



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:07 pm BST

PDB ID : 5IL9  
Title : Crystal structure of Deg9  
Authors : Ouyang, M.; Liu, L.; Li, X.Y.; Zhao, S.; Zhang, L.X.  
Deposited on : 2016-03-04  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

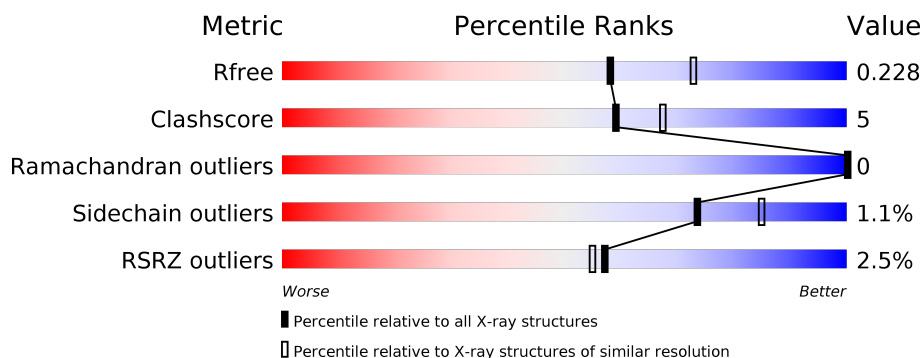
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	566	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 7%, green 75%, grey 18%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>75%</span> <span>7%</span> <span>18%</span> </div> </div>
1	B	566	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 8%, green 72%, grey 20%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>72%</span> <span>8%</span> <span>20%</span> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7670 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 Protease Do-like 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3554	2273	593	674	14			
1	B	455	Total	C	N	O	S	0	1	0
			3448	2209	576	649	14			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP Q9FL12
A	28	GLY	-	expression tag	UNP Q9FL12
A	29	SER	-	expression tag	UNP Q9FL12
A	30	SER	-	expression tag	UNP Q9FL12
A	31	HIS	-	expression tag	UNP Q9FL12
A	32	HIS	-	expression tag	UNP Q9FL12
A	33	HIS	-	expression tag	UNP Q9FL12
A	34	HIS	-	expression tag	UNP Q9FL12
A	35	HIS	-	expression tag	UNP Q9FL12
A	36	HIS	-	expression tag	UNP Q9FL12
A	37	SER	-	expression tag	UNP Q9FL12
A	38	SER	-	expression tag	UNP Q9FL12
A	39	GLY	-	expression tag	UNP Q9FL12
A	40	LEU	-	expression tag	UNP Q9FL12
A	41	VAL	-	expression tag	UNP Q9FL12
A	42	PRO	-	expression tag	UNP Q9FL12
A	43	ARG	-	expression tag	UNP Q9FL12
A	44	GLY	-	expression tag	UNP Q9FL12
A	45	SER	-	expression tag	UNP Q9FL12
A	46	HIS	-	expression tag	UNP Q9FL12
A	47	MET	-	expression tag	UNP Q9FL12
A	48	ALA	-	expression tag	UNP Q9FL12
A	49	SER	-	expression tag	UNP Q9FL12
A	50	MET	-	expression tag	UNP Q9FL12
A	51	THR	-	expression tag	UNP Q9FL12

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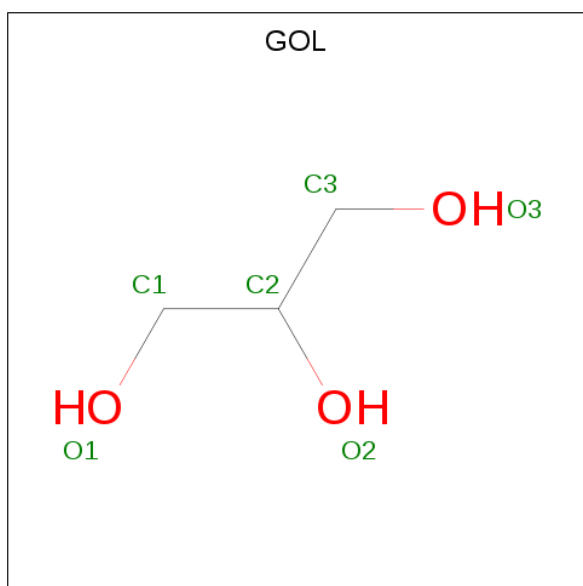
Chain	Residue	Modelled	Actual	Comment	Reference
A	52	GLY	-	expression tag	UNP Q9FL12
A	53	GLY	-	expression tag	UNP Q9FL12
A	54	GLN	-	expression tag	UNP Q9FL12
A	55	GLN	-	expression tag	UNP Q9FL12
A	56	MET	-	expression tag	UNP Q9FL12
A	57	GLY	-	expression tag	UNP Q9FL12
A	58	ARG	-	expression tag	UNP Q9FL12
A	59	GLY	-	expression tag	UNP Q9FL12
A	60	SER	-	expression tag	UNP Q9FL12
A	61	GLU	-	expression tag	UNP Q9FL12
A	62	PHE	-	expression tag	UNP Q9FL12
A	63	GLU	-	expression tag	UNP Q9FL12
A	64	LEU	-	expression tag	UNP Q9FL12
B	27	MET	-	expression tag	UNP Q9FL12
B	28	GLY	-	expression tag	UNP Q9FL12
B	29	SER	-	expression tag	UNP Q9FL12
B	30	SER	-	expression tag	UNP Q9FL12
B	31	HIS	-	expression tag	UNP Q9FL12
B	32	HIS	-	expression tag	UNP Q9FL12
B	33	HIS	-	expression tag	UNP Q9FL12
B	34	HIS	-	expression tag	UNP Q9FL12
B	35	HIS	-	expression tag	UNP Q9FL12
B	36	HIS	-	expression tag	UNP Q9FL12
B	37	SER	-	expression tag	UNP Q9FL12
B	38	SER	-	expression tag	UNP Q9FL12
B	39	GLY	-	expression tag	UNP Q9FL12
B	40	LEU	-	expression tag	UNP Q9FL12
B	41	VAL	-	expression tag	UNP Q9FL12
B	42	PRO	-	expression tag	UNP Q9FL12
B	43	ARG	-	expression tag	UNP Q9FL12
B	44	GLY	-	expression tag	UNP Q9FL12
B	45	SER	-	expression tag	UNP Q9FL12
B	46	HIS	-	expression tag	UNP Q9FL12
B	47	MET	-	expression tag	UNP Q9FL12
B	48	ALA	-	expression tag	UNP Q9FL12
B	49	SER	-	expression tag	UNP Q9FL12
B	50	MET	-	expression tag	UNP Q9FL12
B	51	THR	-	expression tag	UNP Q9FL12
B	52	GLY	-	expression tag	UNP Q9FL12
B	53	GLY	-	expression tag	UNP Q9FL12
B	54	GLN	-	expression tag	UNP Q9FL12
B	55	GLN	-	expression tag	UNP Q9FL12

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Chain	Residue	Modelled	Actual	Comment	Reference
B	56	MET	-	expression tag	UNP Q9FL12
B	57	GLY	-	expression tag	UNP Q9FL12
B	58	ARG	-	expression tag	UNP Q9FL12
B	59	GLY	-	expression tag	UNP Q9FL12
B	60	SER	-	expression tag	UNP Q9FL12
B	61	GLU	-	expression tag	UNP Q9FL12
B	62	PHE	-	expression tag	UNP Q9FL12
B	63	GLU	-	expression tag	UNP Q9FL12
B	64	LEU	-	expression tag	UNP Q9FL12

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	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	343	Total	O	0	0
			343	343		
3	B	313	Total	O	0	0
			313	313		

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

- [illegible]

- Chain B:
- 
- 3% 72% 8% 20%
- MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS HIS SER SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER MET THR GLY GLN MET GLY ARG GLN MET GLY LEU LEU ASN ASN GLU SER GLU GLY ASN GLN ARG THR SER PRO PRO GLU ARG ARG SER SER LEU
- HIS HIS SER ASP THR LYS ASN GLY HIS CYS ASN ASN GLY LEU VAL ILE VAL THR THR GLU SER ALA ILE PRO ALA THR SER TRP GLU THR VAL V119 P123 R146 I158 R163 K180 K187 E198 W212 V215 G221 L226 Q227 D228 A229 E230
- G237 V248 R251 W252 E253 L254 L255 S256 TYR VAL HIS GLY SER T262 T263 L264 L265 G266 A271 A272 I273 I274 N277 S278 D285 K288 F294 Q295 SER LEU HIS GLU ASP ALA GLU N304 I305 G306 Y307 P310 T311 P312 Y327 T328 G329 F330 P331 V332 I335
- R359 I360 I363 E369 V372 L373 D377 N396 Y405 L406 L417 H436 R468 Y471 P480 I512 K549 L586 LYS THR GLU ARG ASN

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.05Å 132.05Å 154.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.93 – 2.20 47.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.3 (39.93-2.20) 89.4 (47.89-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.04 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.180 , 0.228 0.180 , 0.228	Depositor DCC
$R_{free}$ test set	2995 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.040 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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 [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	0.43	1/3630 (0.0%)	0.60	1/4933 (0.0%)
1	B	0.40	0/3522	0.59	2/4790 (0.0%)
All	All	0.41	1/7152 (0.0%)	0.60	3/9723 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	ASP	C-N	6.14	1.48	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ASN	CB-CA-C	-6.64	97.12	110.40
1	B	406	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	359	ARG	NE-CZ-NH2	-5.73	117.44	120.30

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	3554	0	3493	30	0
1	B	3448	0	3372	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	16	2	0
3	A	343	0	0	7	0
3	B	313	0	0	11	0
All	All	7670	0	6881	65	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 5.

All (65) 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:A:274:ASN:O	1:A:277:ASN:ND2	2.10	0.84
1:B:386:ASN:OD1	3:B:701:HOH:O	1.98	0.80
1:A:274:ASN:H	1:A:277:ASN:HD21	1.33	0.76
1:A:156:GLY:HA2	1:A:279:GLY:O	1.87	0.75
1:B:262:THR:N	3:B:704:HOH:O	2.19	0.74
1:B:198:GLU:OE1	1:B:198:GLU:N	2.20	0.72
1:B:549:LYS:HD2	2:B:601:GOL:H2	1.74	0.69
1:A:380:LEU:O	3:A:601:HOH:O	2.13	0.65
1:B:146[A]:ARG:NH2	3:B:709:HOH:O	2.29	0.65
1:B:586:LEU:O	3:B:702:HOH:O	2.15	0.65
1:B:359:ARG:NH2	3:B:705:HOH:O	2.20	0.64
1:B:277:ASN:ND2	3:B:711:HOH:O	2.31	0.64
1:A:158:ILE:HG23	1:A:212:TRP:HZ3	1.66	0.61
1:A:185:ASP:O	3:A:603:HOH:O	2.15	0.59
1:A:274:ASN:ND2	1:A:275:SER:O	2.33	0.59
2:B:602:GOL:O1	3:B:703:HOH:O	2.16	0.56
1:A:277:ASN:HD22	1:A:277:ASN:H	1.54	0.56
1:A:334:GLY:N	3:A:616:HOH:O	2.37	0.54
1:A:181:LYS:NZ	1:A:211:PHE:O	2.30	0.53
1:B:332:VAL:HG21	1:B:436:HIS:HB2	1.92	0.52
1:A:405:TYR:OH	3:A:602:HOH:O	2.15	0.51
1:A:386:ASN:OD1	3:A:601:HOH:O	2.20	0.50
1:A:393:VAL:CG2	1:A:405:TYR:HE1	2.26	0.48
1:B:278:SER:OG	1:B:294:PHE:HA	2.13	0.48
1:B:335:ILE:HG22	1:B:363:ILE:HG12	1.95	0.48
1:A:209:ASP:OD1	3:A:604:HOH:O	2.20	0.47
1:B:512:ILE:HD11	3:B:717:HOH:O	2.14	0.47
1:B:158:ILE:HG23	1:B:212:TRP:HZ3	1.79	0.47
1:A:339:LYS:HG2	1:A:390:ASP:HA	1.96	0.47
1:B:163:ARG:NH1	3:B:708:HOH:O	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:GLY:HA2	1:B:310:PRO:HD3	1.97	0.46
1:B:360:ILE:HD12	1:B:377:ASP:HB2	1.96	0.45
1:B:468:ARG:HD2	3:B:752:HOH:O	2.16	0.45
1:A:332:VAL:HG21	1:A:436:HIS:HB2	1.99	0.45
1:B:274:ASN:H	1:B:277:ASN:HB2	1.81	0.45
1:A:138:PRO:HA	1:A:146:ARG:HD3	1.99	0.44
1:B:226:LEU:HD21	1:B:251:ARG:HA	1.99	0.44
1:B:251:ARG:HH21	1:B:253:GLU:HG3	1.82	0.44
1:B:327:TYR:CZ	1:B:329:GLY:HA2	2.52	0.44
1:B:471:TYR:CZ	1:B:480:PRO:HD3	2.53	0.44
1:A:277:ASN:HD22	1:A:277:ASN:N	2.14	0.44
1:B:311:THR:OG1	1:B:312:PRO:HD3	2.18	0.43
1:A:226:LEU:HD22	1:A:251:ARG:HA	1.99	0.43
1:A:382:PHE:CZ	1:A:407:ILE:HG12	2.53	0.43
1:B:265:LEU:HG	1:B:310:PRO:HG3	2.01	0.43
1:B:180:LYS:HE2	1:B:187:LYS:HG3	2.00	0.43
1:B:254:ILE:HD13	1:B:265:LEU:HA	2.00	0.43
1:A:393:VAL:HG21	1:A:405:TYR:HE1	1.83	0.43
1:B:254:ILE:HA	1:B:264:LEU:O	2.18	0.43
1:A:537:ALA:O	1:A:541:GLU:HG3	2.19	0.43
1:B:417:LEU:HA	1:B:417:LEU:HD23	1.85	0.43
1:A:367:ALA:HB1	1:A:369:GLU:OE1	2.19	0.42
1:A:128:VAL:HG11	1:A:233:VAL:HG12	2.01	0.42
1:B:221:GLY:HA3	1:B:288:LYS:HB3	2.02	0.42
1:A:507:VAL:HG22	1:A:515:GLU:HG2	2.01	0.41
1:A:274:ASN:ND2	1:A:274:ASN:C	2.74	0.41
1:A:213:GLU:OE1	3:A:605:HOH:O	2.22	0.41
1:A:274:ASN:N	1:A:277:ASN:HD21	2.08	0.41
1:B:330:PHE:CD1	1:B:330:PHE:N	2.88	0.41
1:B:549:LYS:HE2	3:B:974:HOH:O	2.20	0.41
1:A:417:LEU:HA	1:A:417:LEU:HD23	1.95	0.40
1:A:233:VAL:O	1:A:281:PRO:HD2	2.22	0.40
1:B:212:TRP:O	1:B:215:VAL:HG22	2.20	0.40
1:B:369:GLU:HB3	1:B:373:LEU:HD12	2.03	0.40
1:B:254:ILE:HD12	1:B:405:TYR:CE1	2.56	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	463/566 (82%)	449 (97%)	14 (3%)	0	100	100
1	B	450/566 (80%)	432 (96%)	18 (4%)	0	100	100
All	All	913/1132 (81%)	881 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	383/490 (78%)	376 (98%)	7 (2%)	59	72
1	B	366/490 (75%)	365 (100%)	1 (0%)	92	97
All	All	749/980 (76%)	741 (99%)	8 (1%)	73	85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	VAL
1	A	182	ARG
1	A	246	SER
1	A	261	SER
1	A	277	ASN
1	A	405	TYR
1	A	452	PHE
1	B	372	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN

### 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 carbohydrates 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	B	602	-	5,5,5	0.37	0	5,5,5	0.32	0
2	GOL	B	601	-	5,5,5	0.42	0	5,5,5	0.17	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	B	602	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	601	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	602	GOL	O1-C1-C2-C3
2	B	601	GOL	O1-C1-C2-O2
2	B	601	GOL	O1-C1-C2-C3
2	B	602	GOL	O1-C1-C2-O2
2	B	601	GOL	O2-C2-C3-O3
2	B	601	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	GOL	1	0
2	B	601	GOL	1	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	465/566 (82%)	-0.31	8 (1%) 70 68	17, 31, 55, 81	1 (0%)
1	B	455/566 (80%)	-0.22	15 (3%) 46 44	17, 33, 62, 73	0
All	All	920/1132 (81%)	-0.27	23 (2%) 57 55	17, 32, 60, 81	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	272	ALA	5.8
1	B	306	GLY	5.1
1	A	272	ALA	4.7
1	A	302	ALA	4.4
1	A	271	ALA	3.9
1	B	248	VAL	3.7
1	A	405	TYR	3.1
1	B	304	ASN	3.1
1	B	273	ILE	3.1
1	B	247	GLY	2.8
1	B	123	PRO	2.7
1	B	246	SER	2.4
1	B	271	ALA	2.4
1	B	307	TYR	2.4
1	B	295	GLN	2.3
1	A	124	SER	2.3
1	B	305	ILE	2.3
1	A	300	GLU	2.2
1	B	229	ALA	2.2
1	B	227	GLN	2.2
1	B	285	ASP	2.1
1	A	274	ASN	2.1
1	A	299	HIS	2.1

## 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	B	601	6/6	0.88	0.15	41,46,49,56	0
2	GOL	B	602	6/6	0.89	0.12	59,65,68,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.