LEU
1	C	223	GLU
1	C	328[A]	ARG
1	C	328[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

2 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	$\# Z  > 2$
2	GOL	C	354	-	5,5,5	0.78	0	5,5,5	1.20	0
2	GOL	C	355	-	5,5,5	0.79	0	5,5,5	1.34	1 (20%)

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	GOL	C	354	-	-	0/4/4/4	0/0/0/0
2	GOL	C	355	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	C	355	GOL	O2-C2-C3	2.43	119.70	108.44

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	347/354 (98%)	-0.27	3 (0%) 81 86	16, 28, 43, 61	0
1	B	343/354 (96%)	-0.08	10 (2%) 49 54	17, 31, 49, 62	0
1	C	346/354 (97%)	-0.31	4 (1%) 75 82	13, 22, 42, 64	0
All	All	1036/1062 (97%)	-0.22	17 (1%) 68 74	13, 27, 46, 64	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	TYR	6.5
1	B	353	GLY	5.7
1	A	286	ASN	5.6
1	C	353	GLY	4.2
1	C	1	MSE	3.3
1	A	353	GLY	3.1
1	B	55	ALA	2.8
1	B	15	TRP	2.8
1	A	1	MSE	2.7
1	B	277	PHE	2.6
1	C	286	ASN	2.2
1	B	257	PHE	2.2
1	B	288	ILE	2.2
1	B	3	ASN	2.2
1	B	66	VAL	2.1
1	C	278	ALA	2.0
1	B	76	ASP	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
2	GOL	C	355	6/6	0.14	5.52	27,31,41,42	0
2	GOL	C	354	6/6	0.08	-0.84	44,48,53,54	0

### 6.5 Other polymers

There are no such residues in this entry.