



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:50 AM UTC

PDB ID : 3WOI / pdb_00003woi
Title : Crystal structure of the DAP BII (S657A)
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 : 2.10 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

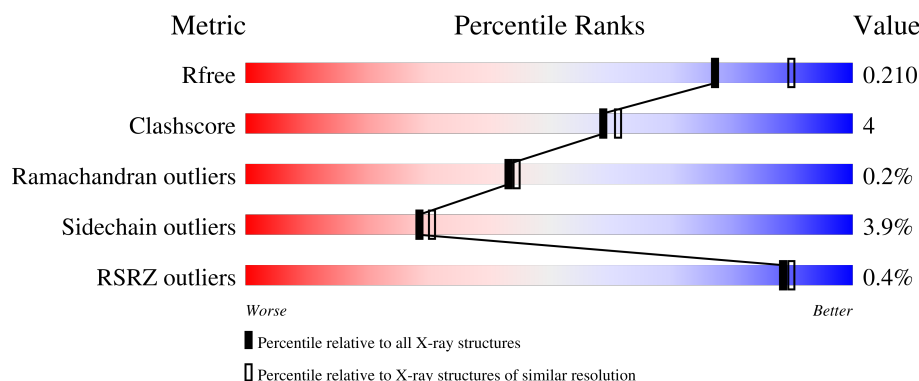
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	% 84% 14% .
1	B	698	90% 9% .

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	B	801	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11790 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.

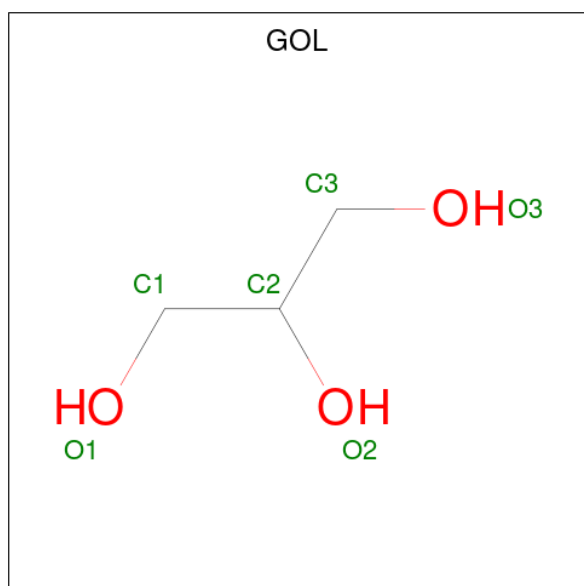
- Molecule 1 is a protein called dipeptidyl aminopeptidase BII.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	697	Total	C	N	O	S	Se	0	0	0
			5367	3396	937	1016	4	14			
1	B	697	Total	C	N	O	S	Se	0	0	0
			5367	3396	937	1016	4	14			

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 (CCD ID: GOL) (formula: C₃H₈O₃).



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	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

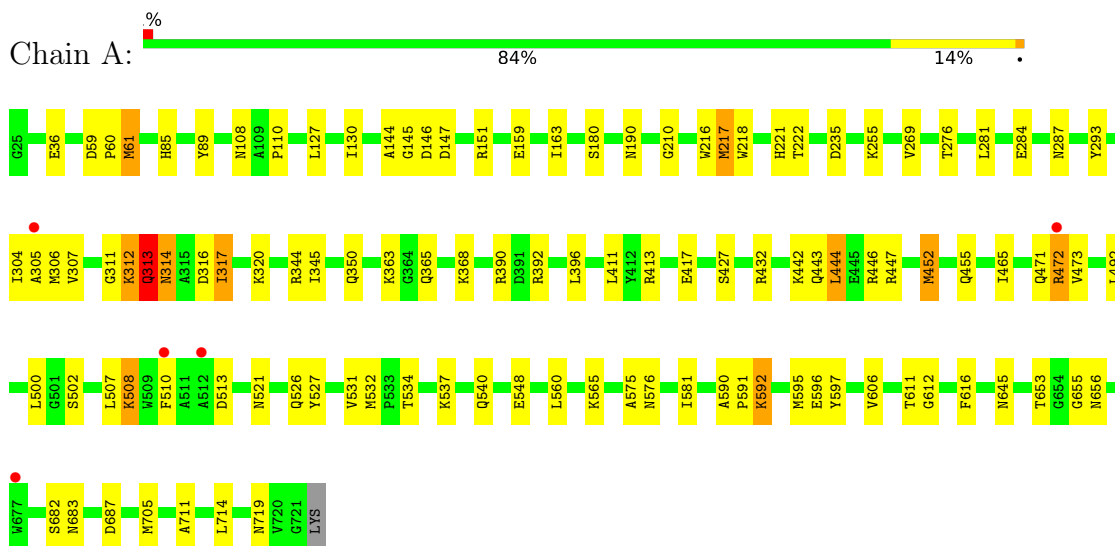
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	317	Total	O	0	0
			317	317		
4	B	691	Total	O	0	0
			691	691		

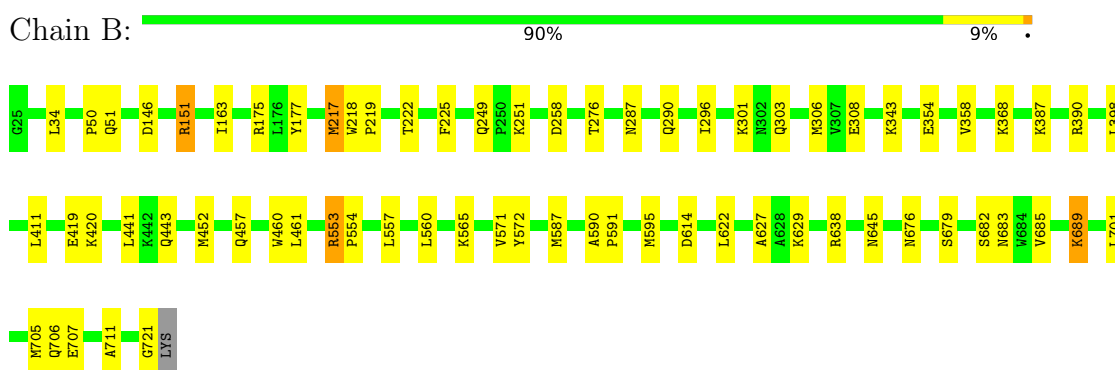
3 Residue-property plots

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	119.90Å 119.90Å 226.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-2.10) 98.1 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.156 , 0.203 0.167 , 0.210	Depositor DCC
R_{free} test set	4754 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11790	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [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	1.15	4/5470 (0.1%)	1.10	10/7391 (0.1%)
1	B	1.34	13/5470 (0.2%)	1.12	5/7391 (0.1%)
All	All	1.25	17/10940 (0.2%)	1.11	15/14782 (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	A	0	3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	590	ALA	C-O	-10.17	1.15	1.24
1	B	308	GLU	CD-OE2	7.04	1.38	1.25
1	B	572	TYR	C-O	-6.41	1.17	1.24
1	B	553	ARG	C-O	-6.33	1.18	1.24
1	A	590	ALA	C-O	-6.23	1.19	1.24
1	B	711	ALA	N-CA	-5.89	1.40	1.46
1	B	457	GLN	C-O	-5.81	1.17	1.24
1	B	638	ARG	C-O	-5.72	1.16	1.24
1	A	575	ALA	CA-C	5.55	1.60	1.52
1	A	89	TYR	C-O	-5.44	1.17	1.24
1	B	151	ARG	CD-NE	-5.32	1.38	1.46
1	B	614	ASP	C-O	-5.31	1.17	1.24
1	B	419	GLU	C-O	-5.24	1.17	1.24
1	A	655	GLY	N-CA	5.07	1.52	1.45
1	B	627	ALA	C-O	-5.03	1.18	1.24
1	B	706	GLN	CA-C	-5.03	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	ILE	CA-CB	-5.01	1.48	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	MSE	CG-SE-CE	-10.66	75.47	98.92
1	A	314	ASN	N-CA-C	7.72	120.55	110.43
1	A	452	MSE	CG-SE-CE	-6.57	84.47	98.92
1	A	217	MSE	CG-SE-CE	6.56	113.36	98.92
1	B	452	MSE	CG-SE-CE	5.85	111.79	98.92
1	B	705	MSE	CG-SE-CE	-5.80	86.17	98.92
1	B	308	GLU	CB-CG-CD	5.71	122.31	112.60
1	A	293	TYR	CA-C-N	-5.52	112.92	119.05
1	A	293	TYR	C-N-CA	-5.52	112.92	119.05
1	A	590	ALA	CA-C-N	-5.41	114.20	120.04
1	A	590	ALA	C-N-CA	-5.41	114.20	120.04
1	B	163	ILE	N-CA-C	5.19	115.40	110.42
1	A	532	MSE	CG-SE-CE	5.12	110.19	98.92
1	A	218	TRP	N-CA-C	-5.11	100.54	109.48
1	A	61	MSE	CG-SE-CE	5.01	109.96	98.92

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	GLN	Peptide
1	A	611	THR	Peptide
1	A	612	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5367	0	5277	62	0
1	B	5367	0	5277	33	0
2	A	12	0	16	0	0
2	B	30	0	40	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	317	0	0	6	1
4	B	691	0	0	13	1
All	All	11790	0	10610	95	1

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 (95) 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:595:MSE:HE2	4:B:1009:HOH:O	1.52	1.09
1:A:591:PRO:HD2	4:A:991:HOH:O	1.65	0.95
1:A:60:PRO:HG2	1:A:61:MSE:HE3	1.50	0.92
1:B:707:GLU:OE2	4:B:1572:HOH:O	1.88	0.91
1:A:595:MSE:HE2	4:A:991:HOH:O	1.83	0.77
1:A:317:ILE:HG23	1:A:452:MSE:HE2	1.67	0.77
1:B:303:GLN:HA	1:B:306:MSE:HE3	1.69	0.76
1:A:307:VAL:HG22	1:A:452:MSE:HE3	1.66	0.75
1:B:287:ASN:OD1	1:B:390:ARG:NH1	2.23	0.70
1:A:527:TYR:CE1	1:A:531:VAL:HG11	2.28	0.69
1:A:60:PRO:HG2	1:A:61:MSE:CE	2.24	0.67
1:A:312:LYS:O	1:A:313:GLN:CB	2.44	0.66
1:B:411:LEU:HD21	1:B:441:LEU:HD11	1.78	0.66
1:B:222:THR:H	1:B:645:ASN:HD21	1.44	0.65
1:A:312:LYS:O	1:A:313:GLN:HB3	1.95	0.65
1:A:307:VAL:HA	1:A:452:MSE:HE1	1.80	0.64
1:A:473:VAL:HG11	1:A:534:THR:HG21	1.81	0.62
1:A:216:TRP:O	1:A:217:MSE:HE2	2.00	0.62
1:A:127:LEU:HD21	1:A:130:ILE:HD11	1.81	0.62
1:B:175:ARG:HD2	1:B:177:TYR:CZ	2.35	0.61
1:A:145:GLY:O	1:A:147:ASP:N	2.29	0.58
1:A:682:SER:HA	4:A:1110:HOH:O	2.03	0.57
1:B:420:LYS:NZ	4:B:1496:HOH:O	2.35	0.57
1:A:61:MSE:HA	1:A:61:MSE:HE2	1.85	0.57
1:A:151:ARG:HD3	4:A:1078:HOH:O	2.04	0.56
1:A:311:GLY:O	1:A:314:ASN:O	2.24	0.56
1:A:221:HIS:HB3	1:A:606:VAL:HG22	1.87	0.56
1:B:290:GLN:NE2	4:B:1569:HOH:O	2.38	0.56
1:A:61:MSE:SE	1:A:581:ILE:HD11	2.55	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:MSE:HE3	1:A:455:GLN:HB3	1.88	0.55
1:B:689:LYS:NZ	1:B:689:LYS:HB3	2.22	0.54
2:B:805:GOL:H31	4:B:1393:HOH:O	2.08	0.54
1:A:222:THR:H	1:A:645:ASN:HD21	1.58	0.52
1:A:345:ILE:O	1:A:350:GLN:NE2	2.41	0.52
1:B:622:LEU:C	1:B:622:LEU:HD23	2.34	0.52
1:B:151:ARG:HD3	4:B:1118:HOH:O	2.09	0.51
1:A:313:GLN:N	1:A:314:ASN:O	2.42	0.51
1:A:210:GLY:HA2	1:A:616:PHE:CE1	2.45	0.51
1:B:676:ASN:OD1	1:B:679:SER:HB3	2.11	0.50
1:B:721:GLY:C	4:B:1573:HOH:O	2.54	0.50
1:A:413:ARG:NH1	1:A:417:GLU:OE2	2.45	0.49
1:A:127:LEU:HA	1:A:190:ASN:HD22	1.77	0.49
1:B:50:PRO:HG2	1:B:51:GLN:HE21	1.77	0.49
1:B:218:TRP:CG	1:B:219:PRO:HA	2.47	0.49
1:A:85:HIS:HE1	4:A:998:HOH:O	1.95	0.49
1:A:108:ASN:O	1:A:110:PRO:HD3	2.13	0.49
1:A:392:ARG:HB2	1:A:471:GLN:HB3	1.93	0.48
1:A:317:ILE:HG23	1:A:452:MSE:CE	2.42	0.48
1:B:301:LYS:HE3	4:B:1317:HOH:O	2.14	0.47
1:A:307:VAL:HA	1:A:452:MSE:CE	2.45	0.47
1:A:314:ASN:HD22	1:A:316:ASP:HB3	1.79	0.47
1:A:281:LEU:HB2	1:A:284:GLU:HG3	1.97	0.47
1:A:314:ASN:HB2	1:A:317:ILE:HB	1.97	0.47
1:A:287:ASN:OD1	1:A:390:ARG:NH1	2.47	0.46
1:A:653:THR:H	1:A:656:ASN:HD22	1.62	0.46
1:B:251:LYS:HE3	4:B:1474:HOH:O	2.15	0.45
1:A:443:GLN:O	1:A:444:LEU:C	2.60	0.45
1:A:235:ASP:HA	1:B:343:LYS:HE3	1.98	0.45
1:A:521:ASN:HA	1:A:526:GLN:NE2	2.32	0.45
1:B:222:THR:H	1:B:645:ASN:ND2	2.12	0.45
1:A:312:LYS:C	1:A:313:GLN:CG	2.90	0.44
1:A:314:ASN:HB3	1:A:317:ILE:H	1.81	0.44
1:A:312:LYS:O	1:A:313:GLN:HG2	2.18	0.44
1:A:592:LYS:HB3	1:A:592:LYS:HE3	1.84	0.44
1:B:225:PHE:CG	1:B:701:LEU:HG	2.53	0.44
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.88	0.43
1:A:276:THR:HA	1:A:683:ASN:OD1	2.19	0.43
1:A:591:PRO:HG3	1:A:597:TYR:CE2	2.54	0.43
1:B:443:GLN:NE2	4:B:1206:HOH:O	2.50	0.43
1:A:392:ARG:H	1:A:471:GLN:NE2	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:MSE:CE	1:A:455:GLN:HB3	2.49	0.43
1:A:159:GLU:O	1:A:163:ILE:HG12	2.19	0.43
1:B:218:TRP:CD2	1:B:219:PRO:HA	2.53	0.43
1:B:591:PRO:HD2	4:B:1009:HOH:O	2.18	0.43
1:A:320:LYS:HG2	1:A:446:ARG:O	2.18	0.42
1:A:320:LYS:O	1:A:447:ARG:HA	2.19	0.42
1:A:507:LEU:O	1:A:508:LYS:C	2.63	0.42
1:A:304:ILE:O	1:A:305:ALA:C	2.61	0.42
1:A:312:LYS:O	1:A:313:GLN:CG	2.67	0.42
1:A:465:ILE:O	1:A:472:ARG:NH2	2.53	0.42
1:A:687:ASP:OD1	1:A:687:ASP:C	2.62	0.42
1:A:705:MSE:HE2	1:A:711:ALA:HB3	2.01	0.41
1:B:354:GLU:O	1:B:358:VAL:HG23	2.20	0.41
1:B:571:VAL:HA	4:B:1337:HOH:O	2.19	0.41
1:B:398:LEU:HD23	1:B:398:LEU:HA	1.94	0.41
1:B:553:ARG:N	1:B:554:PRO:CD	2.84	0.41
1:A:363:LYS:O	1:A:365:GLN:O	2.38	0.41
1:B:303:GLN:NE2	1:B:460:TRP:HE1	2.18	0.41
1:B:276:THR:HA	1:B:683:ASN:ND2	2.35	0.41
1:B:595:MSE:HB3	4:B:1009:HOH:O	2.21	0.41
1:A:396:LEU:HD12	1:A:396:LEU:HA	1.89	0.40
1:A:442:LYS:NZ	4:A:911:HOH:O	2.54	0.40
1:A:527:TYR:CZ	1:A:531:VAL:HG11	2.57	0.40
1:A:411:LEU:HD22	1:A:510:PHE:HA	2.03	0.40
1:B:682:SER:HA	1:B:685:VAL:O	2.21	0.40

All (1) 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)
4:A:1129:HOH:O	4:B:984:HOH:O[6_545]	1.90	0.30

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%)	667 (96%)	25 (4%)	3 (0%)	30	28
1	B	695/698 (100%)	682 (98%)	13 (2%)	0	100	100
All	All	1390/1396 (100%)	1349 (97%)	38 (3%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	ALA
1	A	146	ASP
1	A	313	GLN

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	539/526 (102%)	510 (95%)	29 (5%)	20	18
1	B	539/526 (102%)	526 (98%)	13 (2%)	43	49
All	All	1078/1052 (102%)	1036 (96%)	42 (4%)	28	31

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	59	ASP
1	A	180	SER
1	A	255	LYS
1	A	269	VAL
1	A	312	LYS
1	A	313	GLN
1	A	317	ILE
1	A	344	ARG
1	A	368	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	427	SER
1	A	432	ARG
1	A	444	LEU
1	A	472	ARG
1	A	492	LEU
1	A	500	LEU
1	A	502	SER
1	A	508	LYS
1	A	513	ASP
1	A	537	LYS
1	A	540	GLN
1	A	548	GLU
1	A	560	LEU
1	A	565	LYS
1	A	576	ASN
1	A	592	LYS
1	A	596	GLU
1	A	714	LEU
1	A	719	ASN
1	B	34	LEU
1	B	146	ASP
1	B	217	MSE
1	B	249	GLN
1	B	258	ASP
1	B	368	LYS
1	B	387	LYS
1	B	557	LEU
1	B	560	LEU
1	B	565	LYS
1	B	587	MSE
1	B	629	LYS
1	B	689	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	85	HIS
1	A	190	ASN
1	A	314	ASN
1	A	385	GLN
1	A	400	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	471	GLN
1	A	558	GLN
1	A	576	ASN
1	A	585	ASN
1	A	645	ASN
1	A	656	ASN
1	A	665	HIS
1	B	51	GLN
1	B	84	ASN
1	B	215	ASN
1	B	249	GLN
1	B	290	GLN
1	B	303	GLN
1	B	330	ASN
1	B	483	ASN
1	B	526	GLN
1	B	558	GLN
1	B	585	ASN
1	B	613	GLN
1	B	645	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 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	804	-	5,5,5	0.33	0	5,5,5	1.06	1 (20%)
2	GOL	B	802	-	5,5,5	1.14	0	5,5,5	2.07	1 (20%)
2	GOL	B	805	-	5,5,5	0.45	0	5,5,5	0.92	0
2	GOL	A	802	-	5,5,5	0.35	0	5,5,5	0.89	0
2	GOL	B	801	-	5,5,5	0.50	0	5,5,5	2.02	2 (40%)
2	GOL	A	801	-	5,5,5	0.25	0	5,5,5	0.53	0
2	GOL	B	803	-	5,5,5	0.84	0	5,5,5	0.92	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	B	804	-	-	0/4/4/4	-
2	GOL	B	802	-	-	2/4/4/4	-
2	GOL	B	805	-	-	2/4/4/4	-
2	GOL	A	802	-	-	0/4/4/4	-
2	GOL	B	801	-	-	4/4/4/4	-
2	GOL	A	801	-	-	2/4/4/4	-
2	GOL	B	803	-	-	3/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	GOL	O1-C1-C2	3.92	128.02	110.38
2	B	801	GOL	O3-C3-C2	-3.05	96.64	110.38
2	B	801	GOL	C3-C2-C1	2.70	121.71	111.80
2	B	804	GOL	C3-C2-C1	-2.06	104.23	111.80

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O1-C1-C2-C3
2	B	801	GOL	O1-C1-C2-C3
2	B	801	GOL	C1-C2-C3-O3
2	B	802	GOL	O1-C1-C2-C3
2	B	803	GOL	C1-C2-C3-O3
2	B	805	GOL	C1-C2-C3-O3
2	B	802	GOL	O1-C1-C2-O2
2	B	803	GOL	O2-C2-C3-O3
2	B	805	GOL	O2-C2-C3-O3
2	A	801	GOL	O1-C1-C2-O2
2	B	801	GOL	O1-C1-C2-O2
2	B	801	GOL	O2-C2-C3-O3
2	B	803	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	682/698 (97%)	0.01	5 (0%) 84 86	18, 38, 66, 85	0
1	B	682/698 (97%)	-0.54	0 100 100	14, 25, 41, 61	0
All	All	1364/1396 (97%)	-0.27	5 (0%) 88 90	14, 30, 58, 85	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	677	TRP	2.5
1	A	512	ALA	2.5
1	A	510	PHE	2.2
1	A	472	ARG	2.0
1	A	305	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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
2	GOL	B	803	6/6	0.90	0.11	39,47,50,54	0
2	GOL	B	801	6/6	0.92	0.09	34,38,43,43	0
2	GOL	A	802	6/6	0.92	0.09	34,44,47,53	0
3	ZN	A	805	1/1	0.92	0.06	54,54,54,54	0
2	GOL	B	805	6/6	0.93	0.10	40,44,48,56	0
2	GOL	A	801	6/6	0.93	0.12	37,54,57,64	0
2	GOL	B	802	6/6	0.94	0.11	25,44,51,53	0
3	ZN	A	804	1/1	0.96	0.06	77,77,77,77	0
2	GOL	B	804	6/6	0.96	0.07	27,28,34,42	0
3	ZN	A	803	1/1	0.98	0.03	37,37,37,37	1
3	ZN	B	807	1/1	0.99	0.02	30,30,30,30	0
3	ZN	B	808	1/1	0.99	0.06	24,24,24,24	1
3	ZN	B	806	1/1	1.00	0.01	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.