



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:16 PM GMT

PDB ID : 3WON  
Title : Crystal structure of the DAP BII dipeptide complex III  
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Deposited on : 2013-12-29  
Resolution : 1.75 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

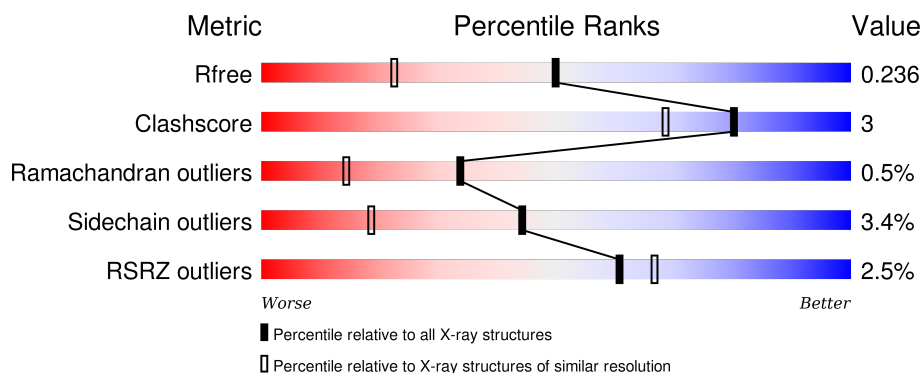
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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>92%</div> <div>7%</div> </div>
1	B	698	<div> <div>5%</div> <div>87%</div> <div>11%</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	VAL	A	801	-	-	-	X
4	GOL	A	804	-	-	X	-
4	GOL	A	805	-	-	-	X
4	GOL	A	806	-	-	-	X
4	GOL	A	807	-	-	-	X
4	GOL	B	804	-	-	-	X
4	GOL	B	806	-	-	-	X

## 2 Entry composition [i](#)

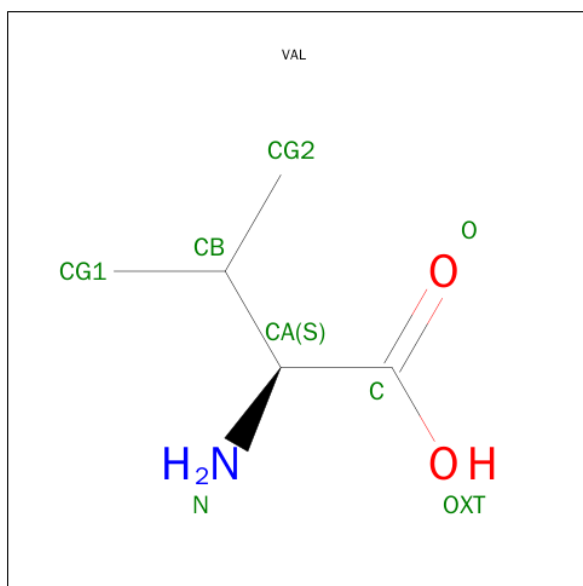
There are 6 unique types of molecules in this entry. The entry contains 11804 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

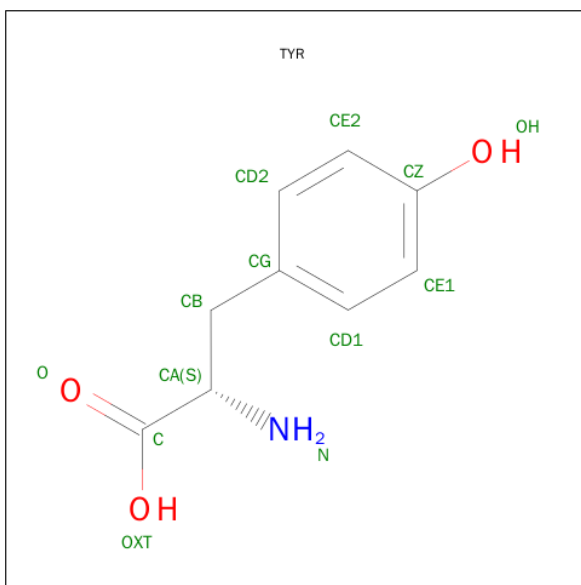
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	697	Total	C	N	O	S	0	0	0
			5371	3398	937	1017	19			
1	B	697	Total	C	N	O	S	0	0	0
			5371	3398	937	1017	19			

- Molecule 2 is VALINE (three-letter code: VAL) (formula:  $C_5H_{11}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	5	1	1		
2	B	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 3 is TYROSINE (three-letter code: TYR) (formula:  $C_9H_{11}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		
3	B	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

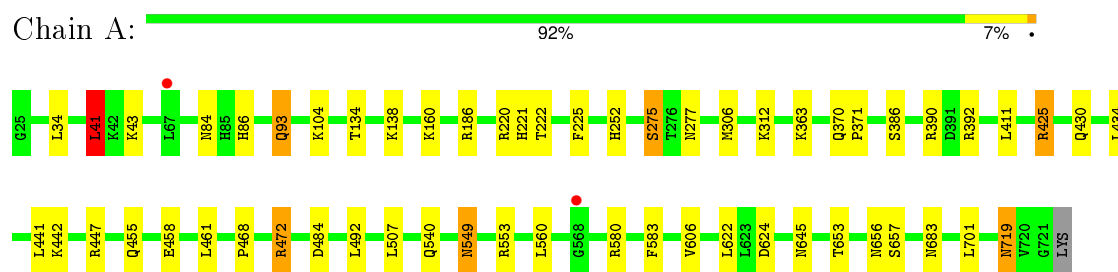
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	583	Total	O	0	0
			583	583		
6	B	381	Total	O	0	0
			381	381		

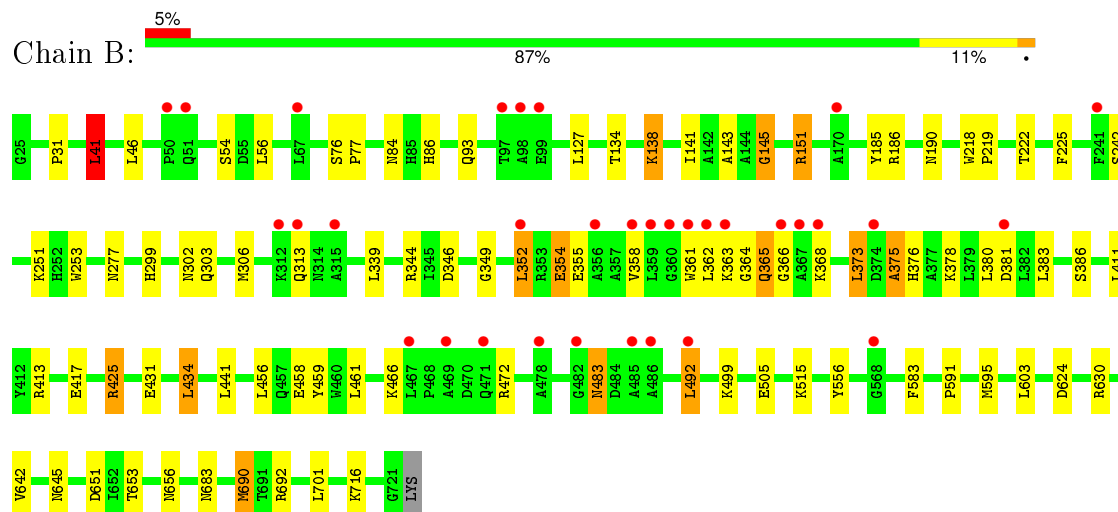
### 3 Residue-property plots

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 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.05Å 122.05Å 219.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.11 – 1.75 39.11 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.11-1.75) 98.8 (39.11-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.188 , 0.229 0.196 , 0.236	Depositor DCC
$R_{free}$ test set	8264 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 164405 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11804	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.39 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.7516e-03.*

<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	0.95	1/5489 (0.0%)	0.95	12/7440 (0.2%)
1	B	0.88	1/5489 (0.0%)	0.93	14/7440 (0.2%)
All	All	0.92	2/10978 (0.0%)	0.94	26/14880 (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	B	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	SER	CB-OG	-5.43	1.35	1.42
1	B	185	TYR	CE1-CZ	-5.22	1.31	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	472	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	B	630	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	B	151	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	A	624	ASP	CB-CG-OD1	7.62	125.16	118.30
1	B	690	MET	CG-SD-CE	-7.11	88.82	100.20
1	B	41	LEU	CB-CG-CD1	7.09	123.05	111.00
1	A	41	LEU	CA-CB-CG	6.55	130.37	115.30
1	A	580	ARG	NE-CZ-NH1	6.38	123.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	383	LEU	CB-CG-CD2	-6.31	100.27	111.00
1	A	392	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	A	484	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	624	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	B	41	LEU	CA-CB-CG	6.08	129.29	115.30
1	B	186	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	B	624	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	41	LEU	CB-CG-CD1	5.93	121.08	111.00
1	B	413	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	151	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	425	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	651	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	580	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	425	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	390	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	B	651	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	692	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	145	GLY	Peptide
1	B	313	GLN	Peptide
1	B	363	LYS	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	5371	0	5284	27	0
1	B	5371	0	5284	41	0
2	A	7	0	8	1	0
2	B	7	0	8	0	0
3	A	13	0	9	0	0
3	B	13	0	9	0	0
4	A	30	0	40	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	32	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	583	0	0	4	0
6	B	381	0	0	1	0
All	All	11804	0	10674	72	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 (72) 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:354:GLU:O	1:B:358:VAL:HG23	1.63	0.96
1:A:252:HIS:ND1	4:A:804:GOL:O1	2.04	0.86
1:A:252:HIS:HD1	4:A:804:GOL:HO1	1.19	0.81
1:A:277:ASN:HD22	1:A:683:ASN:HD21	1.38	0.70
4:A:806:GOL:C1	6:A:1098:HOH:O	2.45	0.63
1:B:591:PRO:HD2	1:B:595:MET:SD	2.39	0.63
4:A:806:GOL:H11	6:A:1098:HOH:O	1.99	0.62
1:B:411:LEU:HD21	1:B:441:LEU:HD11	1.83	0.60
1:A:222:THR:H	1:A:645:ASN:HD21	1.50	0.60
1:B:591:PRO:HG2	1:B:595:MET:SD	2.43	0.59
1:B:222:THR:H	1:B:645:ASN:HD21	1.50	0.59
1:A:160:LYS:NZ	1:A:425:ARG:O	2.32	0.58
1:B:431:GLU:HA	1:B:434:LEU:HD22	1.85	0.57
1:B:362:LEU:HA	1:B:365:GLN:OE1	2.04	0.57
1:B:299:HIS:HD2	1:B:459:TYR:OH	1.88	0.57
1:B:373:LEU:O	1:B:373:LEU:HD23	2.06	0.56
1:A:442:LYS:HE2	1:A:507:LEU:HD21	1.87	0.55
1:B:134:THR:HG22	1:B:138:LYS:HD3	1.88	0.55
1:A:93:GLN:NE2	1:A:447:ARG:HE	2.05	0.54
1:A:41:LEU:HD13	1:A:583:PHE:CG	2.42	0.54
1:A:411:LEU:HD21	1:A:441:LEU:HD11	1.90	0.54
1:A:549:ASN:HD21	1:A:553:ARG:HE	1.55	0.53
1:A:252:HIS:CE1	4:A:804:GOL:HO1	2.26	0.53
1:B:253:TRP:CE2	4:B:805:GOL:H32	2.45	0.52
1:B:344:ARG:NH1	1:B:690:MET:HG3	2.25	0.51
1:A:306:MET:HE3	1:A:455:GLN:HB3	1.92	0.51
1:B:41:LEU:HG	1:B:46:LEU:HD22	1.93	0.51
1:B:84:ASN:HD22	1:B:86:HIS:CE1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ASN:O	1:B:306:MET:HG3	2.09	0.51
1:B:653:THR:H	1:B:656:ASN:HD22	1.59	0.51
1:A:221:HIS:HB3	1:A:606:VAL:HG22	1.95	0.49
1:B:127:LEU:HA	1:B:190:ASN:HD22	1.79	0.48
1:B:277:ASN:HD22	1:B:683:ASN:HD21	1.63	0.47
4:A:806:GOL:H12	6:A:1098:HOH:O	2.11	0.47
1:B:472:ARG:NH2	1:B:483:ASN:HD21	2.13	0.46
4:A:807:GOL:H32	6:A:1421:HOH:O	2.14	0.46
1:A:370:GLN:N	1:A:371:PRO:CD	2.78	0.46
1:B:591:PRO:CG	1:B:595:MET:SD	3.04	0.46
1:A:134:THR:HG22	1:A:138:LYS:HD2	1.98	0.46
1:B:417:GLU:O	1:B:425:ARG:HG2	2.15	0.45
1:A:549:ASN:ND2	1:A:553:ARG:HE	2.13	0.45
1:B:41:LEU:HD13	1:B:583:PHE:CG	2.51	0.45
1:B:218:TRP:CG	1:B:219:PRO:HA	2.52	0.44
1:B:31:PRO:HB3	1:B:56:LEU:HD21	2.00	0.44
1:B:376:HIS:HD2	1:B:556:TYR:CZ	2.36	0.43
1:B:346:ASP:OD2	1:B:349:GLY:HA3	2.18	0.43
1:B:603:LEU:HG	1:B:642:VAL:HB	2.01	0.43
1:A:653:THR:H	1:A:656:ASN:HD22	1.65	0.43
1:B:375:ALA:O	1:B:376:HIS:C	2.55	0.42
1:B:376:HIS:O	1:B:380:LEU:HB2	2.19	0.42
1:B:303:GLN:HE21	1:B:456:LEU:HD22	1.84	0.42
1:A:84:ASN:HD22	1:A:86:HIS:CE1	2.37	0.42
1:B:591:PRO:CD	1:B:595:MET:SD	3.07	0.42
1:A:225:PHE:CG	1:A:701:LEU:HG	2.54	0.42
1:A:622:LEU:C	1:A:622:LEU:HD23	2.40	0.42
1:B:361:TRP:O	1:B:365:GLN:OE1	2.38	0.42
1:A:252:HIS:CE1	4:A:804:GOL:O1	2.69	0.42
1:A:86:HIS:CE1	2:A:801:VAL:HB	2.55	0.42
1:B:458:GLU:HB2	1:B:492:LEU:HD21	2.02	0.41
1:B:134:THR:O	1:B:138:LYS:HG2	2.20	0.41
1:A:86:HIS:CE1	1:A:657:SER:HG	2.38	0.41
1:B:141:ILE:HG23	1:B:151:ARG:HG2	2.02	0.41
1:A:425:ARG:HB2	1:A:430:GLN:HG2	2.03	0.41
1:B:595:MET:C	1:B:595:MET:SD	2.99	0.41
1:B:222:THR:H	1:B:645:ASN:ND2	2.17	0.41
1:B:225:PHE:CG	1:B:701:LEU:HG	2.55	0.41
1:A:458:GLU:HB2	1:A:492:LEU:HD11	2.02	0.41
1:A:220:ARG:HB3	1:A:645:ASN:HD22	1.86	0.41
1:B:499:LYS:HB3	1:B:505:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:GLY:HA2	6:B:1223:HOH:O	2.19	0.41
1:A:468:PRO:O	1:A:472:ARG:HG2	2.20	0.40
1:B:76:SER:HB2	1:B:77:PRO:HD2	2.02	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	695/698 (100%)	678 (98%)	16 (2%)	1 (0%)	56	36
1	B	695/698 (100%)	664 (96%)	25 (4%)	6 (1%)	21	6
All	All	1390/1396 (100%)	1342 (96%)	41 (3%)	7 (0%)	34	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	364	GLY
1	B	466	LYS
1	A	719	ASN
1	B	143	ALA
1	B	352	LEU
1	B	375	ALA
1	B	366	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	541/542 (100%)	526 (97%)	15 (3%)	51	25
1	B	541/542 (100%)	519 (96%)	22 (4%)	37	13
All	All	1082/1084 (100%)	1045 (97%)	37 (3%)	44	18

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	41	LEU
1	A	43	LYS
1	A	93	GLN
1	A	104	LYS
1	A	275	SER
1	A	312	LYS
1	A	363	LYS
1	A	386	SER
1	A	434	LEU
1	A	461	LEU
1	A	540	GLN
1	A	549	ASN
1	A	560	LEU
1	A	719	ASN
1	B	41	LEU
1	B	54	SER
1	B	93	GLN
1	B	138	LYS
1	B	242	SER
1	B	251	LYS
1	B	339	LEU
1	B	352	LEU
1	B	354	GLU
1	B	355	GLU
1	B	365	GLN
1	B	368	LYS
1	B	373	LEU
1	B	378	LYS
1	B	381	ASP
1	B	386	SER
1	B	434	LEU
1	B	461	LEU
1	B	483	ASN

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Mol	Chain	Res	Type
1	B	492	LEU
1	B	515	LYS
1	B	716	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	93	GLN
1	A	215	ASN
1	A	249	GLN
1	A	277	ASN
1	A	303	GLN
1	A	330	ASN
1	A	334	ASN
1	A	338	GLN
1	A	350	GLN
1	A	385	GLN
1	A	471	GLN
1	A	549	ASN
1	A	585	ASN
1	A	645	ASN
1	A	656	ASN
1	B	84	ASN
1	B	93	GLN
1	B	190	ASN
1	B	249	GLN
1	B	277	ASN
1	B	287	ASN
1	B	299	HIS
1	B	303	GLN
1	B	334	ASN
1	B	338	GLN
1	B	350	GLN
1	B	385	GLN
1	B	443	GLN
1	B	540	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 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	VAL	A	801	3	5,6,7	0.79	0	5,7,9	0.56	0
3	TYR	A	802	2	10,13,13	1.33	2 (20%)	11,17,17	0.55	0
4	GOL	A	803	-	5,5,5	0.27	0	5,5,5	0.43	0
4	GOL	A	804	-	5,5,5	0.63	0	5,5,5	2.14	1 (20%)
4	GOL	A	805	-	5,5,5	0.57	0	5,5,5	0.38	0
4	GOL	A	806	-	5,5,5	0.60	0	5,5,5	1.22	0
4	GOL	A	807	-	5,5,5	0.50	0	5,5,5	0.77	0
2	VAL	B	801	3	5,6,7	0.77	0	5,7,9	0.70	0
3	TYR	B	802	2	10,13,13	1.15	0	11,17,17	0.56	0
4	GOL	B	803	-	5,5,5	0.42	0	5,5,5	0.48	0
4	GOL	B	804	-	5,5,5	0.64	0	5,5,5	1.31	0
4	GOL	B	805	-	5,5,5	0.70	0	5,5,5	0.90	0
4	GOL	B	806	-	5,5,5	0.50	0	5,5,5	0.45	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	VAL	A	801	3	-	0/4/6/8	0/0/0/0
3	TYR	A	802	2	-	0/4/8/8	0/1/1/1
4	GOL	A	803	-	-	0/4/4/4	0/0/0/0
4	GOL	A	804	-	-	0/4/4/4	0/0/0/0
4	GOL	A	805	-	-	0/4/4/4	0/0/0/0
4	GOL	A	806	-	-	0/4/4/4	0/0/0/0
4	GOL	A	807	-	-	0/4/4/4	0/0/0/0
2	VAL	B	801	3	-	0/4/6/8	0/0/0/0
3	TYR	B	802	2	-	0/4/8/8	0/1/1/1
4	GOL	B	803	-	-	0/4/4/4	0/0/0/0
4	GOL	B	804	-	-	0/4/4/4	0/0/0/0
4	GOL	B	805	-	-	0/4/4/4	0/0/0/0
4	GOL	B	806	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	TYR	CE2-CZ	-2.20	1.34	1.38
3	A	802	TYR	CD2-CG	2.38	1.43	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	804	GOL	O1-C1-C2	-4.37	88.99	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	VAL	1	0
4	A	804	GOL	4	0
4	A	806	GOL	3	0
4	A	807	GOL	1	0
4	B	805	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	697/698 (99%)	-0.17	2 (0%) 94 95	8, 21, 36, 52	0
1	B	697/698 (99%)	0.28	33 (4%) 35 40	11, 30, 54, 80	0
All	All	1394/1396 (99%)	0.05	35 (2%) 61 67	8, 25, 49, 80	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	367	ALA	4.6
1	B	368	LYS	4.1
1	B	363	LYS	4.0
1	B	98	ALA	4.0
1	B	359	LEU	3.8
1	B	469	ALA	3.7
1	B	486	ALA	3.5
1	B	356	ALA	3.5
1	B	366	GLY	3.4
1	B	471	GLN	3.2
1	B	99	GLU	3.2
1	B	313	GLN	3.0
1	B	482	GLY	3.0
1	B	170	ALA	2.9
1	B	312	LYS	2.7
1	B	97	THR	2.7
1	B	360	GLY	2.7
1	B	361	TRP	2.7
1	A	67	LEU	2.6
1	B	485	ALA	2.5
1	B	467	LEU	2.5
1	B	51	GLN	2.5
1	B	492	LEU	2.5
1	B	381	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	352	LEU	2.3
1	B	67	LEU	2.3
1	B	374	ASP	2.2
1	B	362	LEU	2.2
1	A	568	GLY	2.1
1	B	241	PHE	2.1
1	B	478	ALA	2.1
1	B	315	ALA	2.1
1	B	50	PRO	2.0
1	B	358	VAL	2.0
1	B	568	GLY	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
4	GOL	A	806	6/6	0.93	0.16	18.57	33,46,46,48	0
4	GOL	B	806	6/6	0.87	0.23	4.95	47,51,55,55	0
4	GOL	A	807	6/6	0.93	0.14	4.13	19,33,38,45	0
2	VAL	A	801	7/8	0.99	0.15	3.54	10,11,13,13	0
4	GOL	B	804	6/6	0.93	0.11	2.29	26,35,38,42	0
4	GOL	A	805	6/6	0.90	0.18	2.10	34,38,40,42	0
2	VAL	B	801	7/8	0.98	0.14	1.60	14,14,14,15	0
4	GOL	B	805	6/6	0.89	0.18	0.91	36,47,48,52	0
3	TYR	A	802	13/13	0.96	0.13	0.47	12,18,21,26	0
4	GOL	B	803	6/6	0.97	0.07	-0.93	19,20,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TYR	B	802	13/13	0.96	0.10	-1.04	16,21,27,29	0
4	GOL	A	803	6/6	0.98	0.05	-1.60	16,17,18,21	0
5	ZN	B	807	1/1	0.99	0.03	-	31,31,31,31	0
5	ZN	A	809	1/1	0.97	0.13	-	47,47,47,47	0
5	ZN	A	808	1/1	0.98	0.05	-	26,26,26,26	0
4	GOL	A	804	6/6	0.96	0.12	-	30,35,39,40	0
5	ZN	B	808	1/1	0.97	0.10	-	50,50,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.