



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:16 PM GMT

PDB ID : 3WOJ  
Title : Crystal structure of the DAP BII  
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Deposited on : 2013-12-29  
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  
<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

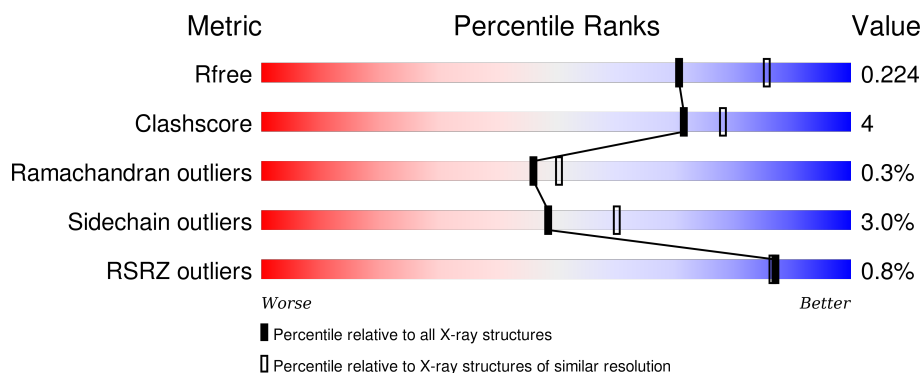
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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. 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	698	<div> <div></div> <div>89% 10% .</div> </div>
1	B	698	<div> <div></div> <div>89% 10% .</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	A	802	-	-	-	X
2	GOL	A	803	-	-	-	X
2	GOL	A	804	-	-	-	X
2	GOL	B	802	-	-	-	X
2	GOL	B	803	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11715 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 dipeptidyl aminopeptidase BII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	698	Total	C	N	O	S	0	0	0
			5381	3404	939	1019	19			
1	B	698	Total	C	N	O	S	0	0	0
			5381	3404	939	1019	19			

- 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	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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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		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	1	Total	Zn	0	0
			1	1		

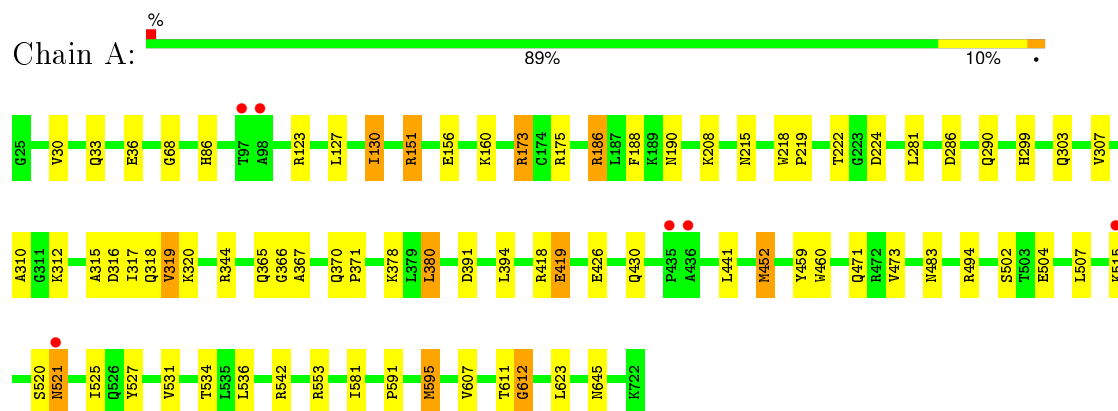
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	462	Total	O	0	0
			462	462		
4	B	446	Total	O	0	0
			446	446		

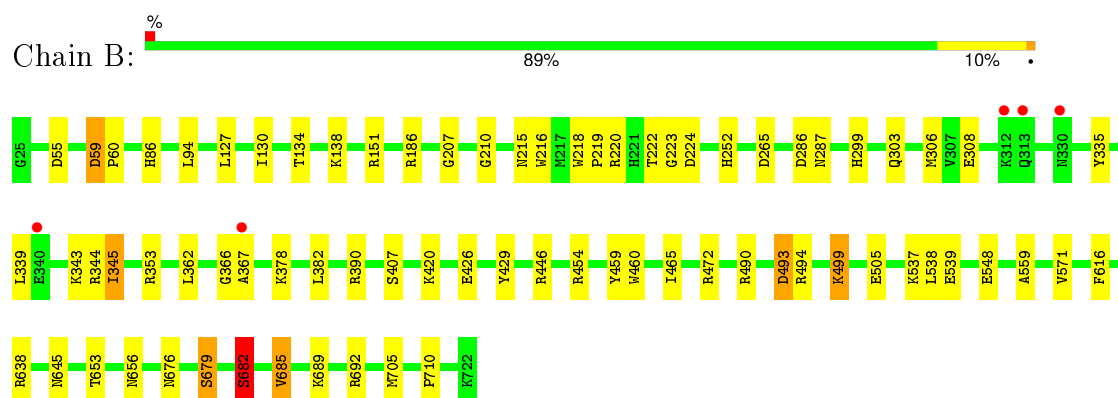
### 3 Residue-property plots

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: dipeptidyl aminopeptidase BII



- Molecule 1: dipeptidyl aminopeptidase BII



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.46Å 130.71Å 170.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.59 – 2.20 29.59 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.59-2.20) 98.6 (29.59-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.40 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.165 , 0.220 0.173 , 0.224	Depositor DCC
$R_{free}$ test set	4318 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.7	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 86106 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, ZN

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	0.92	1/5499 (0.0%)	0.96	16/7451 (0.2%)
1	B	0.94	4/5499 (0.1%)	0.93	13/7451 (0.2%)
All	All	0.93	5/10998 (0.0%)	0.95	29/14902 (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	3
1	B	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	GLU	CD-OE1	7.32	1.33	1.25
1	B	679	SER	CB-OG	-5.95	1.34	1.42
1	B	682	SER	CA-CB	5.68	1.61	1.52
1	B	429	TYR	CE1-CZ	-5.12	1.31	1.38
1	B	539	GLU	CD-OE1	-5.04	1.20	1.25

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	A	156	GLU	OE1-CD-OE2	-9.26	112.19	123.30
1	B	426	GLU	OE1-CD-OE2	-8.83	112.70	123.30
1	A	151	ARG	NE-CZ-NH1	8.41	124.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	494	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	A	186	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	B	685	VAL	CB-CA-C	-7.40	97.35	111.40
1	B	692	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	553	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	344	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	490	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	365	GLN	C-N-CA	-6.54	108.57	122.30
1	B	186	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	553	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	612	GLY	N-CA-C	6.08	128.31	113.10
1	B	55	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	353	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	542	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	123	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	494	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	494	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	692	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	493	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	286	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	581	ILE	CG1-CB-CG2	-5.41	99.49	111.40
1	B	59	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	B	286	ASP	CB-CG-OD1	5.09	122.89	118.30
1	A	494	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	186	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	366	GLY	Peptide
1	A	419	GLU	Peptide
1	A	611	THR	Peptide
1	B	366	GLY	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	5381	0	5297	51	0
1	B	5381	0	5297	42	0
2	A	24	0	32	1	0
2	B	18	0	23	4	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	462	0	0	9	0
4	B	446	0	0	7	0
All	All	11715	0	10649	93	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 4.

All (93) 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:307:VAL:HA	1:A:452:MET:HE3	1.37	1.03
1:A:315:ALA:O	1:A:319:VAL:HG12	1.64	0.96
1:B:224:ASP:OD1	4:B:1323:HOH:O	1.88	0.91
1:B:679:SER:O	1:B:682:SER:HB3	1.73	0.87
1:A:591:PRO:HD2	1:A:595:MET:HE1	1.55	0.86
1:A:591:PRO:HD2	1:A:595:MET:CE	2.05	0.86
1:A:224:ASP:OD1	4:A:1296:HOH:O	1.94	0.86
1:A:86:HIS:N	4:A:1296:HOH:O	1.88	0.84
1:A:591:PRO:CD	1:A:595:MET:HE1	2.12	0.80
1:A:130:ILE:HD11	1:A:186:ARG:HD3	1.65	0.78
1:A:307:VAL:HA	1:A:452:MET:CE	2.18	0.73
1:B:94:LEU:HD23	1:B:94:LEU:O	1.88	0.73
1:B:86:HIS:N	4:B:1323:HOH:O	1.94	0.72
1:B:685:VAL:O	1:B:685:VAL:HG23	1.85	0.72
1:A:173:ARG:HD2	1:A:175:ARG:HH21	1.54	0.72
1:B:682:SER:HA	1:B:685:VAL:O	1.95	0.67
1:A:307:VAL:CA	1:A:452:MET:HE3	2.20	0.67
1:A:299:HIS:HD2	1:A:459:TYR:OH	1.78	0.66
1:B:222:THR:H	1:B:645:ASN:HD21	1.41	0.66
1:B:420:LYS:NZ	4:B:1176:HOH:O	2.28	0.66
1:B:685:VAL:O	1:B:685:VAL:CG2	2.40	0.66
1:A:318:GLN:HG2	4:A:1205:HOH:O	1.95	0.66
1:A:418:ARG:O	1:A:419:GLU:HG2	1.95	0.65
1:B:299:HIS:HD2	1:B:459:TYR:OH	1.81	0.63
1:A:151:ARG:HD3	4:A:1045:HOH:O	2.00	0.62
1:A:307:VAL:HG22	1:A:452:MET:HE3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:PRO:HD2	1:A:595:MET:HE3	1.84	0.60
1:B:287:ASN:OD1	1:B:390:ARG:NH1	2.34	0.60
1:A:86:HIS:CB	4:A:1296:HOH:O	2.51	0.58
1:A:307:VAL:HG22	1:A:452:MET:CE	2.34	0.57
1:B:454:ARG:NH1	1:B:493:ASP:OD1	2.37	0.56
1:B:382:LEU:HD11	1:B:548:GLU:HB3	1.89	0.55
1:B:306:MET:CE	4:B:1161:HOH:O	2.54	0.55
1:B:94:LEU:C	1:B:94:LEU:HD23	2.27	0.55
1:B:306:MET:HE1	4:B:1161:HOH:O	2.07	0.55
1:A:30:VAL:H	1:A:33:GLN:HE21	1.55	0.55
1:A:130:ILE:HD12	1:A:188:PHE:CZ	2.43	0.54
1:A:418:ARG:O	1:A:419:GLU:CB	2.55	0.53
1:B:130:ILE:N	1:B:130:ILE:HD12	2.24	0.52
1:B:335:TYR:O	1:B:339:LEU:HG	2.09	0.52
1:B:345:ILE:HD12	1:B:685:VAL:HG21	1.92	0.50
1:B:499:LYS:HB2	1:B:505:GLU:HG2	1.93	0.50
1:B:220:ARG:HB3	1:B:645:ASN:HD22	1.77	0.50
1:A:591:PRO:CG	1:A:595:MET:HE1	2.43	0.49
1:B:151:ARG:HD3	4:B:923:HOH:O	2.12	0.49
1:B:265:ASP:OD2	2:B:802:GOL:H32	2.14	0.48
1:B:676:ASN:O	1:B:679:SER:HB2	2.13	0.48
1:A:418:ARG:O	1:A:419:GLU:CG	2.61	0.48
1:A:222:THR:H	1:A:645:ASN:HD21	1.60	0.48
1:A:521:ASN:HD22	1:A:521:ASN:H	1.60	0.47
1:B:345:ILE:CD1	1:B:685:VAL:HG21	2.44	0.47
1:A:218:TRP:CG	1:A:219:PRO:HA	2.49	0.47
1:A:281:LEU:HD23	1:A:380:LEU:CD1	2.45	0.47
1:B:653:THR:H	1:B:656:ASN:HD22	1.62	0.47
1:B:362:LEU:HD21	1:B:559:ALA:HB1	1.98	0.46
1:B:638:ARG:HH12	2:B:802:GOL:H31	1.79	0.46
1:A:281:LEU:HD23	1:A:380:LEU:HD13	1.97	0.46
1:A:303:GLN:NE2	4:A:1310:HOH:O	2.46	0.46
1:B:705:MET:O	1:B:710:PRO:HA	2.16	0.46
1:A:303:GLN:NE2	1:A:460:TRP:HE1	2.15	0.45
1:B:215:ASN:O	1:B:216:TRP:HB2	2.17	0.45
1:A:591:PRO:HG2	1:A:595:MET:HE1	1.99	0.45
1:A:391:ASP:HB2	1:A:471:GLN:HE21	1.82	0.44
1:B:465:ILE:O	1:B:472:ARG:NH2	2.50	0.44
1:A:127:LEU:HA	1:A:190:ASN:ND2	2.33	0.44
1:A:317:ILE:HG21	1:A:452:MET:HE1	1.99	0.44
1:B:218:TRP:CG	1:B:219:PRO:HA	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLY:HA2	1:B:616:PHE:CE1	2.53	0.44
1:B:127:LEU:HD21	1:B:130:ILE:HD11	2.00	0.43
1:A:218:TRP:CD2	1:A:219:PRO:HA	2.54	0.43
1:A:307:VAL:CG2	1:A:452:MET:HE3	2.48	0.43
1:A:86:HIS:HB3	4:A:1296:HOH:O	2.16	0.43
1:A:483:ASN:ND2	1:A:483:ASN:O	2.52	0.43
1:B:222:THR:H	1:B:645:ASN:ND2	2.14	0.42
1:A:310:ALA:HB3	1:A:452:MET:HE1	2.00	0.42
1:B:638:ARG:HH12	2:B:802:GOL:C3	2.32	0.42
1:A:160:LYS:HG2	1:A:430:GLN:NE2	2.33	0.42
1:B:303:GLN:NE2	1:B:460:TRP:HE1	2.17	0.42
1:A:370:GLN:N	1:A:371:PRO:CD	2.82	0.42
1:A:378:LYS:HA	1:A:378:LYS:HD3	1.97	0.42
1:A:527:TYR:CE1	1:A:531:VAL:HG11	2.54	0.42
1:A:316:ASP:OD1	1:A:320:LYS:HE2	2.20	0.42
1:B:134:THR:HG22	1:B:138:LYS:HD2	2.01	0.41
1:A:290:GLN:NE2	2:A:802:GOL:H11	2.35	0.41
1:A:607:VAL:HG22	1:A:623:LEU:HD23	2.02	0.41
1:A:394:LEU:C	1:A:394:LEU:HD23	2.40	0.41
1:A:318:GLN:CG	4:A:1205:HOH:O	2.63	0.41
1:A:473:VAL:HG13	1:A:534:THR:HG21	2.02	0.41
1:B:59:ASP:HA	1:B:60:PRO:HA	1.93	0.40
1:B:207:GLY:HA2	1:B:223:GLY:O	2.21	0.40
1:B:252:HIS:CE1	2:B:803:GOL:H32	2.57	0.40
1:B:306:MET:HE3	4:B:1161:HOH:O	2.20	0.40
1:A:86:HIS:ND1	4:A:1296:HOH:O	2.37	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	696/698 (100%)	674 (97%)	19 (3%)	3 (0%)	39	42
1	B	696/698 (100%)	677 (97%)	18 (3%)	1 (0%)	56	64
All	All	1392/1396 (100%)	1351 (97%)	37 (3%)	4 (0%)	46	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	612	GLY
1	B	367	ALA
1	A	367	ALA
1	A	68	GLY

### 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	542/542 (100%)	523 (96%)	19 (4%)	43	53
1	B	542/542 (100%)	529 (98%)	13 (2%)	57	69
All	All	1084/1084 (100%)	1052 (97%)	32 (3%)	48	60

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	130	ILE
1	A	173	ARG
1	A	208	LYS
1	A	215	ASN
1	A	312	LYS
1	A	319	VAL
1	A	380	LEU
1	A	441	LEU
1	A	452	MET
1	A	502	SER
1	A	504	GLU

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Mol	Chain	Res	Type
1	A	507	LEU
1	A	515	LYS
1	A	520	SER
1	A	521	ASN
1	A	525	ILE
1	A	536	LEU
1	A	595	MET
1	B	308	GLU
1	B	343	LYS
1	B	344	ARG
1	B	345	ILE
1	B	378	LYS
1	B	407	SER
1	B	446	ARG
1	B	499	LYS
1	B	537	LYS
1	B	538	LEU
1	B	571	VAL
1	B	682	SER
1	B	689	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	84	ASN
1	A	190	ASN
1	A	259	GLN
1	A	287	ASN
1	A	290	GLN
1	A	299	HIS
1	A	303	GLN
1	A	350	GLN
1	A	430	GLN
1	A	471	GLN
1	A	521	ASN
1	A	567	GLN
1	A	585	ASN
1	A	645	ASN
1	A	656	ASN
1	B	84	ASN
1	B	249	GLN

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Mol	Chain	Res	Type
1	B	252	HIS
1	B	259	GLN
1	B	299	HIS
1	B	303	GLN
1	B	330	ASN
1	B	334	ASN
1	B	338	GLN
1	B	471	GLN
1	B	585	ASN
1	B	645	ASN
1	B	656	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](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

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	801	-	5,5,5	0.22	0	5,5,5	1.04	0
2	GOL	A	802	-	5,5,5	0.48	0	5,5,5	0.49	0
2	GOL	A	803	-	5,5,5	0.52	0	5,5,5	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	A	804	-	5,5,5	0.62	0	5,5,5	1.63	2 (40%)
2	GOL	B	801	-	5,5,5	0.61	0	5,5,5	0.38	0
2	GOL	B	802	-	5,5,5	1.29	0	5,5,5	1.39	1 (20%)
2	GOL	B	803	-	5,5,5	0.87	0	5,5,5	1.28	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	801	-	-	0/4/4/4	0/0/0/0
2	GOL	A	802	-	-	0/4/4/4	0/0/0/0
2	GOL	A	803	-	-	0/4/4/4	0/0/0/0
2	GOL	A	804	-	-	0/4/4/4	0/0/0/0
2	GOL	B	801	-	-	0/4/4/4	0/0/0/0
2	GOL	B	802	-	-	0/4/4/4	0/0/0/0
2	GOL	B	803	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	804	GOL	C3-C2-C1	-2.68	100.60	111.12
2	A	804	GOL	O2-C2-C1	2.36	119.47	108.65
2	B	802	GOL	C3-C2-C1	2.49	120.87	111.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	GOL	1	0
2	B	802	GOL	3	0
2	B	803	GOL	1	0



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 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	698/698 (100%)	-0.40	6 (0%) 85 85	6, 18, 41, 60	0
1	B	698/698 (100%)	-0.43	5 (0%) 89 88	6, 17, 35, 70	0
All	All	1396/1396 (100%)	-0.41	11 (0%) 87 87	6, 17, 38, 70	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	GLN	4.1
1	A	98	ALA	3.5
1	A	97	THR	3.3
1	A	435	PRO	3.3
1	A	515	LYS	2.9
1	A	436	ALA	2.5
1	B	330	ASN	2.4
1	B	312	LYS	2.3
1	A	521	ASN	2.2
1	B	340	GLU	2.1
1	B	367	ALA	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	A	804	6/6	0.85	0.22	10.44	32,41,44,47	0
2	GOL	B	802	6/6	0.95	0.16	3.27	18,20,20,22	0
2	GOL	B	803	6/6	0.85	0.19	3.01	27,32,34,35	0
2	GOL	A	802	6/6	0.91	0.19	2.93	38,40,40,40	0
2	GOL	A	803	6/6	0.94	0.14	2.76	19,19,23,24	0
2	GOL	A	801	6/6	0.96	0.12	0.65	12,14,15,18	0
2	GOL	B	801	6/6	0.96	0.10	-0.85	14,18,20,20	0
3	ZN	B	804	1/1	0.97	0.12	-	36,36,36,36	0
3	ZN	B	805	1/1	1.00	0.05	-	15,15,15,15	0
3	ZN	A	805	1/1	0.95	0.17	-	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.