



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:16 PM GMT

PDB ID : 3WOK  
Title : Crystal structure of the DAP BII (Space)  
Authors : Sakamoto, Y.; Suzuki, Y.; Iizuka, I.; Tateoka, C.; Roppongi, S.; Fujimoto, M.;  
Nonaka, T.; Ogasawara, W.; Tanaka, N.  
Deposited on : 2013-12-29  
Resolution : 1.95 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

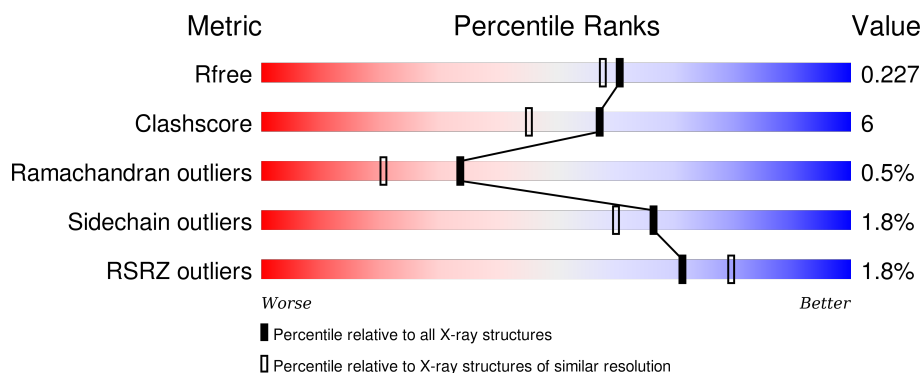
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	
1	B	698	

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	803	-	-	-	X
2	GOL	A	804	-	-	-	X
2	GOL	A	805	-	-	-	X
2	GOL	A	806	-	-	-	X
2	GOL	A	807	-	-	-	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 12092 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	Se	0	0	0
			5380	3404	939	1018	4	15			
1	B	698	Total	C	N	O	S	Se	0	1	0
			5385	3408	939	1018	4	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	657	ALA	SER	ENGINEERED MUTATION	UNP V5YM14
B	657	ALA	SER	ENGINEERED MUTATION	UNP V5YM14

- 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		

*Continued on next page...*

*Continued from previous page...*

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

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

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

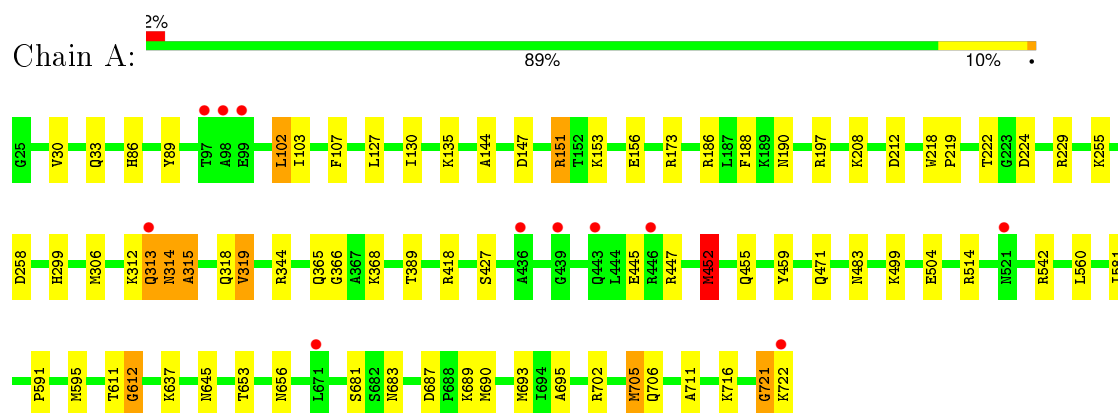
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	638	Total O 638 638	0	0
4	B	619	Total O 619 619	0	0

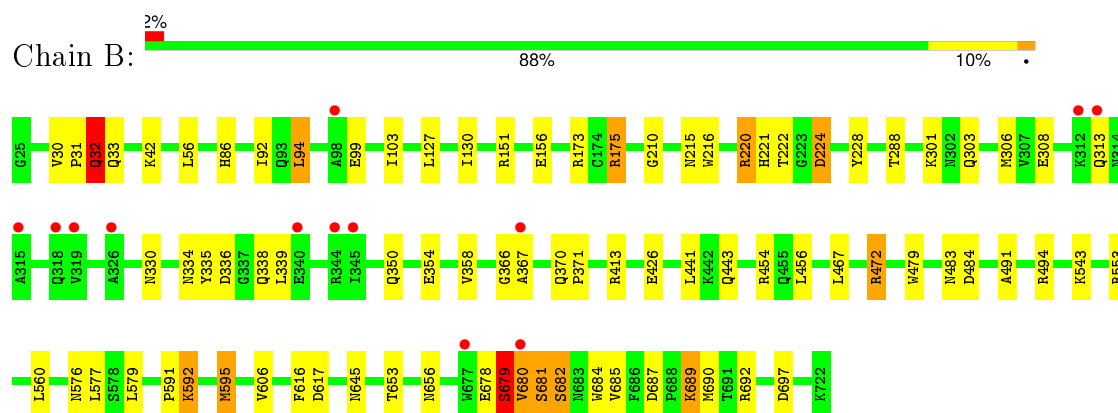
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

#### • 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, $\alpha$ , $\beta$ , $\gamma$	76.74Å 130.44Å 171.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.56 – 1.95 29.56 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.56-1.95) 98.7 (29.56-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.182 , 0.225 0.188 , 0.227	Depositor DCC
$R_{free}$ test set	6223 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 124208 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.88	1/5483 (0.0%)	0.95	19/7405 (0.3%)
1	B	0.92	4/5491 (0.1%)	1.04	30/7415 (0.4%)
All	All	0.90	5/10974 (0.0%)	1.00	49/14820 (0.3%)

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	2
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	220	ARG	CD-NE	-8.31	1.32	1.46
1	B	220	ARG	CA-CB	6.09	1.67	1.53
1	B	220	ARG	NE-CZ	-5.49	1.25	1.33
1	B	32	GLN	CD-OE1	-5.28	1.12	1.24
1	A	504	GLU	CG-CD	5.25	1.59	1.51

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	ARG	NE-CZ-NH2	-23.35	108.63	120.30
1	B	220	ARG	CG-CD-NE	-11.69	87.25	111.80
1	A	151	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	B	224	ASP	CB-CG-OD1	10.57	127.82	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	B	220	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	B	592	LYS	CD-CE-NZ	8.34	130.88	111.70
1	B	595[A]	MSE	CA-CB-CG	8.09	127.05	113.30
1	B	595[B]	MSE	CA-CB-CG	8.09	127.05	113.30
1	A	365	GLN	C-N-CA	-7.70	106.12	122.30
1	B	692	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	B	224	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	B	692	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	B	220	ARG	CB-CG-CD	7.56	131.25	111.60
1	B	494	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	A	147	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	258	ASP	CB-CG-OD1	-7.16	111.86	118.30
1	A	147	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	A	504	GLU	OE1-CD-OE2	-6.76	115.19	123.30
1	A	452	MSE	CG-SE-CE	6.72	113.69	98.90
1	B	220	ARG	NH1-CZ-NH2	6.29	126.33	119.40
1	A	186	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	197	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	542	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	595[A]	MSE	N-CA-CB	5.86	121.16	110.60
1	B	595[B]	MSE	N-CA-CB	5.86	121.16	110.60
1	A	447	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	595[A]	MSE	CG-SE-CE	-5.55	86.68	98.90
1	B	595[B]	MSE	CG-SE-CE	-5.55	86.68	98.90
1	B	220	ARG	N-CA-CB	5.46	120.42	110.60
1	B	484	ASP	CB-CG-OD1	5.45	123.21	118.30
1	B	228	TYR	CB-CG-CD1	5.45	124.27	121.00
1	B	220	ARG	CD-NE-CZ	5.43	131.21	123.60
1	B	32	GLN	CB-CA-C	5.42	121.23	110.40
1	A	229	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	173	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	344	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	553	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	472	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	B	175	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	612	GLY	N-CA-C	5.25	126.24	113.10
1	A	514	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	697	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	344	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	617	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	687	ASP	CB-CG-OD2	-5.06	113.75	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	553	ARG	C-N-CD	5.04	138.98	128.40
1	B	175	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	705	MSE	CG-SE-CE	-5.01	87.88	98.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	GLN	Peptide
1	A	611	THR	Peptide
1	A	721	GLY	Peptide
1	B	366	GLY	Peptide
1	B	679	SER	Peptide

## 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	5380	0	5297	62	1
1	B	5385	0	5306	65	0
2	A	48	0	63	0	0
2	B	18	0	24	1	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
4	A	638	0	0	22	1
4	B	619	0	0	11	2
All	All	12092	0	10690	128	2

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 6.

All (128) 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:B:224:ASP:OD1	4:B:1504:HOH:O	1.70	1.06

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:NZ	4:A:901:HOH:O	1.81	0.99
1:A:591:PRO:HD2	1:A:595:MSE:SE	2.13	0.98
1:B:127:LEU:HD21	1:B:130:ILE:HD11	1.45	0.98
1:A:452:MSE:SE	4:A:1323:HOH:O	2.33	0.95
1:B:591:PRO:HD2	1:B:595[B]:MSE:SE	2.17	0.93
1:A:224:ASP:OD1	4:A:1525:HOH:O	1.89	0.90
1:B:31:PRO:HG2	1:B:56:LEU:HD21	1.55	0.89
1:A:318:GLN:HG2	4:A:912:HOH:O	1.74	0.87
1:B:350:GLN:O	1:B:354:GLU:HG3	1.75	0.84
1:B:680:VAL:O	1:B:682:SER:N	2.12	0.81
1:B:30:VAL:H	1:B:33:GLN:HE21	1.29	0.80
1:B:682:SER:HA	1:B:685:VAL:O	1.81	0.79
1:B:94:LEU:HD23	1:B:94:LEU:O	1.82	0.79
1:B:130:ILE:N	1:B:130:ILE:HD12	1.97	0.79
1:A:595:MSE:HE3	4:B:1259:HOH:O	1.85	0.77
1:B:56:LEU:HD22	1:B:579:LEU:HD23	1.64	0.77
1:B:678:GLU:HG2	1:B:690:MSE:HE3	1.69	0.75
1:A:689:LYS:O	1:A:690:MSE:HE2	1.85	0.75
1:B:156:GLU:OE1	4:B:901:HOH:O	2.05	0.74
1:A:30:VAL:H	1:A:33:GLN:HE21	1.35	0.74
1:A:151:ARG:HD3	4:A:1002:HOH:O	1.89	0.72
1:B:426:GLU:OE2	4:B:901:HOH:O	2.08	0.70
1:B:86:HIS:N	4:B:1504:HOH:O	1.92	0.69
1:A:306:MSE:HE1	4:A:1300:HOH:O	1.92	0.68
1:A:705:MSE:HE2	1:A:711:ALA:HB3	1.75	0.68
1:A:130:ILE:HD12	1:A:188:PHE:CE2	2.28	0.68
1:A:156:GLU:OE1	4:A:901:HOH:O	2.11	0.67
1:B:680:VAL:C	1:B:682:SER:H	1.98	0.67
1:A:86:HIS:N	4:A:1525:HOH:O	2.02	0.65
1:B:56:LEU:HD22	1:B:579:LEU:CD2	2.27	0.64
1:B:32:GLN:H	1:B:32:GLN:NE2	1.95	0.64
1:B:31:PRO:CG	1:B:56:LEU:HD21	2.27	0.64
1:B:56:LEU:CD2	1:B:579:LEU:HD23	2.27	0.64
1:B:413:ARG:NH2	1:B:426:GLU:HG3	2.12	0.64
1:A:389:THR:HA	1:A:471:GLN:HE22	1.61	0.64
1:B:678:GLU:O	1:B:679:SER:HB3	1.99	0.62
1:B:303:GLN:HA	1:B:306:MSE:HE2	1.82	0.62
1:B:222:THR:H	1:B:645:ASN:HD21	1.48	0.61
1:A:222:THR:H	1:A:645:ASN:HD21	1.47	0.61
1:B:86:HIS:ND1	4:B:1504:HOH:O	2.22	0.61
1:A:86:HIS:ND1	4:A:1525:HOH:O	2.06	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASN:OD1	1:B:338:GLN:OE1	2.19	0.60
1:B:653:THR:H	1:B:656:ASN:HD22	1.51	0.59
1:B:32:GLN:HE21	1:B:32:GLN:H	1.48	0.59
1:A:306:MSE:HE2	1:A:455:GLN:HB3	1.84	0.59
1:A:716:LYS:HA	1:A:722:LYS:HB3	1.85	0.58
1:A:721:GLY:HA3	1:A:722:LYS:HB3	1.87	0.57
1:A:452:MSE:CE	1:A:452:MSE:HA	2.35	0.57
1:A:389:THR:HA	1:A:471:GLN:NE2	2.21	0.56
1:A:722:LYS:HE3	4:A:1444:HOH:O	2.06	0.56
1:A:683:ASN:OD1	4:A:1531:HOH:O	2.18	0.56
1:A:427:SER:HB2	4:A:1456:HOH:O	2.07	0.54
1:A:315:ALA:O	1:A:319:VAL:HG12	2.07	0.54
1:B:591:PRO:CD	1:B:595[B]:MSE:SE	3.00	0.54
1:B:592:LYS:HE2	1:B:595[B]:MSE:HG2	1.89	0.54
1:B:313:GLN:OE1	1:B:313:GLN:N	2.39	0.53
1:A:721:GLY:CA	1:A:722:LYS:HB3	2.38	0.53
1:A:127:LEU:HA	1:A:190:ASN:HD22	1.74	0.53
1:A:312:LYS:NZ	4:A:1081:HOH:O	2.43	0.51
1:A:418:ARG:NH1	4:A:1117:HOH:O	2.43	0.51
1:A:89:TYR:CE1	1:A:103:ILE:HD12	2.45	0.51
1:A:313:GLN:HG3	1:A:314:ASN:H	1.76	0.51
1:B:151:ARG:HD3	4:B:957:HOH:O	2.11	0.51
1:A:313:GLN:CG	1:A:314:ASN:N	2.74	0.50
1:A:218:TRP:CG	1:A:219:PRO:HA	2.46	0.50
1:B:454:ARG:HD2	4:B:1483:HOH:O	2.12	0.50
1:A:144:ALA:HB3	1:A:151:ARG:HG2	1.95	0.49
1:B:472:ARG:NH2	1:B:483:ASN:OD1	2.45	0.49
1:A:722:LYS:HD2	4:A:1137:HOH:O	2.12	0.48
2:B:803:GOL:H32	4:B:1490:HOH:O	2.13	0.48
1:A:299:HIS:HD2	1:A:459:TYR:OH	1.97	0.48
1:A:721:GLY:CA	1:A:722:LYS:CB	2.92	0.48
1:A:689:LYS:C	1:A:690:MSE:HE2	2.34	0.48
1:A:452:MSE:HE3	1:A:452:MSE:HA	1.96	0.48
1:A:313:GLN:CG	1:A:314:ASN:H	2.27	0.48
1:B:42:LYS:HD2	4:B:1029:HOH:O	2.13	0.47
1:B:680:VAL:C	1:B:682:SER:N	2.66	0.47
1:B:335:TYR:O	1:B:339:LEU:HG	2.14	0.47
1:A:452:MSE:CE	4:A:1323:HOH:O	2.62	0.46
1:A:306:MSE:CE	4:A:1300:HOH:O	2.57	0.46
1:A:637:LYS:HE2	4:A:951:HOH:O	2.15	0.46
1:A:595:MSE:HB2	1:A:595:MSE:HE2	1.75	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:HIS:HB3	1:B:606:VAL:HG22	1.98	0.46
1:B:288:THR:HG21	1:B:684:TRP:CZ2	2.52	0.45
1:A:483:ASN:ND2	1:A:483:ASN:O	2.49	0.45
1:A:218:TRP:CD2	1:A:219:PRO:HA	2.52	0.45
1:B:370:GLN:N	1:B:371:PRO:CD	2.80	0.45
1:B:30:VAL:HB	1:B:32:GLN:HE22	1.82	0.45
1:B:220:ARG:HD2	1:B:222:THR:OG1	2.17	0.45
1:B:441:LEU:HD12	1:B:441:LEU:C	2.37	0.45
1:B:130:ILE:N	1:B:130:ILE:CD1	2.71	0.44
1:A:366:GLY:HA3	4:A:915:HOH:O	2.16	0.44
1:A:212:ASP:HB3	4:A:949:HOH:O	2.16	0.44
1:B:30:VAL:N	1:B:33:GLN:HE21	2.07	0.44
1:B:595[B]:MSE:HB2	1:B:595[B]:MSE:HE2	1.75	0.44
1:A:452:MSE:CE	1:A:455:GLN:CD	2.87	0.43
1:A:693:MSE:HE3	1:A:695:ALA:HB2	2.01	0.43
1:B:130:ILE:H	1:B:130:ILE:HD12	1.81	0.43
1:A:222:THR:H	1:A:645:ASN:ND2	2.15	0.43
1:A:595:MSE:SE	1:A:595:MSE:C	3.08	0.42
1:B:358:VAL:HG11	1:B:560:LEU:HD23	2.01	0.42
1:A:581:ILE:N	1:A:581:ILE:HD12	2.33	0.42
1:B:576:ASN:O	1:B:577:LEU:HB2	2.19	0.42
1:A:681:SER:HB2	4:A:936:HOH:O	2.18	0.42
1:B:94:LEU:C	1:B:94:LEU:HD23	2.37	0.42
1:A:653:THR:H	1:A:656:ASN:HD22	1.68	0.42
1:A:722:LYS:CE	4:A:1444:HOH:O	2.66	0.42
1:A:702:ARG:O	1:A:706:GLN:HG3	2.20	0.42
1:B:301:LYS:NZ	1:B:336:ASP:OD2	2.37	0.42
1:A:102:LEU:HG	1:A:107:PHE:HB2	2.01	0.42
1:A:595:MSE:HG2	4:B:1259:HOH:O	2.20	0.41
1:B:479:TRP:CH2	1:B:491:ALA:HB1	2.55	0.41
1:A:153:LYS:NZ	1:A:156:GLU:OE1	2.51	0.41
1:B:210:GLY:HA2	1:B:616:PHE:CE1	2.55	0.41
1:A:306:MSE:CE	1:A:455:GLN:HB3	2.50	0.41
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.55	0.41
1:B:467:LEU:HB2	1:B:472:ARG:HE	1.84	0.41
1:B:354:GLU:O	1:B:358:VAL:HG23	2.20	0.41
1:B:30:VAL:H	1:B:33:GLN:NE2	2.08	0.41
1:B:156:GLU:OE2	1:B:543:LYS:NZ	2.51	0.41
1:B:306:MSE:HE1	1:B:456:LEU:HD23	2.02	0.41
1:B:220:ARG:HB3	1:B:645:ASN:HD22	1.85	0.41
1:B:92:ILE:CG2	1:B:103:ILE:HD13	2.51	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:ASP:OD1	1:B:689:LYS:HD2	2.21	0.40
1:B:687:ASP:OD1	1:B:689:LYS:CD	2.70	0.40
1:B:215:ASN:O	1:B:216:TRP:HB2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LYS:NZ	4:B:1428:HOH:O[3_655]	1.83	0.37
4:A:908:HOH:O	4:B:1428:HOH:O[3_655]	2.15	0.05

## 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%)	673 (97%)	20 (3%)	3 (0%)	39	27
1	B	697/698 (100%)	671 (96%)	22 (3%)	4 (1%)	30	16
All	All	1393/1396 (100%)	1344 (96%)	42 (3%)	7 (0%)	34	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	ASN
1	A	612	GLY
1	B	680	VAL
1	A	315	ALA
1	B	681	SER
1	B	367	ALA
1	B	679	SER

### 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	541/526 (103%)	531 (98%)	10 (2%)	66	60
1	B	542/526 (103%)	532 (98%)	10 (2%)	66	60
All	All	1083/1052 (103%)	1063 (98%)	20 (2%)	66	60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	135	LYS
1	A	173	ARG
1	A	208	LYS
1	A	319	VAL
1	A	368	LYS
1	A	445	GLU
1	A	452	MSE
1	A	499	LYS
1	A	560	LEU
1	B	32	GLN
1	B	94	LEU
1	B	99	GLU
1	B	175	ARG
1	B	308	GLU
1	B	330	ASN
1	B	443	GLN
1	B	681	SER
1	B	682	SER
1	B	689	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	84	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	190	ASN
1	A	299	HIS
1	A	338	GLN
1	A	350	GLN
1	A	365	GLN
1	A	471	GLN
1	A	483	ASN
1	A	585	ASN
1	A	645	ASN
1	A	656	ASN
1	B	32	GLN
1	B	33	GLN
1	B	84	ASN
1	B	121	ASN
1	B	249	GLN
1	B	303	GLN
1	B	338	GLN
1	B	443	GLN
1	B	521	ASN
1	B	567	GLN
1	B	585	ASN
1	B	645	ASN
1	B	656	ASN

### 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 ⓘ

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	0.38	0	5,5,5	0.93	0
2	GOL	A	802	-	5,5,5	0.64	0	5,5,5	0.91	0
2	GOL	A	803	3	5,5,5	1.47	1 (20%)	5,5,5	2.53	4 (80%)
2	GOL	A	804	-	5,5,5	0.70	0	5,5,5	1.33	0
2	GOL	A	805	-	5,5,5	0.67	0	5,5,5	1.43	1 (20%)
2	GOL	A	806	-	5,5,5	0.44	0	5,5,5	0.14	0
2	GOL	A	807	-	5,5,5	0.23	0	5,5,5	0.43	0
2	GOL	A	808	-	5,5,5	0.43	0	5,5,5	0.73	0
2	GOL	B	801	-	5,5,5	0.27	0	5,5,5	0.52	0
2	GOL	B	802	-	5,5,5	0.40	0	5,5,5	0.91	0
2	GOL	B	803	-	5,5,5	0.48	0	5,5,5	1.26	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	3	-	0/4/4/4	0/0/0/0
2	GOL	A	804	-	-	0/4/4/4	0/0/0/0
2	GOL	A	805	-	-	0/4/4/4	0/0/0/0
2	GOL	A	806	-	-	0/4/4/4	0/0/0/0
2	GOL	A	807	-	-	0/4/4/4	0/0/0/0
2	GOL	A	808	-	-	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	803	GOL	O2-C2	2.87	1.52	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	803	GOL	C3-C2-C1	-2.71	100.48	111.12
2	A	803	GOL	O1-C1-C2	-2.10	99.99	110.18
2	A	803	GOL	O3-C3-C2	2.14	120.55	110.18
2	A	805	GOL	O2-C2-C1	2.29	119.16	108.65
2	A	803	GOL	O2-C2-C3	3.83	126.23	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	803	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	683/698 (97%)	-0.05	11 (1%) 74 83	7, 17, 39, 66	0
1	B	683/698 (97%)	-0.04	13 (1%) 70 78	7, 18, 38, 69	0
All	All	1366/1396 (97%)	-0.04	24 (1%) 71 80	7, 18, 38, 69	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	ALA	5.5
1	B	315	ALA	4.4
1	A	97	THR	4.4
1	B	313	GLN	3.6
1	B	367	ALA	3.5
1	A	722	LYS	3.1
1	B	677	TRP	3.1
1	A	436	ALA	3.0
1	B	345	ILE	3.0
1	B	319	VAL	2.9
1	A	521	ASN	2.9
1	B	318	GLN	2.9
1	A	313	GLN	2.8
1	B	98	ALA	2.6
1	A	99	GLU	2.6
1	B	340	GLU	2.5
1	B	326	ALA	2.5
1	B	680	VAL	2.4
1	A	446	ARG	2.3
1	B	312	LYS	2.3
1	A	439	GLY	2.1
1	A	671	LEU	2.1
1	A	443	GLN	2.1
1	B	344	ARG	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. 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	B	802	6/6	0.97	0.15	6.86	14,17,17,18	0
2	GOL	A	806	6/6	0.81	0.20	5.27	37,41,42,43	0
2	GOL	A	804	6/6	0.95	0.15	3.88	25,29,30,34	0
2	GOL	B	803	6/6	0.94	0.13	3.12	17,26,27,33	0
2	GOL	A	807	6/6	0.84	0.22	3.03	29,30,40,41	0
2	GOL	A	805	6/6	0.94	0.14	2.71	23,25,27,27	0
2	GOL	A	803	6/6	0.92	0.14	2.49	17,23,24,27	0
2	GOL	A	808	6/6	0.88	0.15	1.77	22,23,25,26	0
2	GOL	A	802	6/6	0.97	0.09	0.65	14,17,20,24	0
3	ZN	B	804	1/1	1.00	0.11	0.34	12,12,12,12	0
2	GOL	B	801	6/6	0.96	0.09	-0.09	13,16,17,20	0
2	GOL	A	801	6/6	0.97	0.08	-0.20	12,13,14,15	0
3	ZN	A	809	1/1	0.99	0.09	-	14,14,14,14	0
3	ZN	A	811	1/1	1.00	0.04	-	20,20,20,20	0
3	ZN	A	810	1/1	0.99	0.05	-	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.