



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:16 PM GMT

PDB ID : 3WOI
Title : Crystal structure of the DAP BII (S657A)
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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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

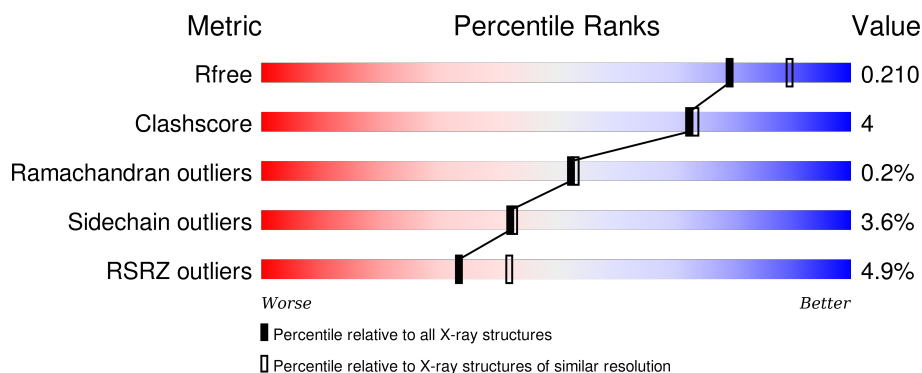
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>8%</div> <div>86%</div> <div>13%</div> </div>
1	B	698	<div> <div>2%</div> <div>90%</div> <div>9%</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	GOL	A	802	-	-	-	X
2	GOL	B	801	-	-	-	X
2	GOL	B	803	-	-	-	X
2	GOL	B	805	-	-	-	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 (three-letter code: GOL) (formula: C₃H₈O₃).



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

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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 (three-letter code: ZN) (formula: Zn).

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

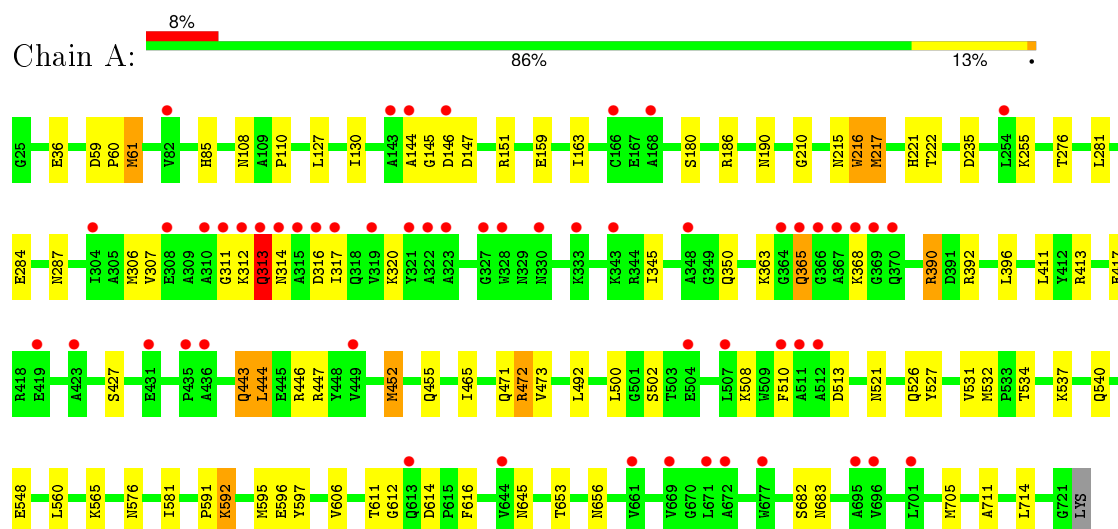
- Molecule 4 is water.

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

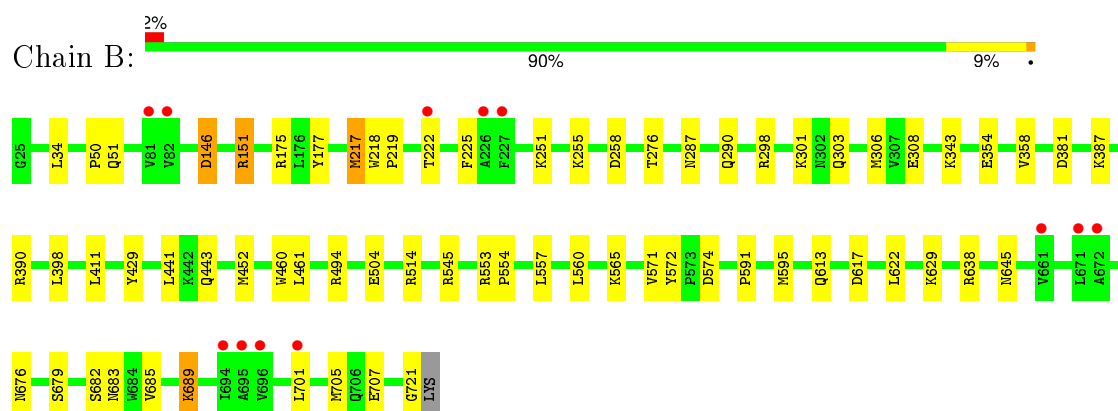
3 Residue-property plots

These plots are drawn for all protein, RNA 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, α , β , γ	119.90Å 119.90Å 226.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-2.10) 98.2 (29.99-2.10)	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 (5.26%)	DCC
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 95090 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	1/5470 (0.0%)	0.90	6/7391 (0.1%)
1	B	1.03	6/5470 (0.1%)	0.96	15/7391 (0.2%)
All	All	0.94	7/10940 (0.1%)	0.94	21/14782 (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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	308	GLU	CD-OE2	11.89	1.38	1.25
1	B	429	TYR	CE1-CZ	-6.17	1.30	1.38
1	B	308	GLU	CG-CD	6.04	1.61	1.51
1	B	504	GLU	CG-CD	6.00	1.60	1.51
1	A	216	TRP	CB-CG	-5.66	1.40	1.50
1	B	146	ASP	CB-CG	-5.30	1.40	1.51
1	B	572	TYR	CE1-CZ	-5.12	1.31	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	B	217	MSE	CG-SE-CE	-10.65	75.47	98.90
1	B	151	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	B	494	ARG	NE-CZ-NH1	7.32	123.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	MSE	CG-SE-CE	6.57	113.36	98.90
1	A	452	MSE	CG-SE-CE	-6.56	84.47	98.90
1	B	638	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	B	381	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	452	MSE	CG-SE-CE	5.86	111.79	98.90
1	B	705	MSE	CG-SE-CE	-5.79	86.17	98.90
1	A	390	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	B	574	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	638	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	A	186	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	514	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	298	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	617	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	532	MSE	CG-SE-CE	5.13	110.19	98.90
1	B	545	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	217	MSE	CB-CA-C	-5.07	100.27	110.40
1	A	61	MSE	CG-SE-CE	5.03	109.96	98.90

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	57	0
1	B	5367	0	5277	32	0
2	A	12	0	16	0	0
2	B	30	0	40	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	317	0	0	5	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	691	0	0	12	1
All	All	11790	0	10610	89	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 (89) 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:HB3	1.95	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: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:A:61:MSE:HE2	1:A:61:MSE:HA	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
1:A:306:MSE:HE3	1:A:455:GLN:HB3	1.88	0.55
2:B:805:GOL:H31	4:B:1393:HOH:O	2.08	0.54
1:B:689:LYS:NZ	1:B:689:LYS:HB3	2.22	0.54
1:A:222:THR:H	1:A:645:ASN:HD21	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ILE:O	1:A:350:GLN:NE2	2.41	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: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:218:TRP:CG	1:B:219:PRO:HA	2.47	0.49
1:B:50:PRO:HG2	1:B:51:GLN:HE21	1.77	0.49
1:A:108:ASN:O	1:A:110:PRO:HD3	2.13	0.49
1:A:85:HIS:HE1	4:A:998:HOH:O	1.95	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:B:622:LEU:HD23	1:B:622:LEU:C	2.34	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:B:721:GLY:C	4:B:1573:HOH:O	2.54	0.45
1:B:222:THR:H	1:B:645:ASN:ND2	2.12	0.45
1:A:521:ASN:HA	1:A:526:GLN:NE2	2.32	0.45
1:A:235:ASP:HA	1:B:343:LYS:HE3	1.98	0.45
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
1:A:306:MSE:CE	1:A:455:GLN:HB3	2.49	0.43
1:B:591:PRO:HD2	4:B:1009:HOH:O	2.18	0.43
1:B:218:TRP:CD2	1:B:219:PRO:HA	2.53	0.43
1:A:159:GLU:O	1:A:163:ILE:HG12	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:553:ARG:N	1:B:554:PRO:CD	2.84	0.41
1:B:398:LEU:HA	1:B:398:LEU:HD23	1.94	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:595:MSE:HB3	4:B:1009:HOH:O	2.21	0.41
1:B:276:THR:HA	1:B:683:ASN:ND2	2.35	0.41
1:A:443:GLN:O	1:A:444:LEU:C	2.60	0.40
1:A:396:LEU:HA	1:A:396:LEU:HD12	1.89	0.40
1:A:527:TYR:CZ	1:A:531:VAL:HG11	2.57	0.40
1:B:682:SER:HA	1:B:685:VAL:O	2.21	0.40
1:A:411:LEU:HD22	1:A:510:PHE:HA	2.03	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 ⓘ

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	695/698 (100%)	667 (96%)	25 (4%)	3 (0%)	39	37
1	B	695/698 (100%)	682 (98%)	13 (2%)	0	100	100
All	All	1390/1396 (100%)	1349 (97%)	38 (3%)	3 (0%)	52	53

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%)	512 (95%)	27 (5%)	30	27
1	B	539/526 (102%)	527 (98%)	12 (2%)	60	64
All	All	1078/1052 (102%)	1039 (96%)	39 (4%)	42	43

All (39) 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	215	ASN
1	A	255	LYS
1	A	313	GLN
1	A	365	GLN
1	A	368	LYS
1	A	427	SER
1	A	443	GLN
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

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Mol	Chain	Res	Type
1	A	560	LEU
1	A	565	LYS
1	A	576	ASN
1	A	592	LYS
1	A	596	GLU
1	A	614	ASP
1	A	714	LEU
1	B	34	LEU
1	B	146	ASP
1	B	217	MSE
1	B	255	LYS
1	B	258	ASP
1	B	387	LYS
1	B	557	LEU
1	B	560	LEU
1	B	565	LYS
1	B	613	GLN
1	B	629	LYS
1	B	689	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	85	HIS
1	A	95	ASN
1	A	190	ASN
1	A	249	GLN
1	A	314	ASN
1	A	338	GLN
1	A	385	GLN
1	A	400	ASN
1	A	471	GLN
1	A	576	ASN
1	A	645	ASN
1	A	656	ASN
1	A	665	HIS
1	B	51	GLN
1	B	78	ASN
1	B	84	ASN
1	B	95	ASN
1	B	277	ASN

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Mol	Chain	Res	Type
1	B	290	GLN
1	B	303	GLN
1	B	334	ASN
1	B	338	GLN
1	B	443	GLN
1	B	526	GLN
1	B	585	ASN
1	B	645	ASN
1	B	683	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 carbohydrates 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	A	801	-	5,5,5	0.26	0	5,5,5	0.44	0
2	GOL	A	802	-	5,5,5	0.33	0	5,5,5	0.80	0
2	GOL	B	801	-	5,5,5	0.48	0	5,5,5	1.91	2 (40%)
2	GOL	B	802	-	5,5,5	1.07	0	5,5,5	1.97	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	803	-	5,5,5	0.77	0	5,5,5	0.88	0
2	GOL	B	804	-	5,5,5	0.31	0	5,5,5	0.92	0
2	GOL	B	805	-	5,5,5	0.46	0	5,5,5	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	801	-	-	0/4/4/4	0/0/0/0
2	GOL	A	802	-	-	0/4/4/4	0/0/0/0
2	GOL	B	801	-	-	0/4/4/4	0/0/0/0
2	GOL	B	802	-	-	0/4/4/4	0/0/0/0
2	GOL	B	803	-	-	0/4/4/4	0/0/0/0
2	GOL	B	804	-	-	0/4/4/4	0/0/0/0
2	GOL	B	805	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	GOL	O3-C3-C2	-2.79	96.64	110.18
2	B	801	GOL	C3-C2-C1	2.70	121.71	111.12
2	B	802	GOL	O1-C1-C2	3.68	128.02	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	805	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	682/698 (97%)	0.32	55 (8%)	15 20	18, 38, 66, 85	0
1	B	682/698 (97%)	-0.21	12 (1%)	71 76	14, 25, 41, 61	0
All	All	1364/1396 (97%)	0.06	67 (4%)	33 42	14, 30, 58, 85	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	364	GLY	5.4
1	A	367	ALA	5.4
1	A	315	ALA	5.1
1	A	313	GLN	4.6
1	B	671	LEU	4.0
1	A	343	LYS	4.0
1	A	308	GLU	3.7
1	A	146	ASP	3.7
1	A	368	LYS	3.6
1	B	696	VAL	3.5
1	A	644	VAL	3.3
1	A	143	ALA	3.3
1	B	82	VAL	3.3
1	A	366	GLY	3.2
1	A	323	ALA	3.2
1	A	144	ALA	3.2
1	B	672	ALA	3.2
1	B	695	ALA	3.2
1	A	511	ALA	3.1
1	B	81	VAL	3.1
1	A	671	LEU	3.1
1	A	310	ALA	3.1
1	A	423	ALA	3.1
1	A	319	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	510	PHE	3.1
1	A	370	GLN	3.0
1	A	661	VAL	3.0
1	B	661	VAL	2.9
1	A	322	ALA	2.8
1	A	321	TYR	2.8
1	A	512	ALA	2.8
1	B	701	LEU	2.8
1	A	435	PRO	2.7
1	A	369	GLY	2.7
1	A	168	ALA	2.7
1	A	613	GLN	2.7
1	A	677	TRP	2.7
1	A	449	VAL	2.6
1	A	365	GLN	2.6
1	A	166	CYS	2.6
1	A	317	ILE	2.6
1	A	696	VAL	2.6
1	A	431	GLU	2.5
1	A	314	ASN	2.5
1	A	312	LYS	2.5
1	A	82	VAL	2.4
1	A	254	LEU	2.4
1	A	311	GLY	2.4
1	B	226	ALA	2.4
1	A	333	LYS	2.3
1	A	504	GLU	2.3
1	B	694	ILE	2.3
1	A	316	ASP	2.3
1	A	348	ALA	2.3
1	A	419	GLU	2.3
1	A	327	GLY	2.3
1	A	436	ALA	2.3
1	A	330	ASN	2.2
1	A	701	LEU	2.2
1	A	672	ALA	2.2
1	A	695	ALA	2.2
1	B	227	PHE	2.1
1	A	304	ILE	2.1
1	A	669	VAL	2.1
1	A	328	TRP	2.0
1	A	507	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	222	THR	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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	B	801	6/6	0.95	0.13	3.42	34,38,43,43	0
2	GOL	B	805	6/6	0.92	0.21	2.30	40,44,48,56	0
2	GOL	A	802	6/6	0.93	0.15	2.13	34,44,47,53	0
2	GOL	B	803	6/6	0.85	0.14	2.02	39,47,50,54	0
2	GOL	A	801	6/6	0.93	0.15	1.95	37,54,57,64	0
2	GOL	B	804	6/6	0.95	0.11	0.05	27,28,34,42	0
3	ZN	B	807	1/1	0.99	0.07	-0.94	30,30,30,30	0
3	ZN	A	803	1/1	0.97	0.05	-	37,37,37,37	1
3	ZN	B	806	1/1	0.99	0.07	-	23,23,23,23	0
3	ZN	A	804	1/1	0.95	0.08	-	77,77,77,77	0
2	GOL	B	802	6/6	0.90	0.25	-	25,44,51,53	0
3	ZN	A	805	1/1	0.93	0.06	-	54,54,54,54	0
3	ZN	B	808	1/1	0.99	0.05	-	24,24,24,24	1

6.5 Other polymers [i](#)

There are no such residues in this entry.