



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:48 PM UTC

PDB ID : 3WOL / pdb_00003wol
Title : Crystal structure of the DAP BII dipeptide complex I
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 : 1.74 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

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>.

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

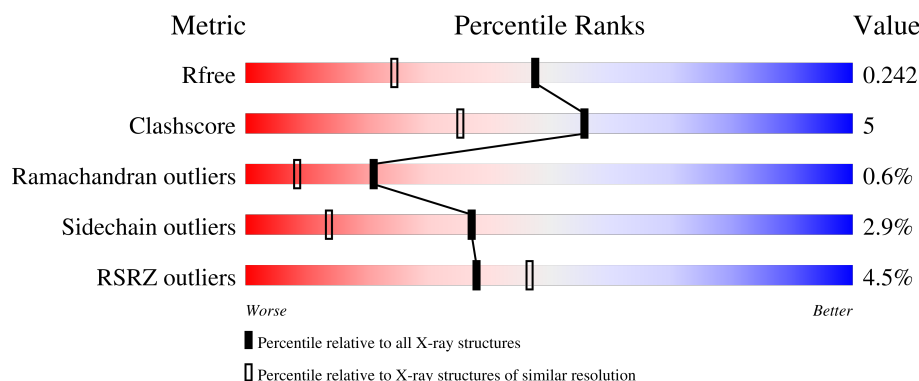
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

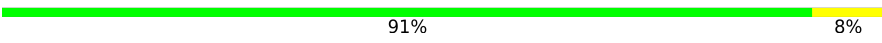
The reported resolution of this entry is 1.74 Å.

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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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 ≥ 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	 91% 8%
1	B	698	 9% 82% 17%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12085 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.

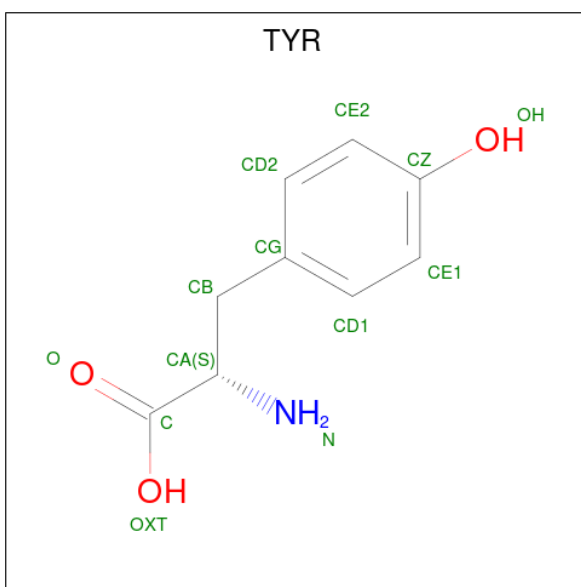
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	696	Total	C	N	O	S	0	0	0
			5367	3396	936	1016	19			
1	B	696	Total	C	N	O	S	0	0	0
			5367	3396	936	1016	19			

- Molecule 2 is VALINE (CCD ID: 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 (CCD ID: 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 (CCD ID: 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	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 (CCD ID: ZN) (formula: Zn).

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

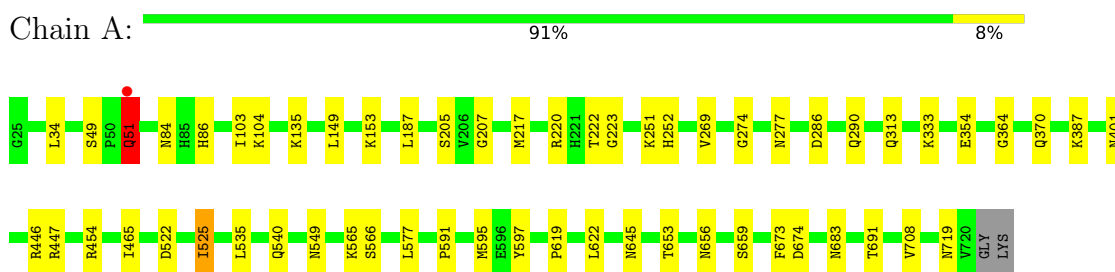
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	769	Total	O	0	0
			769	769		
6	B	501	Total	O	0	0
			501	501		

3 Residue-property plots

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, α , β , γ	121.86Å 121.86Å 219.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.56 – 1.74 29.56 – 1.74	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.56-1.74) 98.3 (29.56-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.192 , 0.239 0.199 , 0.242	Depositor DCC
R_{free} test set	8341 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12085	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 20.84 % 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 7.9631e-03.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	1.30	8/5485 (0.1%)	1.15	7/7435 (0.1%)
1	B	1.17	7/5485 (0.1%)	1.10	6/7435 (0.1%)
All	All	1.23	15/10970 (0.1%)	1.12	13/14870 (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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	291	TRP	CA-C	6.81	1.59	1.52
1	A	220	ARG	N-CA	-6.78	1.37	1.46
1	A	674	ASP	N-CA	5.83	1.53	1.46
1	A	401	ASN	N-CA	5.69	1.53	1.46
1	A	691	THR	N-CA	-5.60	1.39	1.46
1	B	176	LEU	N-CA	-5.43	1.39	1.46
1	A	673	PHE	C-O	-5.43	1.18	1.24
1	A	708	VAL	C-O	-5.43	1.17	1.24
1	B	577	LEU	CA-C	-5.39	1.46	1.52
1	B	684	TRP	CA-C	5.31	1.57	1.52
1	B	206	VAL	CA-C	5.24	1.59	1.52
1	B	203	PRO	N-CA	-5.13	1.40	1.47
1	A	187	LEU	N-CA	-5.06	1.40	1.46
1	A	719	ASN	CA-C	-5.02	1.46	1.53
1	B	250	PRO	C-O	-5.01	1.18	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	GLN	CA-C-N	-6.10	112.72	119.19
1	A	370	GLN	C-N-CA	-6.10	112.72	119.19
1	A	674	ASP	CA-C-N	6.09	126.30	121.61
1	A	674	ASP	C-N-CA	6.09	126.30	121.61
1	B	498	THR	N-CA-C	5.76	117.72	110.24
1	A	566	SER	N-CA-C	-5.46	106.12	112.89
1	B	595	MET	CB-CG-SD	-5.45	96.37	112.70
1	B	313	GLN	N-CA-C	5.43	119.53	113.02
1	B	606	VAL	N-CA-C	-5.38	105.48	110.53
1	B	325	MET	N-CA-C	5.27	117.03	111.28
1	A	51	GLN	N-CA-CB	5.22	118.37	110.28
1	B	465	ILE	N-CA-CB	5.14	117.53	110.54
1	A	103	ILE	N-CA-C	-5.10	105.52	110.42

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	145	GLY	Peptide
1	B	363	LYS	Peptide
1	B	374	ASP	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	5367	0	5281	32	0
1	B	5367	0	5281	69	0
2	A	7	0	8	1	0
2	B	7	0	8	1	0
3	A	13	0	9	0	0
3	B	13	0	9	1	0
4	A	24	0	32	2	0
4	B	12	0	16	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	769	0	0	12	0
6	B	501	0	0	9	0
All	All	12085	0	10644	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (101) 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:446:ARG:HD2	6:B:1331:HOH:O	1.55	1.05
1:A:595:MET:HE3	1:B:595:MET:HE2	1.38	1.02
1:B:310:ALA:HB3	1:B:452:MET:HE1	1.44	1.00
1:A:217:MET:HE1	6:A:1393:HOH:O	1.68	0.91
1:B:217:MET:HE1	6:B:1395:HOH:O	1.70	0.90
1:A:549:ASN:HB3	6:A:1124:HOH:O	1.79	0.82
1:A:595:MET:HE3	1:B:595:MET:CE	2.14	0.77
1:A:277:ASN:HD22	1:A:683:ASN:HD21	1.32	0.76
1:A:217:MET:HE2	1:A:333:LYS:NZ	2.08	0.68
1:A:252:HIS:NE2	6:A:1667:HOH:O	2.29	0.66
1:A:387:LYS:NZ	6:A:1559:HOH:O	2.24	0.65
1:A:354:GLU:HG2	6:A:1543:HOH:O	1.95	0.65
1:B:217:MET:HE2	1:B:333:LYS:NZ	2.15	0.62
1:B:591:PRO:HG2	1:B:595:MET:SD	2.40	0.62
1:B:549:ASN:ND2	6:B:1169:HOH:O	2.33	0.61
1:B:287:ASN:HD22	1:B:383:LEU:HD11	1.70	0.57
1:B:388:ALA:O	1:B:471:GLN:OE1	2.22	0.57
1:A:446:ARG:HD2	6:A:1666:HOH:O	2.04	0.56
1:B:61:MET:CE	1:B:581:ILE:HD11	2.36	0.56
1:B:317:ILE:HG21	1:B:452:MET:CE	2.37	0.55
1:B:620:LYS:HG2	6:B:1067:HOH:O	2.06	0.55
1:B:469:ALA:O	1:B:472:ARG:HG2	2.07	0.55
1:B:317:ILE:HD13	1:B:452:MET:HE2	1.88	0.55
1:B:222:THR:H	1:B:645:ASN:HD21	1.56	0.54
1:A:149:LEU:HG	1:A:153:LYS:HE2	1.90	0.53
1:B:142:ALA:O	1:B:144:ALA:O	2.26	0.53
4:A:804:GOL:C1	6:A:1642:HOH:O	2.55	0.53
1:B:156:GLU:OE2	1:B:543:LYS:NZ	2.41	0.53
1:B:197:ARG:HD2	1:B:231:TYR:CE1	2.44	0.53
1:B:127:LEU:HA	1:B:190:ASN:HD22	1.74	0.51
1:B:61:MET:HE1	1:B:581:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:MET:HE1	1:B:581:ILE:CD1	2.41	0.51
1:A:49:SER:HB2	1:A:51:GLN:HE21	1.76	0.50
1:B:653:THR:H	1:B:656:ASN:HD22	1.58	0.49
1:B:159:GLU:HG2	1:B:163:ILE:HD12	1.93	0.49
1:B:657:SER:OG	3:B:802:TYR:C	2.56	0.49
1:B:132:ASP:OD1	1:B:134:THR:OG1	2.18	0.49
1:B:464:TYR:CD1	1:B:467:LEU:HD12	2.47	0.49
1:B:558:GLN:O	1:B:558:GLN:HG3	2.12	0.49
1:B:317:ILE:HG21	1:B:452:MET:HE2	1.95	0.49
1:B:411:LEU:HD21	1:B:441:LEU:HD11	1.95	0.49
1:B:361:TRP:O	1:B:365:GLN:OE1	2.32	0.48
1:B:620:LYS:CG	6:B:1067:HOH:O	2.62	0.48
1:A:86:HIS:CE1	2:A:801:VAL:HB	2.49	0.48
1:A:222:THR:H	1:A:645:ASN:HD21	1.60	0.48
4:A:804:GOL:H12	6:A:1642:HOH:O	2.13	0.48
1:A:540:GLN:HG2	6:A:1255:HOH:O	2.14	0.48
1:A:286:ASP:O	1:A:290:GLN:HG3	2.14	0.47
1:B:346:ASP:OD2	1:B:349:GLY:HA3	2.14	0.47
1:A:217:MET:HE2	1:A:333:LYS:CE	2.45	0.47
1:A:446:ARG:HD3	6:A:1148:HOH:O	2.15	0.47
1:B:517:PHE:CD2	1:B:525:ILE:HD12	2.49	0.46
1:B:660:PRO:HG2	6:B:987:HOH:O	2.15	0.46
1:B:417:GLU:O	1:B:425:ARG:HG2	2.16	0.46
1:A:135:LYS:NZ	6:A:1485:HOH:O	2.43	0.46
1:B:591:PRO:CG	1:B:595:MET:SD	3.04	0.46
1:A:454:ARG:NH1	6:A:1197:HOH:O	2.26	0.45
1:A:591:PRO:HG3	1:A:597:TYR:CE2	2.52	0.45
1:A:149:LEU:HD21	1:A:540:GLN:HE22	1.82	0.45
1:B:89:TYR:OH	6:B:1068:HOH:O	2.19	0.45
1:B:434:LEU:N	1:B:435:PRO:CD	2.80	0.45
1:A:84:ASN:HD22	1:A:86:HIS:CE1	2.35	0.45
1:B:287:ASN:ND2	1:B:383:LEU:HD11	2.31	0.45
1:B:670:GLY:HA2	1:B:696:VAL:O	2.17	0.45
1:A:653:THR:H	1:A:656:ASN:HD22	1.63	0.44
1:B:301:LYS:HA	1:B:304:ILE:HD12	1.98	0.44
1:A:205:SER:OG	1:A:619:PRO:HD3	2.18	0.44
1:B:109:ALA:HB1	1:B:114:ASP:HB2	2.00	0.44
1:B:135:LYS:HA	1:B:135:LYS:HD2	1.80	0.44
1:B:225:PHE:CG	1:B:701:LEU:HG	2.52	0.44
1:B:461:LEU:HD12	1:B:492:LEU:HD11	1.99	0.43
1:B:84:ASN:HD22	1:B:86:HIS:CE1	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:MET:HE2	1:A:333:LYS:HZ1	1.78	0.43
1:B:61:MET:HE2	1:B:581:ILE:HD11	2.01	0.43
1:A:446:ARG:C	1:A:447:ARG:HG3	2.44	0.43
1:B:207:GLY:HA2	1:B:223:GLY:O	2.17	0.43
1:B:302:ASN:O	1:B:306:MET:HG3	2.19	0.43
1:B:193:ILE:HG21	1:B:230:ALA:HB1	2.00	0.42
1:B:591:PRO:HD2	1:B:595:MET:SD	2.58	0.42
1:B:591:PRO:HG3	1:B:597:TYR:CE2	2.54	0.42
1:A:207:GLY:HA2	1:A:223:GLY:O	2.18	0.42
1:B:383:LEU:HD12	1:B:383:LEU:O	2.20	0.42
1:B:411:LEU:HD23	1:B:411:LEU:HA	1.91	0.42
1:B:484:ASP:OD1	1:B:484:ASP:N	2.53	0.42
1:B:359:LEU:O	1:B:360:GLY:C	2.63	0.42
1:B:576:ASN:O	1:B:577:LEU:HB2	2.19	0.42
1:B:599:PRO:O	1:B:646:TYR:HA	2.20	0.42
1:B:376:HIS:HD2	1:B:556:TYR:CZ	2.38	0.42
1:A:522:ASP:HB3	1:A:525:ILE:HG13	2.01	0.41
1:A:269:VAL:HG13	1:A:659:SER:HB3	2.02	0.41
1:A:622:LEU:HD23	1:A:622:LEU:C	2.46	0.41
1:B:622:LEU:HD23	1:B:622:LEU:C	2.45	0.41
1:B:141:ILE:HG23	1:B:151:ARG:HG2	2.02	0.41
1:B:127:LEU:HA	1:B:190:ASN:ND2	2.34	0.41
1:B:218:TRP:HA	1:B:219:PRO:C	2.46	0.41
1:B:455:GLN:NE2	6:B:1249:HOH:O	2.46	0.41
1:B:461:LEU:HD12	1:B:492:LEU:CD1	2.51	0.41
1:B:86:HIS:CE1	2:B:801:VAL:HB	2.57	0.40
1:A:274:GLY:HA2	1:A:577:LEU:HG	2.02	0.40
1:B:447:ARG:HD3	6:B:1048:HOH:O	2.21	0.40
1:B:468:PRO:HG2	1:B:471:GLN:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	694/698 (99%)	679 (98%)	14 (2%)	1 (0%)	48	34
1	B	694/698 (99%)	661 (95%)	26 (4%)	7 (1%)	12	2
All	All	1388/1396 (99%)	1340 (96%)	40 (3%)	8 (1%)	21	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	ALA
1	B	364	GLY
1	B	375	ALA
1	A	364	GLY
1	B	145	GLY
1	B	146	ASP
1	B	366	GLY
1	B	482	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	541/542 (100%)	532 (98%)	9 (2%)	53	32
1	B	541/542 (100%)	519 (96%)	22 (4%)	27	6
All	All	1082/1084 (100%)	1051 (97%)	31 (3%)	37	14

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	51	GLN
1	A	104	LYS
1	A	251	LYS
1	A	313	GLN
1	A	465	ILE
1	A	525	ILE
1	A	535	LEU

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Mol	Chain	Res	Type
1	A	565	LYS
1	B	34	LEU
1	B	47	LYS
1	B	54	SER
1	B	60	PRO
1	B	99	GLU
1	B	135	LYS
1	B	180	SER
1	B	242	SER
1	B	251	LYS
1	B	352	LEU
1	B	365	GLN
1	B	373	LEU
1	B	380	LEU
1	B	424	GLU
1	B	466	LYS
1	B	472	ARG
1	B	492	LEU
1	B	515	LYS
1	B	545	ARG
1	B	549	ASN
1	B	620	LYS
1	B	689	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	84	ASN
1	A	95	ASN
1	A	249	GLN
1	A	277	ASN
1	A	303	GLN
1	A	334	ASN
1	A	400	ASN
1	A	471	GLN
1	A	540	GLN
1	A	549	ASN
1	A	585	ASN
1	A	645	ASN
1	A	656	ASN
1	A	719	ASN

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Mol	Chain	Res	Type
1	B	84	ASN
1	B	95	ASN
1	B	190	ASN
1	B	277	ASN
1	B	303	GLN
1	B	334	ASN
1	B	338	GLN
1	B	443	GLN
1	B	455	GLN
1	B	483	ASN
1	B	540	GLN
1	B	549	ASN
1	B	585	ASN
1	B	645	ASN
1	B	656	ASN
1	B	665	HIS

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 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	B	801	3	4,6,7	0.90	0	6,7,9	0.74	0
2	VAL	A	801	3	4,6,7	1.20	0	6,7,9	1.06	1 (16%)
4	GOL	A	804	-	5,5,5	0.55	0	5,5,5	0.41	0
4	GOL	A	803	-	5,5,5	0.25	0	5,5,5	1.48	1 (20%)
3	TYR	A	802	2	12,13,13	1.43	2 (16%)	13,17,17	0.91	1 (7%)
4	GOL	B	803	-	5,5,5	0.51	0	5,5,5	0.73	0
4	GOL	B	804	-	5,5,5	0.61	0	5,5,5	0.70	0
4	GOL	A	806	-	5,5,5	0.66	0	5,5,5	0.79	0
4	GOL	A	805	-	5,5,5	0.35	0	5,5,5	0.67	0
3	TYR	B	802	2	12,13,13	0.94	0	13,17,17	0.84	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	B	801	3	-	0/5/6/8	-
2	VAL	A	801	3	-	0/5/6/8	-
4	GOL	A	804	-	-	0/4/4/4	-
4	GOL	A	803	-	-	2/4/4/4	-
3	TYR	A	802	2	-	4/8/8/8	0/1/1/1
4	GOL	B	803	-	-	2/4/4/4	-
4	GOL	B	804	-	-	0/4/4/4	-
4	GOL	A	806	-	-	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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	TYR	CE2-CZ	-3.43	1.32	1.39
3	A	802	TYR	CD2-CG	2.13	1.43	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	TYR	OXT-C-O	-2.39	118.66	124.08
2	A	801	VAL	CB-CA-C	-2.14	109.94	112.87
4	A	803	GOL	O2-C2-C3	2.00	117.47	109.18

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	GOL	O1-C1-C2-C3
4	A	806	GOL	O1-C1-C2-C3
4	B	803	GOL	O1-C1-C2-C3
4	A	803	GOL	O1-C1-C2-O2
3	A	802	TYR	OXT-C-CA-CB
3	B	802	TYR	O-C-CA-CB
3	B	802	TYR	OXT-C-CA-CB
3	B	802	TYR	CA-CB-CG-CD1
3	A	802	TYR	CA-CB-CG-CD1
3	A	802	TYR	CA-CB-CG-CD2
4	A	806	GOL	O1-C1-C2-O2
3	A	802	TYR	O-C-CA-CB
3	B	802	TYR	CA-CB-CG-CD2
4	B	803	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	VAL	1	0
2	A	801	VAL	1	0
4	A	804	GOL	2	0
3	B	802	TYR	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, 95th 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 ²)	Q<0.9
1	A	696/698 (99%)	-0.31	1 (0%) 92 93	7, 20, 34, 51	0
1	B	696/698 (99%)	0.43	61 (8%) 15 20	10, 28, 52, 78	0
All	All	1392/1396 (99%)	0.06	62 (4%) 38 47	7, 23, 46, 78	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	469	ALA	6.3
1	B	467	LEU	4.5
1	B	478	ALA	4.3
1	B	482	GLY	4.1
1	B	366	GLY	4.0
1	B	555	VAL	3.9
1	B	381	ASP	3.4
1	B	373	LEU	3.3
1	B	98	ALA	3.2
1	B	361	TRP	3.1
1	B	481	GLY	3.0
1	B	483	ASN	3.0
1	B	367	ALA	3.0
1	B	474	ALA	3.0
1	B	380	LEU	3.0
1	B	492	LEU	3.0
1	B	143	ALA	2.9
1	B	487	ALA	2.9
1	B	309	ALA	2.8
1	B	377	ALA	2.8
1	B	485	ALA	2.8
1	B	563	TYR	2.8
1	B	375	ALA	2.7
1	B	557	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	560	LEU	2.6
1	B	354	GLU	2.6
1	B	315	ALA	2.5
1	B	356	ALA	2.5
1	B	358	VAL	2.5
1	B	468	PRO	2.5
1	B	486	ALA	2.5
1	B	364	GLY	2.5
1	B	376	HIS	2.5
1	B	491	ALA	2.4
1	B	374	ASP	2.4
1	B	359	LEU	2.4
1	B	465	ILE	2.4
1	B	352	LEU	2.4
1	B	473	VAL	2.4
1	B	360	GLY	2.3
1	B	371	PRO	2.3
1	B	369	GLY	2.3
1	A	51	GLN	2.3
1	B	368	LYS	2.3
1	B	372	ALA	2.3
1	B	554	PRO	2.2
1	B	149	LEU	2.2
1	B	243	LYS	2.2
1	B	568	GLY	2.2
1	B	476	VAL	2.2
1	B	479	TRP	2.2
1	B	493	ASP	2.2
1	B	349	GLY	2.2
1	B	313	GLN	2.2
1	B	549	ASN	2.2
1	B	566	SER	2.2
1	B	362	LEU	2.1
1	B	94	LEU	2.1
1	B	488	VAL	2.1
1	B	552	ALA	2.0
1	B	246	VAL	2.0
1	B	282	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	A	808	1/1	0.88	0.11	74,74,74,74	0
4	GOL	A	804	6/6	0.90	0.11	36,37,38,39	0
4	GOL	A	805	6/6	0.92	0.10	30,37,39,40	0
4	GOL	A	806	6/6	0.93	0.09	24,35,35,36	0
4	GOL	B	803	6/6	0.94	0.07	27,32,37,40	0
4	GOL	A	803	6/6	0.96	0.06	15,19,23,25	0
3	TYR	A	802	13/13	0.96	0.06	10,16,22,24	0
4	GOL	B	804	6/6	0.96	0.06	15,17,18,19	0
3	TYR	B	802	13/13	0.96	0.06	16,19,24,27	0
5	ZN	B	805	1/1	0.96	0.17	46,46,46,46	0
2	VAL	B	801	7/8	0.97	0.05	12,12,12,13	0
5	ZN	A	807	1/1	0.97	0.04	27,27,27,27	0
5	ZN	B	806	1/1	0.97	0.06	36,36,36,36	0
2	VAL	A	801	7/8	0.98	0.05	8,8,10,11	0
5	ZN	A	809	1/1	0.98	0.13	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.