



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:47 PM UTC

PDB ID : 3DB2 / pdb_00003db2
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

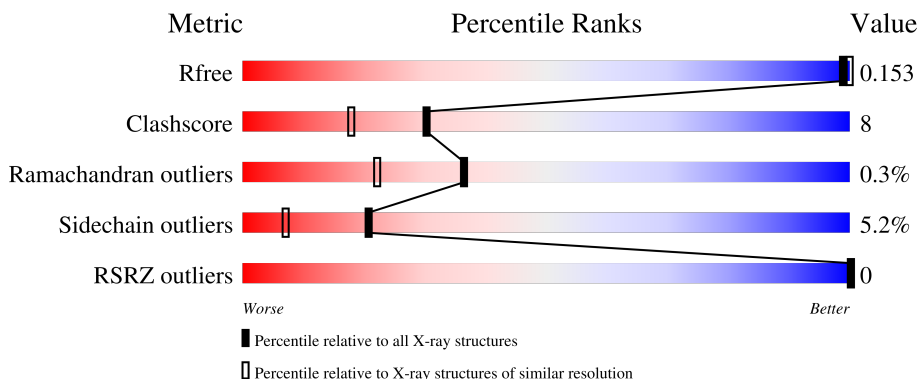
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 69% 25% . .
1	B	354	 69% 23% 5% .
1	C	354	 75% 20% . .

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.

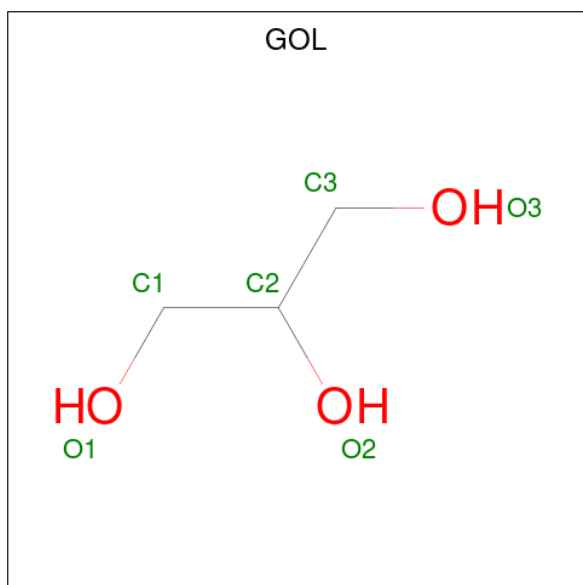
- Molecule 1 is a protein called putative NADPH-dependent oxidoreductase.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q18XG3
B	0	GLY	-	expression tag	UNP Q18XG3
C	0	GLY	-	expression tag	UNP Q18XG3

- Molecule 2 is GLYCEROL (CCD ID: 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		

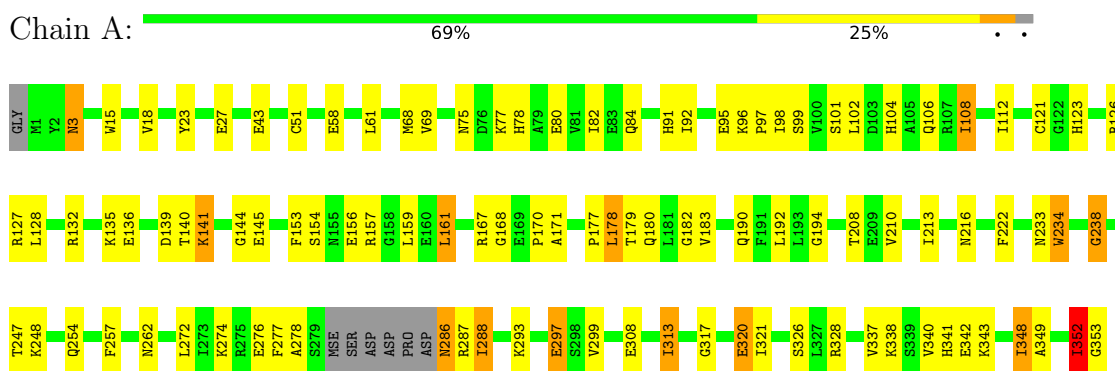
- Molecule 3 is water.

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		

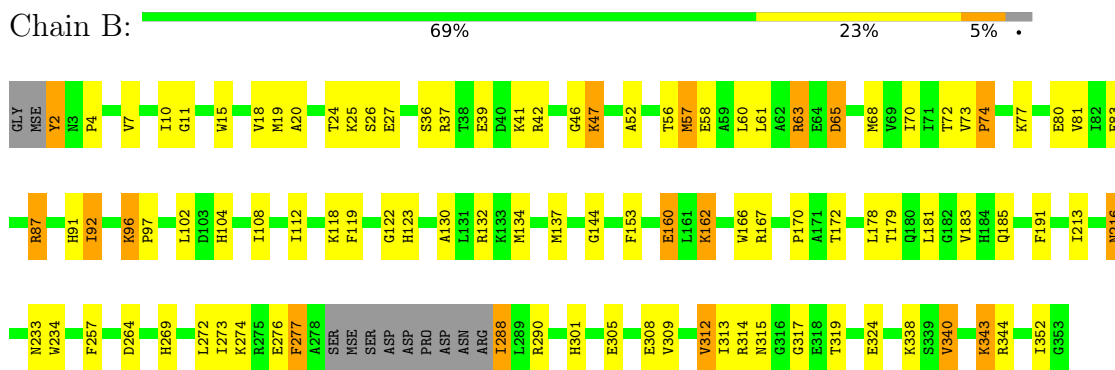
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

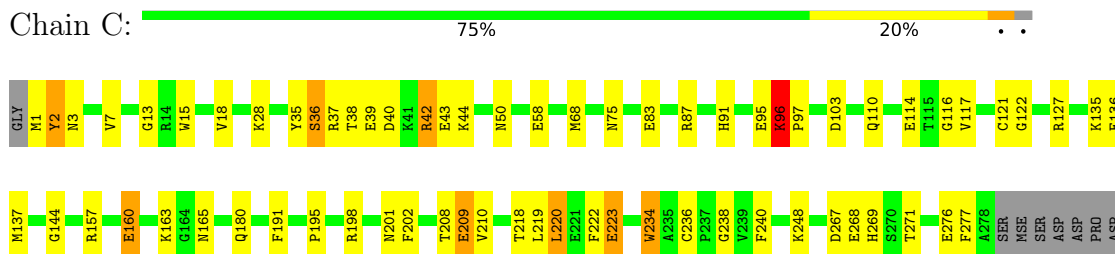
- Molecule 1: putative NADPH-dependent oxidoreductase



- Molecule 1: putative NADPH-dependent oxidoreductase



- Molecule 1: putative NADPH-dependent oxidoreductase





4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.62Å 104.62Å 173.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.75 – 1.70 29.75 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.75-1.70) 97.7 (29.75-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.70Å)	Xtrriage
Refinement program	SHELXL-97, PHENIX, SHELX	Depositor
R, R_{free}	0.142 , 0.174 0.135 , 0.153	Depositor DCC
R_{free} test set	6076 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.380 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	8697	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 i

5.1 Standard geometry i

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	0.58	0/2740	1.69	55/3697 (1.5%)
1	B	0.59	0/2720	1.68	45/3673 (1.2%)
1	C	0.62	0/2802	1.56	32/3779 (0.8%)
All	All	0.60	0/8262	1.65	132/11149 (1.2%)

There are no bond length outliers.

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	SER	CA-C-N	12.90	137.21	120.44
1	B	26	SER	C-N-CA	12.90	137.21	120.44
1	B	96	LYS	O-C-N	-11.57	109.34	121.60
1	A	96	LYS	O-C-N	-11.35	109.04	121.53
1	A	144	GLY	CA-C-N	11.15	138.11	122.72
1	A	144	GLY	C-N-CA	11.15	138.11	122.72
1	C	96	LYS	CA-C-O	-10.25	109.53	120.70
1	B	233	ASN	CA-CB-CG	8.88	121.47	112.60
1	C	50	ASN	CA-CB-CG	-8.14	104.46	112.60
1	B	144	GLY	CA-C-N	8.07	134.04	122.09
1	B	144	GLY	C-N-CA	8.07	134.04	122.09
1	B	96	LYS	CA-C-O	-8.06	112.00	120.87
1	A	27	GLU	CA-C-N	7.99	137.16	121.58
1	A	27	GLU	C-N-CA	7.99	137.16	121.58
1	B	132	ARG	CD-NE-CZ	7.90	135.46	124.40
1	A	58	GLU	CA-C-O	7.82	128.84	120.55
1	B	37	ARG	CA-C-N	7.53	134.87	122.07
1	B	37	ARG	C-N-CA	7.53	134.87	122.07
1	A	153	PHE	CA-CB-CG	7.51	121.31	113.80
1	A	96	LYS	CA-C-O	-7.49	112.54	120.70
1	B	269	HIS	CA-CB-CG	-7.47	106.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	269	HIS	CA-CB-CG	-7.34	106.46	113.80
1	B	264	ASP	CA-CB-CG	7.28	119.88	112.60
1	C	222	PHE	CA-CB-CG	-7.25	106.55	113.80
1	A	262	ASN	CA-C-N	7.24	130.71	120.28
1	A	262	ASN	C-N-CA	7.24	130.71	120.28
1	C	117	VAL	CA-C-N	7.22	130.96	120.71
1	C	117	VAL	C-N-CA	7.22	130.96	120.71
1	C	341	HIS	CA-CB-CG	-7.10	106.70	113.80
1	B	344	ARG	O-C-N	7.05	126.80	121.65
1	C	301	HIS	CA-CB-CG	7.00	120.80	113.80
1	B	27	GLU	CA-C-N	6.94	134.92	121.18
1	B	27	GLU	C-N-CA	6.94	134.92	121.18
1	C	97	PRO	N-CA-C	-6.93	94.08	112.10
1	A	352	ILE	CA-C-N	6.75	133.85	121.70
1	A	352	ILE	C-N-CA	6.75	133.85	121.70
1	C	236	CYS	N-CA-C	6.72	114.05	108.07
1	A	320	GLU	CA-C-N	-6.66	116.64	122.96
1	A	320	GLU	C-N-CA	-6.66	116.64	122.96
1	C	314	ARG	NE-CZ-NH2	6.59	125.13	119.20
1	A	238	GLY	CA-C-N	6.55	132.15	122.71
1	A	238	GLY	C-N-CA	6.55	132.15	122.71
1	C	75	ASN	CA-CB-CG	-6.33	106.27	112.60
1	A	340	VAL	CB-CA-C	-6.26	103.96	111.97
1	B	301	HIS	CA-CB-CG	6.25	120.05	113.80
1	C	13	GLY	O-C-N	-6.25	117.44	122.81
1	B	102	LEU	O-C-N	6.22	128.71	122.12
1	B	92	ILE	CA-C-N	6.19	131.55	123.00
1	B	92	ILE	C-N-CA	6.19	131.55	123.00
1	A	216	ASN	CA-CB-CG	6.14	118.74	112.60
1	A	58	GLU	O-C-N	-6.12	115.64	122.12
1	A	98	ILE	CA-C-N	6.11	133.90	122.84
1	A	98	ILE	C-N-CA	6.11	133.90	122.84
1	C	2	TYR	CA-CB-CG	6.10	124.88	113.90
1	B	96	LYS	CA-C-N	6.07	141.57	127.00
1	B	96	LYS	C-N-CA	6.07	141.57	127.00
1	A	128	LEU	CA-C-O	-6.06	115.13	121.55
1	B	52	ALA	CA-C-N	6.01	126.72	122.33
1	B	52	ALA	C-N-CA	6.01	126.72	122.33
1	B	305	GLU	CA-CB-CG	6.01	126.11	114.10
1	A	238	GLY	N-CA-C	5.97	118.34	111.36
1	A	3	ASN	CA-CB-CG	5.95	118.55	112.60
1	B	181	LEU	CA-C-N	5.93	126.69	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	LEU	C-N-CA	5.93	126.69	119.99
1	A	278	ALA	CA-C-N	5.90	132.32	121.70
1	A	278	ALA	C-N-CA	5.90	132.32	121.70
1	A	352	ILE	O-C-N	5.89	128.24	121.94
1	B	104	HIS	CA-CB-CG	-5.89	107.91	113.80
1	C	351	ILE	N-CA-C	-5.80	106.05	111.45
1	A	126	ARG	CD-NE-CZ	5.78	132.49	124.40
1	B	70	ILE	CA-C-O	5.76	126.56	120.51
1	B	119	PHE	CA-CB-CG	5.75	119.55	113.80
1	B	277	PHE	CA-CB-CG	-5.74	108.06	113.80
1	A	96	LYS	N-CA-CB	5.70	118.44	110.11
1	A	233	ASN	CA-CB-CG	5.69	118.29	112.60
1	A	317	GLY	CA-C-O	-5.67	117.08	122.13
1	A	96	LYS	CA-C-N	5.67	140.61	127.00
1	A	96	LYS	C-N-CA	5.67	140.61	127.00
1	B	46	GLY	CA-C-N	-5.67	112.73	120.44
1	B	46	GLY	C-N-CA	-5.67	112.73	120.44
1	B	290	ARG	O-C-N	5.65	129.71	123.33
1	B	47	LYS	N-CA-C	-5.63	105.06	111.14
1	A	108	ILE	CA-C-O	5.63	126.81	120.85
1	C	127	ARG	CD-NE-CZ	5.62	132.27	124.40
1	C	35	TYR	CA-C-N	5.57	131.23	122.21
1	C	35	TYR	C-N-CA	5.57	131.23	122.21
1	C	58	GLU	CA-C-O	5.54	126.42	120.55
1	C	240	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	159	LEU	CA-C-N	-5.50	113.96	122.49
1	A	159	LEU	C-N-CA	-5.50	113.96	122.49
1	A	254	GLN	CB-CG-CD	5.50	121.95	112.60
1	B	314	ARG	CA-C-O	-5.49	115.05	120.82
1	A	23	TYR	CA-CB-CG	5.49	123.78	113.90
1	C	96	LYS	CA-C-N	5.48	140.15	127.00
1	C	96	LYS	C-N-CA	5.48	140.15	127.00
1	A	272	LEU	CA-C-O	-5.46	114.45	120.24
1	A	192	LEU	CA-C-O	-5.43	114.22	120.24
1	A	123	HIS	CA-CB-CG	5.42	119.22	113.80
1	B	191	PHE	O-C-N	-5.42	116.28	122.08
1	B	340	VAL	CB-CA-C	-5.41	104.99	112.24
1	A	222	PHE	CA-CB-CG	-5.36	108.44	113.80
1	C	350	GLU	CA-C-O	5.32	126.11	120.10
1	B	123	HIS	CA-CB-CG	5.31	119.11	113.80
1	A	272	LEU	O-C-N	5.31	129.48	123.27
1	C	144	GLY	O-C-N	5.29	127.99	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	THR	O-C-N	5.27	129.57	123.30
1	B	74	PRO	CA-C-N	5.25	131.56	121.54
1	B	74	PRO	C-N-CA	5.25	131.56	121.54
1	B	97	PRO	N-CA-CB	5.24	108.36	102.60
1	C	103	ASP	CA-C-N	5.23	127.29	120.28
1	C	103	ASP	C-N-CA	5.23	127.29	120.28
1	A	108	ILE	O-C-N	-5.21	116.47	121.83
1	B	137	MSE	CA-C-O	5.20	125.95	119.97
1	A	171	ALA	CA-C-N	5.18	131.05	121.52
1	A	171	ALA	C-N-CA	5.18	131.05	121.52
1	A	297	GLU	CA-CB-CG	5.17	124.44	114.10
1	A	308	GLU	CA-C-O	5.15	126.01	120.55
1	C	96	LYS	O-C-N	-5.15	115.87	121.53
1	A	257	PHE	CA-CB-CG	-5.14	108.66	113.80
1	B	87	ARG	CD-NE-CZ	5.14	131.60	124.40
1	B	27	GLU	O-C-N	5.13	127.35	122.07
1	C	97	PRO	N-CA-CB	5.13	108.24	102.60
1	C	202	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	92	ILE	N-CA-C	5.09	115.18	107.75
1	A	51	CYS	CA-C-O	-5.09	115.68	121.58
1	C	201	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	B	216	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	58	GLU	CA-C-N	5.03	127.28	120.44
1	A	58	GLU	C-N-CA	5.03	127.28	120.44
1	A	313	ILE	O-C-N	-5.02	116.66	121.83
1	A	213	ILE	O-C-N	-5.01	117.31	122.63
1	C	198	ARG	NE-CZ-NH2	-5.01	114.69	119.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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	46	0
1	B	2666	0	2621	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2736	0	2732	40	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	136	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 (136) 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: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
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:160:GLU:O	1:C:160:GLU:HG3	1.95	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE2	1:C:43:GLU:HA	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
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:C:28:LYS:HZ3	1:C:311:ASP:CG	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:274:LYS:HE3	1:B:276:GLU:CD	2.40	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:O	1:C:96:LYS:HD3	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:132[A]:ARG:HH22	1:A:320:GLU:CD	2.24	0.45
1:A:75:ASN:CG	1:A:97:PRO:HG2	2.42	0.45
1:A:104:HIS:O	1:A:108:ILE:HD12	2.16	0.45
1:B:65:ASP:OD1	1:B:65:ASP:N	2.50	0.45
1:C:110:GLN:NE2	1:C:114:GLU:OE2	2.50	0.44
1:B:25:LYS:NZ	3:B:385:HOH:O	2.49	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:C:219:LEU:C	1:C:220[B]:LEU:HD13	2.42	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:91:HIS:C	1:B:92:ILE:HD13	2.43	0.43
1:B:185:GLN:OE1	1:B:185:GLN:HA	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:A:274:LYS:HE2	1:A:276:GLU:OE1	2.18	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:B:338:LYS:O	1:B:338:LYS:HG2	2.19	0.42
1:C:248[A]:LYS:HE3	3:C:538:HOH:O	2.19	0.42
1:B:91:HIS:CD2	1:B:313:ILE:HG12	2.55	0.42
1:A:328:ARG:O	1:A:328:ARG:HG2	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: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:287:ARG:C	1:A:288:ILE:HD12	2.46	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	100 100
1	B	344/354 (97%)	324 (94%)	18 (5%)	2 (1%)	21 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	350/354 (99%)	341 (97%)	8 (2%)	1 (0%)	36 22
All	All	1042/1062 (98%)	1001 (96%)	38 (4%)	3 (0%)	36 22

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 [i](#)

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%)	264 (95%)	15 (5%)	20 6
1	B	278/291 (96%)	263 (95%)	15 (5%)	20 6
1	C	292/291 (100%)	276 (94%)	16 (6%)	19 6
All	All	849/873 (97%)	803 (95%)	46 (5%)	21 6

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	43	GLU
1	A	101	SER
1	A	141	LYS
1	A	161	LEU
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	321	ILE

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Mol	Chain	Res	Type
1	A	343	LYS
1	A	348	ILE
1	A	352	ILE
1	B	2	TYR
1	B	47	LYS
1	B	56	THR
1	B	57	MSE
1	B	58	GLU
1	B	65	ASP
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	36	SER
1	C	37	ARG
1	C	42[A]	ARG
1	C	42[B]	ARG
1	C	96	LYS
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	234	TRP
1	C	271	THR
1	C	328[A]	ARG
1	C	328[B]	ARG
1	C	352	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	HIS
1	B	315	ASN
1	C	315	ASN
1	C	341	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.86	0	5,5,5	1.23	0
2	GOL	C	355	-	5,5,5	0.85	0	5,5,5	1.37	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	-	-	4/4/4/4	-
2	GOL	C	355	-	-	2/4/4/4	-

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	2.54	119.70	109.18

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	355	GOL	O2-C2-C3-O3
2	C	354	GOL	O1-C1-C2-C3
2	C	354	GOL	C1-C2-C3-O3
2	C	355	GOL	C1-C2-C3-O3
2	C	354	GOL	O1-C1-C2-O2
2	C	354	GOL	O2-C2-C3-O3

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	340/354 (96%)	-1.13	0 100 100	13, 28, 43, 61	5 (1%)
1	B	337/354 (95%)	-1.04	0 100 100	14, 30, 50, 62	5 (1%)
1	C	339/354 (95%)	-1.25	0 100 100	10, 22, 42, 63	8 (2%)
All	All	1016/1062 (95%)	-1.14	0 100 100	10, 27, 46, 63	18 (1%)

There are no RSRZ outliers to report.

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	GOL	C	354	6/6	0.98	0.04	44,48,53,54	0
2	GOL	C	355	6/6	0.99	0.03	27,31,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.