



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2017 – 11:29 AM EDT

PDB ID : 5HY0  
Title : orotic acid hydrolase  
Authors : Peat, T.S.; Balotra, S.; Wilding, M.; Newman, J.; Scott, C.  
Deposited on : 2016-02-01  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029077

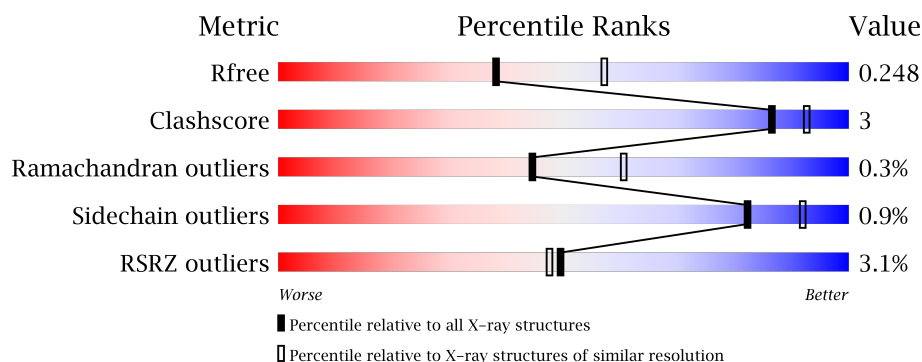
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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. 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	410	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>12%</div> </div> </div>
1	B	410	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>5%</div> <div>12%</div> </div> </div>
1	C	410	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>6%</div> <div>11%</div> </div> </div>
1	D	410	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>6%</div> <div>11%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	401	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10739 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 Ring-opening amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	2	0
			2576	1599	466	500	11			
1	B	359	Total	C	N	O	S	0	5	0
			2590	1607	467	505	11			
1	C	364	Total	C	N	O	S	0	1	0
			2610	1621	474	504	11			
1	D	363	Total	C	N	O	S	0	2	0
			2601	1614	469	507	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP E3JD18
A	-18	GLY	-	expression tag	UNP E3JD18
A	-17	SER	-	expression tag	UNP E3JD18
A	-16	SER	-	expression tag	UNP E3JD18
A	-15	HIS	-	expression tag	UNP E3JD18
A	-14	HIS	-	expression tag	UNP E3JD18
A	-13	HIS	-	expression tag	UNP E3JD18
A	-12	HIS	-	expression tag	UNP E3JD18
A	-11	HIS	-	expression tag	UNP E3JD18
A	-10	HIS	-	expression tag	UNP E3JD18
A	-9	SER	-	expression tag	UNP E3JD18
A	-8	SER	-	expression tag	UNP E3JD18
A	-7	GLY	-	expression tag	UNP E3JD18
A	-6	LEU	-	expression tag	UNP E3JD18
A	-5	VAL	-	expression tag	UNP E3JD18
A	-4	PRO	-	expression tag	UNP E3JD18
A	-3	ARG	-	expression tag	UNP E3JD18
A	-2	GLY	-	expression tag	UNP E3JD18
A	-1	SER	-	expression tag	UNP E3JD18
A	0	HIS	-	expression tag	UNP E3JD18
B	-19	MET	-	initiating methionine	UNP E3JD18

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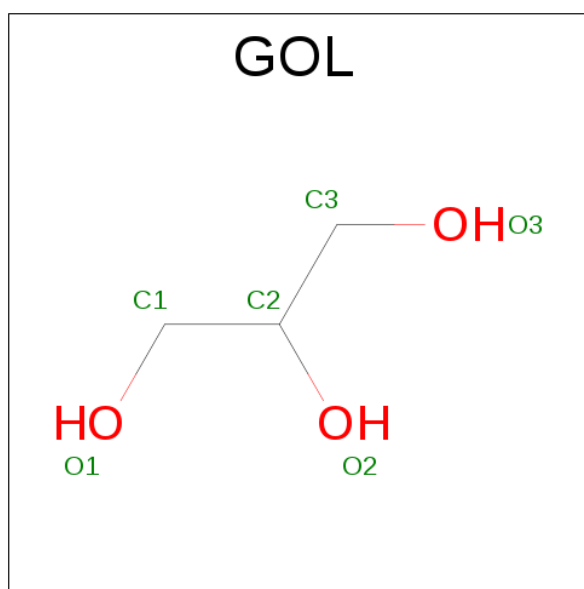
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP E3JD18
B	-17	SER	-	expression tag	UNP E3JD18
B	-16	SER	-	expression tag	UNP E3JD18
B	-15	HIS	-	expression tag	UNP E3JD18
B	-14	HIS	-	expression tag	UNP E3JD18
B	-13	HIS	-	expression tag	UNP E3JD18
B	-12	HIS	-	expression tag	UNP E3JD18
B	-11	HIS	-	expression tag	UNP E3JD18
B	-10	HIS	-	expression tag	UNP E3JD18
B	-9	SER	-	expression tag	UNP E3JD18
B	-8	SER	-	expression tag	UNP E3JD18
B	-7	GLY	-	expression tag	UNP E3JD18
B	-6	LEU	-	expression tag	UNP E3JD18
B	-5	VAL	-	expression tag	UNP E3JD18
B	-4	PRO	-	expression tag	UNP E3JD18
B	-3	ARG	-	expression tag	UNP E3JD18
B	-2	GLY	-	expression tag	UNP E3JD18
B	-1	SER	-	expression tag	UNP E3JD18
B	0	HIS	-	expression tag	UNP E3JD18
C	-19	MET	-	initiating methionine	UNP E3JD18
C	-18	GLY	-	expression tag	UNP E3JD18
C	-17	SER	-	expression tag	UNP E3JD18
C	-16	SER	-	expression tag	UNP E3JD18
C	-15	HIS	-	expression tag	UNP E3JD18
C	-14	HIS	-	expression tag	UNP E3JD18
C	-13	HIS	-	expression tag	UNP E3JD18
C	-12	HIS	-	expression tag	UNP E3JD18
C	-11	HIS	-	expression tag	UNP E3JD18
C	-10	HIS	-	expression tag	UNP E3JD18
C	-9	SER	-	expression tag	UNP E3JD18
C	-8	SER	-	expression tag	UNP E3JD18
C	-7	GLY	-	expression tag	UNP E3JD18
C	-6	LEU	-	expression tag	UNP E3JD18
C	-5	VAL	-	expression tag	UNP E3JD18
C	-4	PRO	-	expression tag	UNP E3JD18
C	-3	ARG	-	expression tag	UNP E3JD18
C	-2	GLY	-	expression tag	UNP E3JD18
C	-1	SER	-	expression tag	UNP E3JD18
C	0	HIS	-	expression tag	UNP E3JD18
D	-19	MET	-	initiating methionine	UNP E3JD18
D	-18	GLY	-	expression tag	UNP E3JD18
D	-17	SER	-	expression tag	UNP E3JD18

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP E3JD18
D	-15	HIS	-	expression tag	UNP E3JD18
D	-14	HIS	-	expression tag	UNP E3JD18
D	-13	HIS	-	expression tag	UNP E3JD18
D	-12	HIS	-	expression tag	UNP E3JD18
D	-11	HIS	-	expression tag	UNP E3JD18
D	-10	HIS	-	expression tag	UNP E3JD18
D	-9	SER	-	expression tag	UNP E3JD18
D	-8	SER	-	expression tag	UNP E3JD18
D	-7	GLY	-	expression tag	UNP E3JD18
D	-6	LEU	-	expression tag	UNP E3JD18
D	-5	VAL	-	expression tag	UNP E3JD18
D	-4	PRO	-	expression tag	UNP E3JD18
D	-3	ARG	-	expression tag	UNP E3JD18
D	-2	GLY	-	expression tag	UNP E3JD18
D	-1	SER	-	expression tag	UNP E3JD18
D	0	HIS	-	expression tag	UNP E3JD18

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



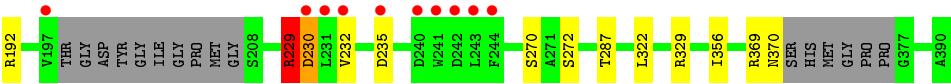
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total 75	O 75	0	0
3	B	81	Total 81	O 81	0	0
3	C	105	Total 105	O 105	0	0
3	D	89	Total 89	O 89	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.58Å 85.66Å 87.23Å 96.47° 114.94° 111.77°	Depositor
Resolution (Å)	41.50 – 2.40 39.05 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.8 (41.50-2.40) 86.3 (39.05-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.72 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.194 , 0.236 0.205 , 0.248	Depositor DCC
$R_{free}$ test set	3259 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.73	0/2616	0.89	7/3565 (0.2%)
1	B	0.71	1/2633 (0.0%)	0.87	7/3591 (0.2%)
1	C	0.78	2/2653 (0.1%)	0.90	5/3616 (0.1%)
1	D	0.74	0/2642	0.90	7/3601 (0.2%)
All	All	0.74	3/10544 (0.0%)	0.89	26/14373 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	267	SER	CB-OG	-7.56	1.32	1.42
1	B	267	SER	CB-OG	-6.07	1.34	1.42
1	C	47	SER	CB-OG	-5.72	1.34	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	C	369	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	66[A]	ARG	NE-CZ-NH1	6.26	123.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66[B]	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	D	66	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	218	LEU	CB-CG-CD2	-5.96	100.86	111.00
1	D	369	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	387	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	235	ASP	CB-CG-OD1	5.76	123.49	118.30
1	C	81	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	D	329	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	66[A]	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	66[B]	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	369	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	81	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	D	192	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	387	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	209	MET	CG-SD-CE	5.35	108.76	100.20
1	D	81	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	66[A]	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	66[B]	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	81	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	C	167	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	66[A]	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	66[B]	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	184	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ILE	Peptide
1	C	376	PRO	Peptide
1	D	229	ARG	Peptide

## 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	2576	0	2549	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2590	0	2546	9	0
1	C	2610	0	2590	14	0
1	D	2601	0	2574	14	0
2	A	6	0	8	2	0
2	B	6	0	8	0	0
3	A	75	0	0	2	0
3	B	81	0	0	1	0
3	C	105	0	0	2	0
3	D	89	0	0	0	0
All	All	10739	0	10275	52	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 3.

All (52) 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:D:135:THR:HG22	1:D:136:GLU:O	1.77	0.83
1:C:173:LEU:HD21	1:C:175:MET:HG3	1.59	0.83
1:C:230:ASP:N	1:C:230:ASP:OD1	2.22	0.63
1:C:370:ASN:ND2	3:C:403:HOH:O	2.34	0.60
1:B:132:ARG:HD3	3:B:507:HOH:O	2.01	0.60
1:D:87:ASP:O	1:D:89:ALA:N	2.35	0.59
1:C:210:CYS:HB3	1:C:238:ARG:HH12	1.68	0.58
1:B:68:PHE:CD1	1:D:68:PHE:CD1	2.92	0.57
1:A:188:ASP:OD2	1:A:192:ARG:NH1	2.39	0.55
1:D:135:THR:HG23	1:D:151:LYS:HB3	1.89	0.54
1:B:322:LEU:O	1:B:370:ASN:HB2	2.08	0.54
1:D:186:VAL:O	1:D:190:LEU:HB2	2.07	0.53
1:D:135:THR:CG2	1:D:151:LYS:HB3	2.38	0.53
1:A:68:PHE:CD1	1:C:68:PHE:CD1	2.97	0.53
1:D:182:SER:O	1:D:186:VAL:HG23	2.09	0.52
1:A:145:ARG:NH2	1:A:195:THR:O	2.42	0.51
2:A:401:GOL:O1	3:A:501:HOH:O	2.06	0.51
1:C:182:SER:O	1:C:186:VAL:HG23	2.11	0.51
1:D:322:LEU:O	1:D:370:ASN:HB2	2.12	0.50
1:A:14:ARG:NH2	1:A:117:ALA:HB2	2.27	0.50
1:B:182:SER:O	1:B:186:VAL:HG23	2.12	0.50
1:C:238:ARG:O	1:C:238:ARG:HG2	2.12	0.50
1:D:229:ARG:O	1:D:232:VAL:N	2.40	0.48
1:C:322:LEU:O	1:C:370:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:THR:HB	1:D:356:ILE:HD11	1.96	0.47
1:A:287:THR:HB	1:A:356:ILE:HD11	1.96	0.47
1:A:322:LEU:O	1:A:370:ASN:HB2	2.15	0.46
1:D:87:ASP:C	1:D:89:ALA:H	2.19	0.46
1:A:188:ASP:O	1:A:191:SER:HB2	2.16	0.46
1:B:287:THR:HB	1:B:356:ILE:HD11	1.98	0.45
1:A:237:ILE:HG22	1:A:237:ILE:O	2.17	0.45
1:A:181:LEU:HD12	1:A:208:SER:HB2	1.98	0.45
1:C:287:THR:HB	1:C:356:ILE:HD11	1.99	0.44
1:A:115:TRP:HE1	2:A:401:GOL:H12	1.84	0.43
1:D:188:ASP:O	1:D:191:SER:HB2	2.19	0.43
1:D:270:SER:OG	1:D:272:SER:HB3	2.19	0.43
1:A:77:LEU:HD23	1:A:88:LEU:HD21	1.99	0.42
1:C:173:LEU:C	1:C:173:LEU:HD23	2.40	0.42
1:D:18:ALA:H	1:D:272:SER:HB2	1.84	0.42
1:B:270:SER:OG	1:B:272[A]:SER:HB3	2.18	0.42
1:A:237:ILE:CG2	1:A:237:ILE:O	2.68	0.42
1:B:114:GLU:HG2	1:B:114:GLU:H	1.78	0.41
1:C:122:GLY:O	1:C:389:PRO:HA	2.20	0.41
1:A:60:LEU:O	1:A:66[A]:ARG:NH2	2.53	0.41
1:C:244:PHE:HA	1:C:372:HIS:O	2.21	0.41
1:C:210:CYS:HB3	1:C:238:ARG:NH1	2.35	0.41
1:A:342:HIS:ND1	3:A:502:HOH:O	2.37	0.41
1:B:281:THR:O	1:B:378:GLY:HA2	2.21	0.41
1:C:35[A]:ARG:HH11	1:C:35[A]:ARG:HD2	1.75	0.41
1:A:141:GLU:OE1	1:A:192:ARG:NH2	2.54	0.40
1:A:186:VAL:HG22	1:A:196:VAL:HG11	2.03	0.40
1:B:329:ARG:HD2	3:C:477:HOH:O	2.20	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	356/410 (87%)	343 (96%)	13 (4%)	0	100	100
1	B	358/410 (87%)	351 (98%)	7 (2%)	0	100	100
1	C	359/410 (88%)	349 (97%)	9 (2%)	1 (0%)	44	60
1	D	359/410 (88%)	347 (97%)	9 (2%)	3 (1%)	22	33
All	All	1432/1640 (87%)	1390 (97%)	38 (3%)	4 (0%)	44	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	377	GLY
1	D	230	ASP
1	D	88	LEU
1	D	229	ARG

### 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	265/310 (86%)	261 (98%)	4 (2%)	70	85
1	B	267/310 (86%)	264 (99%)	3 (1%)	78	90
1	C	270/310 (87%)	268 (99%)	2 (1%)	87	94
1	D	269/310 (87%)	268 (100%)	1 (0%)	93	97
All	All	1071/1240 (86%)	1061 (99%)	10 (1%)	82	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	183	SER
1	A	218	LEU
1	A	369	ARG
1	B	267	SER
1	B	282	ARG
1	B	369	ARG

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Mol	Chain	Res	Type
1	C	230	ASP
1	C	267	SER
1	D	230	ASP

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	A	401	-	5,5,5	0.45	0	5,5,5	1.04	0
2	GOL	B	401	-	5,5,5	0.46	0	5,5,5	1.07	0

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	A	401	-	-	0/4/4/4	0/0/0/0
2	GOL	B	401	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	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	362/410 (88%)	-0.47	10 (2%) 53 51	9, 22, 65, 109	0
1	B	359/410 (87%)	-0.45	11 (3%) 49 47	8, 20, 73, 104	0
1	C	364/410 (88%)	-0.53	9 (2%) 58 55	7, 18, 66, 93	0
1	D	363/410 (88%)	-0.50	15 (4%) 38 36	9, 20, 71, 100	0
All	All	1448/1640 (88%)	-0.49	45 (3%) 49 47	7, 20, 69, 109	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	PRO	5.3
1	D	183	SER	4.9
1	B	390	ALA	4.8
1	A	183	SER	4.2
1	C	182	SER	4.2
1	A	390	ALA	3.8
1	D	242	ASP	3.6
1	B	183	SER	3.6
1	B	184	ARG	3.6
1	D	241	TRP	3.6
1	A	373	MET	3.4
1	A	375	PRO	3.1
1	C	190	LEU	2.8
1	B	241	TRP	2.7
1	B	190	LEU	2.7
1	D	243	LEU	2.7
1	A	230	ASP	2.6
1	D	230	ASP	2.6
1	D	184	ARG	2.5
1	D	187	ALA	2.5
1	D	244	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	239	SER	2.5
1	C	241	TRP	2.4
1	D	197	VAL	2.4
1	B	187	ALA	2.4
1	B	182	SER	2.4
1	B	376	PRO	2.3
1	C	82	GLY	2.3
1	D	240	ASP	2.3
1	A	228	LYS	2.3
1	D	231	LEU	2.3
1	A	255	GLU	2.2
1	A	374	GLY	2.2
1	B	242	ASP	2.2
1	D	235	ASP	2.2
1	C	195	THR	2.1
1	A	190	LEU	2.1
1	C	191	SER	2.1
1	C	90	ASP	2.1
1	D	232	VAL	2.1
1	B	239	SER	2.1
1	D	190	LEU	2.1
1	C	188	ASP	2.0
1	D	191	SER	2.0
1	B	230	ASP	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( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	401	6/6	0.86	0.16	4.59	30,33,35,50	0
2	GOL	B	401	6/6	0.90	0.13	0.71	29,30,33,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.