



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:55 PM UTC

PDB ID : 3WON / pdb\_00003won  
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

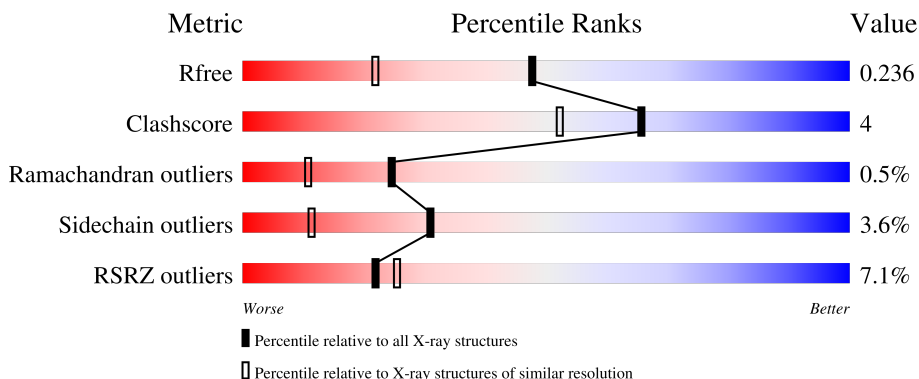
# 1 Overall quality at a glance

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))
$R_{free}$	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 of 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	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
4	GOL	A	804	-	-	X	-

## 2 Entry composition [i](#)

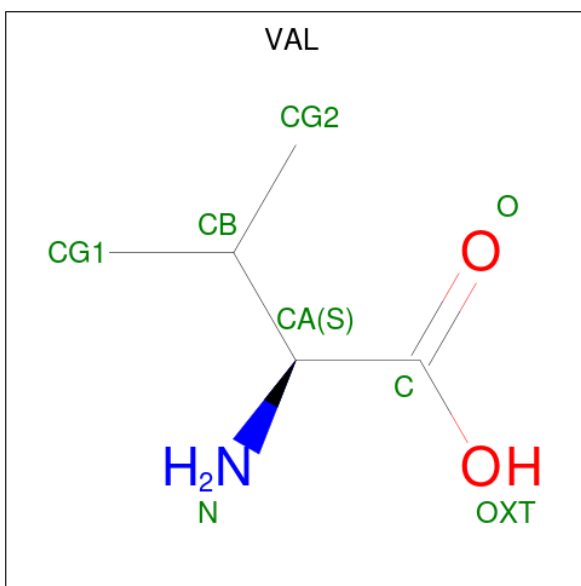
There are 6 unique types of molecules in this entry. The entry contains 11804 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

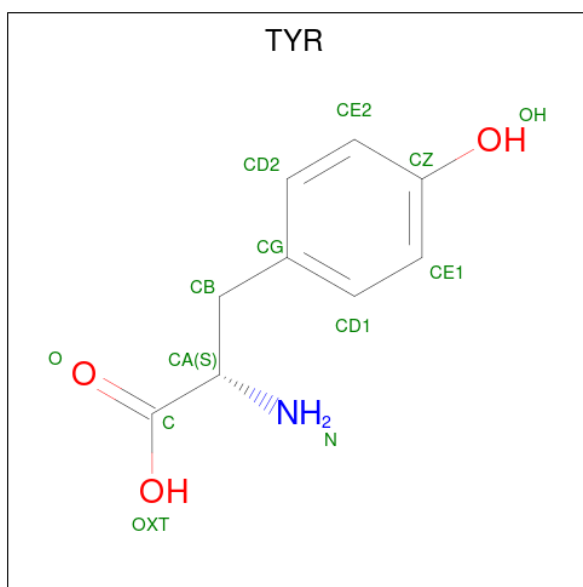
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	697	5371	3398	937	1017	19	0	0	0
1	B	697	5371	3398	937	1017	19	0	0	0

- Molecule 2 is VALINE (CCD ID: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



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

- Molecule 3 is TYROSINE (CCD ID: TYR) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>3</sub>).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

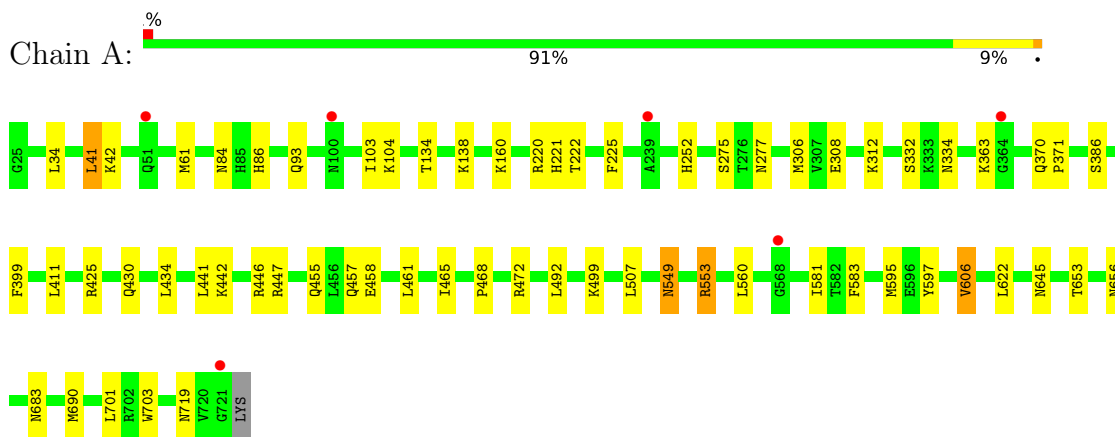
- Molecule 6 is water.

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

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 ( $RSRZ > 2$ ). 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)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.188 , 0.229 0.196 , 0.236	Depositor DCC
$R_{free}$ test set	8264 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11804	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage'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, 0.333 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: ZN, 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	1.24	5/5489 (0.1%)	1.09	3/7440 (0.0%)
1	B	1.16	4/5489 (0.1%)	1.11	11/7440 (0.1%)
All	All	1.20	9/10978 (0.1%)	1.10	14/14880 (0.1%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	291	TRP	CA-C	7.16	1.59	1.52
1	A	334	ASN	CG-ND2	-5.86	1.21	1.33
1	A	703	TRP	N-CA	-5.82	1.39	1.46
1	A	399	PHE	C-O	-5.52	1.17	1.24
1	B	601	THR	N-CA	-5.39	1.39	1.45
1	B	226	ALA	N-CA	5.32	1.52	1.46
1	A	332	SER	N-CA	-5.26	1.40	1.46
1	B	590	ALA	C-O	-5.10	1.20	1.25
1	A	457	GLN	N-CA	5.03	1.52	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ASN	N-CA-C	6.94	120.41	112.57
1	B	709	TYR	CA-C-N	-6.20	113.56	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	709	TYR	C-N-CA	-6.20	113.56	120.14
1	A	103	ILE	N-CA-C	-6.20	104.47	110.42
1	B	313	GLN	N-CA-C	6.17	118.80	111.71
1	B	317	ILE	N-CA-C	5.93	116.67	110.62
1	B	284	GLU	CB-CG-CD	5.87	122.57	112.60
1	B	690	MET	CG-SD-CE	-5.49	88.82	100.90
1	A	553	ARG	CB-CG-CD	5.28	123.44	111.30
1	A	606	VAL	N-CA-C	-5.12	105.72	110.53
1	B	340	GLU	N-CA-C	5.10	117.50	111.33
1	B	590	ALA	CA-C-N	5.05	124.54	119.19
1	B	590	ALA	C-N-CA	5.05	124.54	119.19
1	B	345	ILE	CB-CA-C	-5.01	105.49	111.85

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 [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	5371	0	5284	32	0
1	B	5371	0	5284	47	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	1	0
4	A	30	0	40	8	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11804	0	10674	81	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 (81) 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:A:595:MET:HE3	1:B:595:MET:HE2	1.84	0.59
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:A:61:MET:HE1	1:A:581:ILE:HD11	1.86	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:HD23	1:B:373:LEU:O	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:306:MET:HE3	1:A:455:GLN:HB3	1.89	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: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
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:B:111:THR:OG1	1:B:114:ASP:OD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ALA:O	1:B:690:MET:HE1	2.12	0.50
1:A:595:MET:HE3	1:B:595:MET:CE	2.42	0.49
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
1:A:622:LEU:C	1:A:622:LEU:HD23	2.40	0.47
1:B:375:ALA:O	1:B:376:HIS:C	2.55	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:595:MET:SD	1:B:595:MET:C	2.99	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:657:SER:OG	3:B:802:TYR:C	2.61	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:A:446:ARG:C	1:A:447:ARG:HG3	2.43	0.42
1:B:376:HIS:O	1:B:380:LEU:HB2	2.19	0.42
1:A:84:ASN:HD22	1:A:86:HIS:CE1	2.37	0.42
1:B:303:GLN:HE21	1:B:456:LEU:HD22	1.84	0.42
1:A:225:PHE:CG	1:A:701:LEU:HG	2.54	0.42
1:B:591:PRO:CD	1:B:595:MET:SD	3.07	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:595:MET:HE2	1:A:597:TYR:CE1	2.54	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:B:141:ILE:HG23	1:B:151:ARG:HG2	2.02	0.41
1:A:61:MET:HE3	1:A:61:MET:HB3	1.94	0.41
1:A:425:ARG:HB2	1:A:430:GLN:HG2	2.03	0.41
1:A:458:GLU:HB2	1:A:492:LEU:HD11	2.02	0.41
1:B:222:THR:H	1:B:645:ASN:ND2	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PHE:CG	1:B:701:LEU:HG	2.55	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
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
1:B:218:TRP:HA	1:B:219:PRO:C	2.46	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%)	48 32
1	B	695/698 (100%)	664 (96%)	25 (4%)	6 (1%)	14 4
All	All	1390/1396 (100%)	1342 (96%)	41 (3%)	7 (0%)	24 11

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%)	525 (97%)	16 (3%)	36	16
1	B	541/542 (100%)	518 (96%)	23 (4%)	26	8
All	All	1082/1084 (100%)	1043 (96%)	39 (4%)	31	11

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	41	LEU
1	A	42	LYS
1	A	104	LYS
1	A	275	SER
1	A	308	GLU
1	A	312	LYS
1	A	363	LYS
1	A	386	SER
1	A	434	LEU
1	A	461	LEU
1	A	465	ILE
1	A	499	LYS
1	A	549	ASN
1	A	560	LEU
1	A	690	MET
1	B	41	LEU
1	B	47	LYS
1	B	54	SER
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

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Mol	Chain	Res	Type
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
1	B	492	LEU
1	B	515	LYS
1	B	545	ARG
1	B	716	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	93	GLN
1	A	277	ASN
1	A	290	GLN
1	A	303	GLN
1	A	334	ASN
1	A	385	GLN
1	A	457	GLN
1	A	471	GLN
1	A	540	GLN
1	A	585	ASN
1	A	645	ASN
1	A	656	ASN
1	B	84	ASN
1	B	93	GLN
1	B	95	ASN
1	B	190	ASN
1	B	277	ASN
1	B	287	ASN
1	B	299	HIS
1	B	303	GLN
1	B	334	ASN
1	B	567	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
4	GOL	A	803	-	5,5,5	0.28	0	5,5,5	0.43	0
4	GOL	A	807	-	5,5,5	0.51	0	5,5,5	0.90	0
2	VAL	A	801	3	4,6,7	1.00	0	6,7,9	0.52	0
4	GOL	A	806	-	5,5,5	0.64	0	5,5,5	1.30	0
3	TYR	A	802	2	12,13,13	1.41	2 (16%)	13,17,17	0.97	1 (7%)
4	GOL	B	805	-	5,5,5	0.76	0	5,5,5	0.95	0
4	GOL	B	806	-	5,5,5	0.55	0	5,5,5	0.45	0
4	GOL	B	804	-	5,5,5	0.70	0	5,5,5	1.39	0
4	GOL	A	805	-	5,5,5	0.60	0	5,5,5	0.45	0
3	TYR	B	802	2	12,13,13	1.25	1 (8%)	13,17,17	0.99	1 (7%)
4	GOL	B	803	-	5,5,5	0.44	0	5,5,5	0.53	0
2	VAL	B	801	3	4,6,7	0.95	0	6,7,9	0.72	0
4	GOL	A	804	-	5,5,5	0.58	0	5,5,5	2.33	1 (20%)

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
4	GOL	A	803	-	-	0/4/4/4	-
4	GOL	A	807	-	-	2/4/4/4	-
2	VAL	A	801	3	-	0/5/6/8	-
4	GOL	A	806	-	-	4/4/4/4	-
3	TYR	A	802	2	-	6/8/8/8	0/1/1/1
4	GOL	B	805	-	-	2/4/4/4	-
4	GOL	B	806	-	-	2/4/4/4	-
4	GOL	B	804	-	-	2/4/4/4	-
4	GOL	A	805	-	-	0/4/4/4	-
3	TYR	B	802	2	-	4/8/8/8	0/1/1/1
4	GOL	B	803	-	-	0/4/4/4	-
2	VAL	B	801	3	-	0/5/6/8	-
4	GOL	A	804	-	-	1/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	TYR	CD2-CG	2.51	1.43	1.38
3	A	802	TYR	CE2-CZ	-2.43	1.34	1.39
3	B	802	TYR	CE2-CZ	-2.01	1.35	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	804	GOL	O1-C1-C2	-4.75	88.99	110.38
3	B	802	TYR	OXT-C-O	-2.82	117.67	124.08
3	A	802	TYR	OXT-C-O	-2.50	118.41	124.08

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	807	GOL	C1-C2-C3-O3
4	B	804	GOL	O1-C1-C2-O2
4	B	805	GOL	O1-C1-C2-C3
4	A	806	GOL	O1-C1-C2-C3
4	A	806	GOL	C1-C2-C3-O3
4	B	804	GOL	O1-C1-C2-C3
4	A	807	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	805	GOL	O1-C1-C2-O2
4	A	806	GOL	O2-C2-C3-O3
3	B	802	TYR	OXT-C-CA-CB
4	B	806	GOL	C1-C2-C3-O3
3	A	802	TYR	OXT-C-CA-CB
3	A	802	TYR	O-C-CA-CB
3	A	802	TYR	CA-CB-CG-CD1
3	B	802	TYR	CA-CB-CG-CD1
3	B	802	TYR	O-C-CA-CB
3	B	802	TYR	CA-CB-CG-CD2
4	A	806	GOL	O1-C1-C2-O2
4	B	806	GOL	O2-C2-C3-O3
3	A	802	TYR	CA-CB-CG-CD2
4	A	804	GOL	O2-C2-C3-O3
3	A	802	TYR	OXT-C-CA-N
3	A	802	TYR	O-C-CA-N

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	807	GOL	1	0
2	A	801	VAL	1	0
4	A	806	GOL	3	0
4	B	805	GOL	1	0
3	B	802	TYR	1	0
4	A	804	GOL	4	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%)	-0.14	6 (0%) <span style="border: 1px solid blue; padding: 2px;">81</span> <span style="border: 1px solid blue; padding: 2px;">86</span>	8, 21, 36, 52	0
1	B	697/698 (99%)	0.69	93 (13%) <span style="border: 1px solid red; padding: 2px;">7</span> <span style="border: 1px solid red; padding: 2px;">8</span>	11, 30, 54, 80	0
All	All	1394/1396 (99%)	0.27	99 (7%) <span style="border: 1px solid red; padding: 2px;">22</span> <span style="border: 1px solid red; padding: 2px;">25</span>	8, 25, 48, 80	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	469	ALA	5.3
1	B	373	LEU	4.6
1	B	309	ALA	4.4
1	B	549	ASN	4.2
1	B	366	GLY	4.2
1	B	478	ALA	4.1
1	B	361	TRP	3.9
1	B	368	LYS	3.9
1	B	555	VAL	3.9
1	B	352	LEU	3.9
1	B	381	ASP	3.7
1	B	473	VAL	3.6
1	B	374	ASP	3.6
1	B	315	ALA	3.5
1	B	486	ALA	3.5
1	B	358	VAL	3.5
1	B	246	VAL	3.5
1	B	467	LEU	3.3
1	B	376	HIS	3.3
1	B	377	ALA	3.3
1	B	481	GLY	3.2
1	B	557	LEU	3.1
1	B	98	ALA	3.1
1	B	356	ALA	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	100	ASN	3.1
1	B	482	GLY	3.1
1	B	143	ALA	3.1
1	B	364	GLY	3.1
1	B	362	LEU	3.0
1	B	139	ALA	3.0
1	B	148	ALA	3.0
1	B	312	LYS	3.0
1	B	474	ALA	3.0
1	B	551	ALA	3.0
1	B	492	LEU	2.9
1	B	359	LEU	2.9
1	B	375	ALA	2.9
1	B	94	LEU	2.9
1	B	371	PRO	2.9
1	B	284	GLU	2.8
1	B	479	TRP	2.8
1	B	559	ALA	2.8
1	B	380	LEU	2.7
1	B	369	GLY	2.7
1	B	360	GLY	2.7
1	B	282	ALA	2.7
1	B	47	LYS	2.7
1	B	99	GLU	2.6
1	B	465	ILE	2.6
1	A	721	GLY	2.6
1	B	497	GLY	2.5
1	B	560	LEU	2.5
1	A	568	GLY	2.5
1	B	367	ALA	2.5
1	B	552	ALA	2.5
1	B	234	LYS	2.5
1	B	349	GLY	2.5
1	A	51	GLN	2.4
1	B	568	GLY	2.4
1	B	563	TYR	2.4
1	B	131	THR	2.4
1	B	313	GLN	2.4
1	B	471	GLN	2.4
1	B	235	ASP	2.4
1	B	472	ARG	2.4
1	B	145	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	100	ASN	2.4
1	B	370	GLN	2.3
1	B	146	ASP	2.3
1	B	135	LYS	2.3
1	B	468	PRO	2.3
1	B	357	ALA	2.3
1	B	487	ALA	2.3
1	B	567	GLN	2.3
1	B	137	ALA	2.2
1	B	142	ALA	2.2
1	B	310	ALA	2.2
1	B	485	ALA	2.2
1	B	149	LEU	2.2
1	B	346	ASP	2.2
1	A	364	GLY	2.2
1	B	291	TRP	2.2
1	A	239	ALA	2.2
1	B	470	ASP	2.2
1	B	170	ALA	2.2
1	B	166	CYS	2.2
1	B	355	GLU	2.1
1	B	423	ALA	2.1
1	B	480	LEU	2.1
1	B	566	SER	2.1
1	B	147	ASP	2.1
1	B	241	PHE	2.1
1	B	721	GLY	2.0
1	B	445	GLU	2.0
1	B	133	VAL	2.0
1	B	476	VAL	2.0
1	B	383	LEU	2.0
1	B	353	ARG	2.0
1	B	488	VAL	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 oligosaccharides 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(Å <sup>2</sup> )	Q<0.9
4	GOL	B	806	6/6	0.81	0.17	47,51,55,55	0
4	GOL	B	805	6/6	0.86	0.16	36,47,48,52	0
4	GOL	A	806	6/6	0.90	0.13	33,46,46,48	0
4	GOL	A	805	6/6	0.91	0.12	34,38,40,42	0
4	GOL	B	804	6/6	0.91	0.10	26,35,38,42	0
4	GOL	A	807	6/6	0.92	0.11	19,33,38,45	0
4	GOL	A	804	6/6	0.94	0.12	30,35,39,40	0
3	TYR	B	802	13/13	0.95	0.07	16,21,27,29	0
3	TYR	A	802	13/13	0.95	0.06	12,18,21,26	0
2	VAL	B	801	7/8	0.96	0.06	14,14,14,15	0
4	GOL	A	803	6/6	0.96	0.06	16,17,18,21	0
4	GOL	B	803	6/6	0.96	0.06	19,20,23,23	0
5	ZN	A	809	1/1	0.96	0.18	47,47,47,47	0
5	ZN	B	808	1/1	0.96	0.14	50,50,50,50	0
2	VAL	A	801	7/8	0.98	0.05	10,11,13,13	0
5	ZN	B	807	1/1	0.98	0.07	31,31,31,31	0
5	ZN	A	808	1/1	0.98	0.04	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.