



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:06 AM GMT

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 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

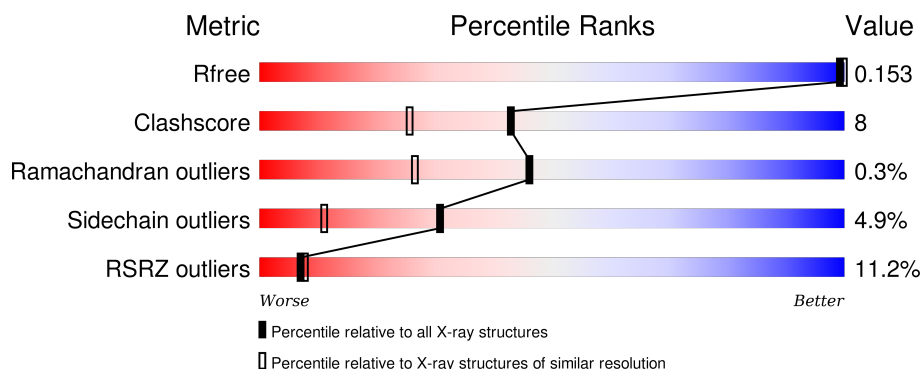
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (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. 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	354	<div> <div>9%</div> <div>73%</div> <div>23%</div> <div>• •</div> </div>
1	B	354	<div> <div>15%</div> <div>73%</div> <div>20%</div> <div>• •</div> </div>
1	C	354	<div> <div>8%</div> <div>80%</div> <div>15%</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
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 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.

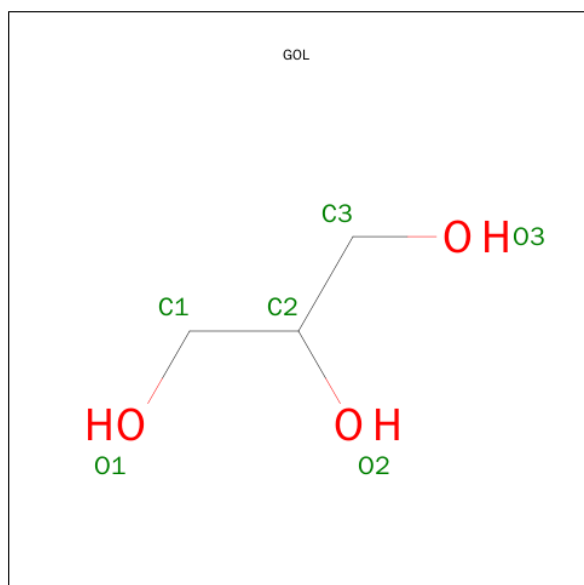
- Molecule 1 is a protein called putative NADPH-dependent oxidoreductase.

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		

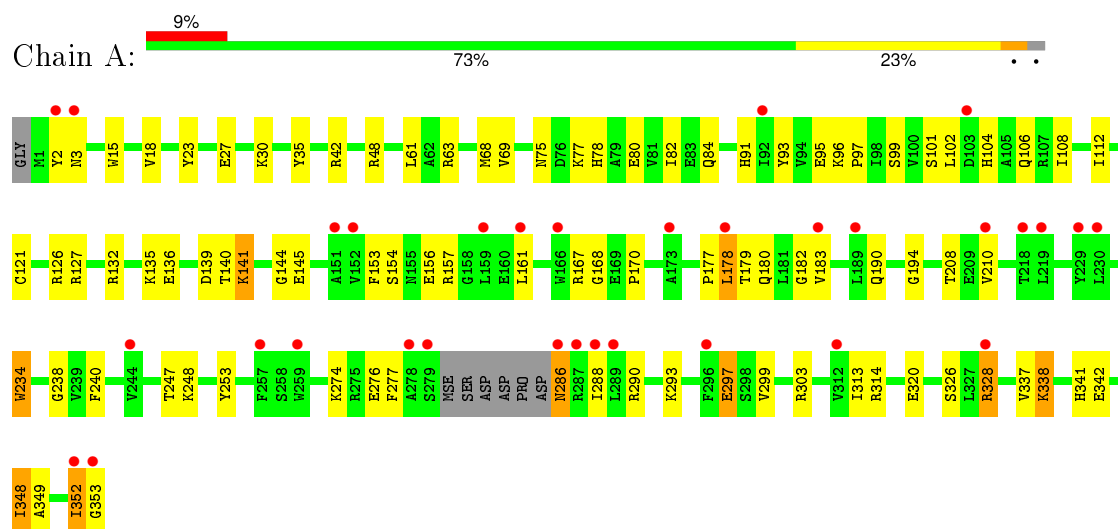
- Molecule 3 is water.

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		

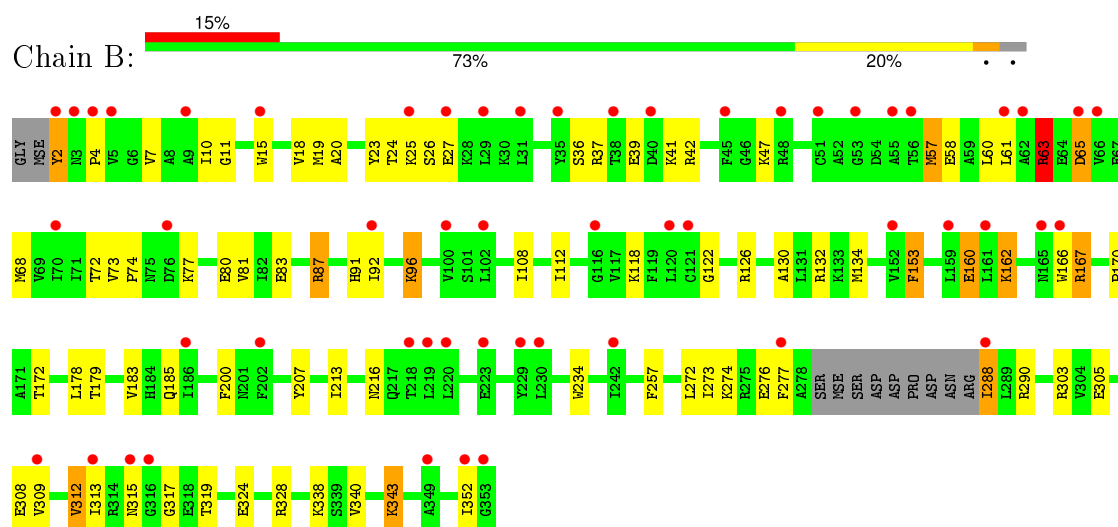
### 3 Residue-property plots

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.

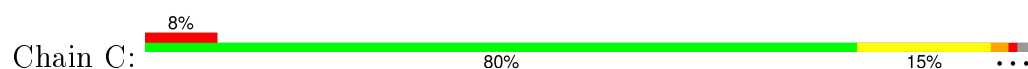
- Molecule 1: putative NADPH-dependent oxidoreductase

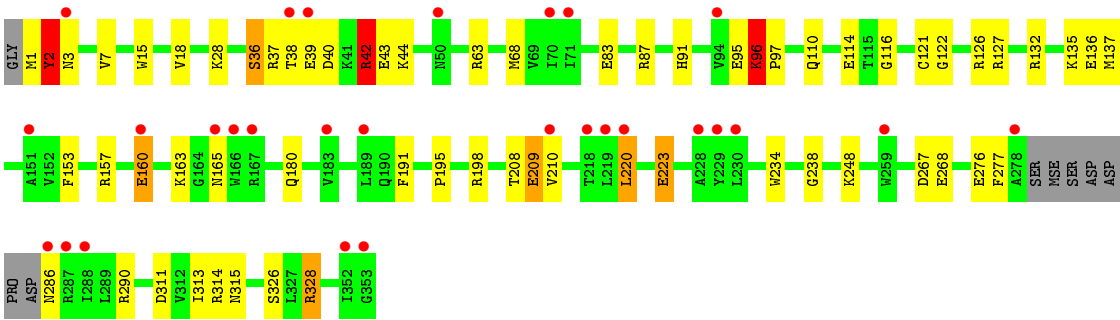


- Molecule 1: putative NADPH-dependent oxidoreductase



- Molecule 1: putative NADPH-dependent oxidoreductase





## 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 0.135 , 0.153	Depositor DCC
$R_{free}$ test set	5943 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> )	0.36 , 71.7	EDS
Estimated twinning fraction	0.380 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 120815 reflections	Xtriage
$F_o, F_c$ correlation	0.90	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

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 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	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (133) 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: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	Interatomic distance (Å)	Clash overlap (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:OE1	1:B:160:GLU:HA	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:C:39:GLU:HA	1:C:42[A]:ARG:NE	2.23	0.54
1:B:10:ILE:HD13	1:B:57:MSE:SE	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LYS:HB3	1:B:122:GLY:O	2.13	0.48
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:15:TRP:CD1	1:A:95:GLU:HG3	2.49	0.47
1:A:145:GLU:O	1:A:247:THR:HG23	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:165:ASN:HA	3:C:572:HOH:O	2.13	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:75:ASN:ND2	1:A:97:PRO:HG2	2.31	0.46
1:A:78:HIS:O	1:A:82:ILE:HG13	2.16	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:C:116:GLY:HA2	3:C:539:HOH:O	2.19	0.43
1:B:11:GLY:O	1:B:72:THR:OG1	2.37	0.43
1:C:315:ASN:ND2	3:C:552:HOH:O	2.50	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248[A]:LYS:HE3	3:C:538:HOH:O	2.19	0.42
1:B:338:LYS:HG2	1:B:338:LYS:O	2.19	0.42
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:C:15:TRP:CD1	1:C:95:GLU:HG3	2.55	0.41
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: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:A:170:PRO:HB2	3:A:507:HOH: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:B:274:LYS:HE3	1:B:276:GLU:OE1	2.20	0.41
1:A:154:SER:O	1:A:238:GLY:HA2	2.20	0.41
1:B:166:TRP:CE2	1:B:167:ARG:HG3	2.55	0.41
1:A:179:THR:O	1:A:183:VAL:HG23	2.21	0.41
1:B:91:HIS:O	1:B:92:ILE:HD13	2.20	0.40
1:A:132[A]:ARG:HH22	1:A:320:GLU:CD	2.24	0.40
1:B:10:ILE:HD11	1:B:57:MSE:HE1	2.02	0.40
1:A:178:LEU:O	1:A:182:GLY:HA3	2.21	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 [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	348/354 (98%)	336 (97%)	12 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	344/354 (97%)	324 (94%)	18 (5%)	2 (1%)	30	12
1	C	350/354 (99%)	341 (97%)	8 (2%)	1 (0%)	46	26
All	All	1042/1062 (98%)	1001 (96%)	38 (4%)	3 (0%)	46	26

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%)	30	11
1	B	278/291 (96%)	263 (95%)	15 (5%)	27	9
1	C	292/291 (100%)	277 (95%)	15 (5%)	29	10
All	All	849/873 (97%)	805 (95%)	44 (5%)	31	10

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

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Mol	Chain	Res	Type
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
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 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 ⓘ

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	0.81	0	5,5,5	1.18	0
2	GOL	C	355	-	5,5,5	0.81	0	5,5,5	1.30	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(°)	Ideal(°)
2	C	355	GOL	O2-C2-C3	2.41	119.70	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	354	GOL	1	0
2	C	355	GOL	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	340/354 (96%)	0.80	32 (9%) <b>11</b> <b>12</b>	16, 28, 43, 61	0
1	B	337/354 (95%)	1.01	54 (16%) <b>3</b> <b>3</b>	17, 31, 50, 62	0
1	C	339/354 (95%)	0.58	28 (8%) <b>14</b> <b>16</b>	13, 22, 42, 63	0
All	All	1016/1062 (95%)	0.80	114 (11%) <b>7</b> <b>8</b>	13, 27, 46, 63	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	ASN	8.9
1	B	353	GLY	7.8
1	B	53	GLY	6.2
1	B	5	VAL	5.8
1	B	288	ILE	5.6
1	C	287	ARG	5.5
1	B	316	GLY	5.1
1	B	38	THR	5.0
1	A	230	LEU	4.8
1	B	2	TYR	4.7
1	A	166	TRP	4.5
1	A	287	ARG	4.3
1	C	166	TRP	4.2
1	A	353	GLY	4.2
1	C	210	VAL	3.9
1	B	277	PHE	3.8
1	A	229	TYR	3.7
1	A	288	ILE	3.7
1	C	230	LEU	3.6
1	B	65	ASP	3.5
1	B	70	ILE	3.4
1	B	352	ILE	3.4
1	A	2	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	278	ALA	3.3
1	C	353	GLY	3.3
1	B	4	PRO	3.3
1	B	219	LEU	3.3
1	A	352	ILE	3.2
1	B	230	LEU	3.2
1	B	92	ILE	3.1
1	A	3	ASN	3.1
1	C	286	ASN	3.1
1	C	39	GLU	3.0
1	A	151	ALA	3.0
1	B	35	TYR	2.9
1	A	161	LEU	2.9
1	A	219	LEU	2.9
1	C	219	LEU	2.9
1	B	9	ALA	2.9
1	B	61	LEU	2.8
1	A	278	ALA	2.7
1	B	55	ALA	2.7
1	B	313	ILE	2.7
1	B	45	PHE	2.7
1	C	151	ALA	2.7
1	B	223	GLU	2.7
1	A	312	VAL	2.7
1	C	183	VAL	2.7
1	B	62	ALA	2.7
1	B	31	LEU	2.6
1	C	50	ASN	2.6
1	C	220[A]	LEU	2.6
1	C	165	ASN	2.6
1	A	159	LEU	2.6
1	C	167	ARG	2.6
1	A	279	SER	2.5
1	B	100	VAL	2.5
1	C	352	ILE	2.5
1	B	161	LEU	2.5
1	B	15	TRP	2.5
1	B	165	ASN	2.5
1	B	159	LEU	2.5
1	B	186	ILE	2.5
1	B	242	ILE	2.5
1	A	210	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	189	LEU	2.4
1	B	3	ASN	2.4
1	A	289	LEU	2.4
1	C	229	TYR	2.4
1	B	166	TRP	2.4
1	B	25	LYS	2.4
1	C	71	ILE	2.3
1	B	66	VAL	2.3
1	B	48	ARG	2.3
1	B	76	ASP	2.3
1	B	29	LEU	2.3
1	C	259	TRP	2.3
1	B	220	LEU	2.3
1	B	218	THR	2.2
1	A	152	VAL	2.2
1	A	218	THR	2.2
1	B	56	THR	2.2
1	B	27	GLU	2.2
1	C	160	GLU	2.2
1	B	349	ALA	2.2
1	A	257	PHE	2.2
1	B	121	CYS	2.2
1	C	70	ILE	2.2
1	A	173	ALA	2.2
1	C	228	ALA	2.2
1	C	94	VAL	2.2
1	C	218	THR	2.1
1	B	120	LEU	2.1
1	A	103	ASP	2.1
1	B	40	ASP	2.1
1	C	189	LEU	2.1
1	B	51	CYS	2.1
1	A	183	VAL	2.1
1	B	152	VAL	2.1
1	C	3	ASN	2.1
1	A	296	PHE	2.1
1	B	116	GLY	2.1
1	A	259	TRP	2.1
1	A	328	ARG	2.1
1	A	92	ILE	2.1
1	B	309	VAL	2.0
1	B	229	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	202	PHE	2.0
1	B	102	LEU	2.0
1	B	315	ASN	2.0
1	C	38	THR	2.0
1	C	288	ILE	2.0
1	A	244	VAL	2.0
1	A	178	LEU	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
2	GOL	C	355	6/6	0.86	0.17	4.89	27,31,41,42	0
2	GOL	C	354	6/6	0.80	0.14	-0.05	44,48,53,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.