Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:06 am BST

PDB ID	:	3WOP
Title	:	Crystal structure of the DAP BII hexapeptide complex II
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	:	1.95 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 following versions of software and data (see references ⓘ) were used in the production of this report:

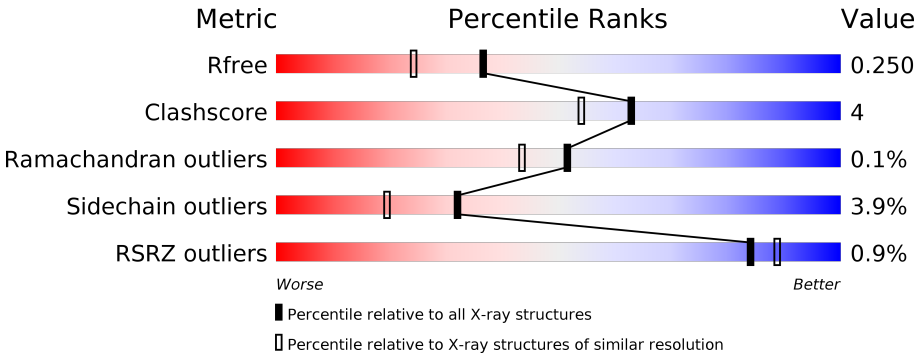
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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 <=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	% 88% 10% ·
1	B	698	% 88% 11% ·
2	C	6	67% 17% 17%
2	D	6	50% 33% 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11619 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called dipeptidyl aminopeptidase BII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	697	Total	C	N	O	S	0	0	0
			5366	3395	935	1017	19			
1	B	697	Total	C	N	O	S	0	0	0
			5366	3395	935	1017	19			

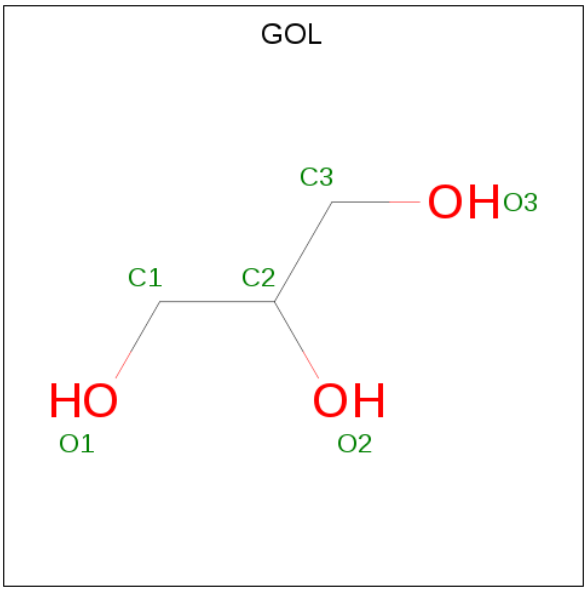
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	ALA	HIS	ENGINEERED MUTATION	UNP V5YM14
B	86	ALA	HIS	ENGINEERED MUTATION	UNP V5YM14

- Molecule 2 is a protein called Angiotensin IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			44	31	7	6			
2	D	5	Total	C	N	O	0	0	0
			44	31	7	6			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is water.

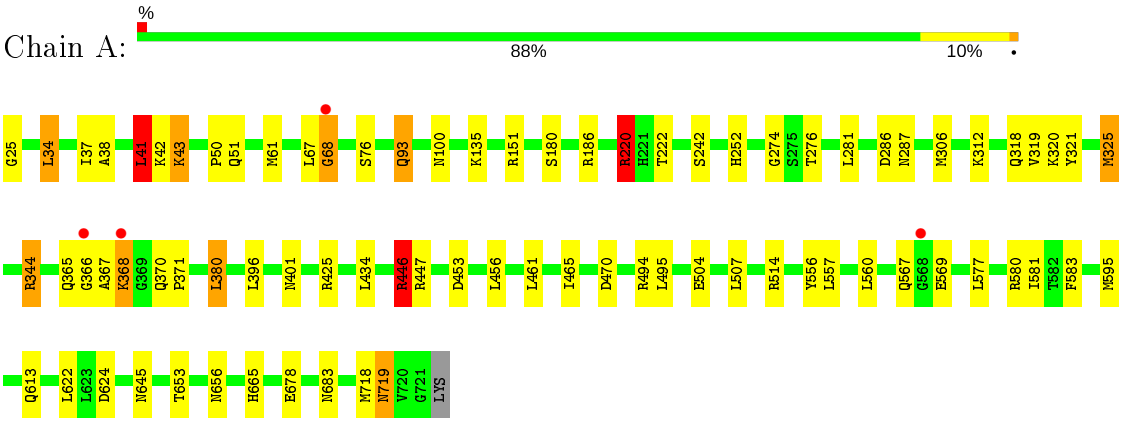
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	412	Total O 412 412	0	0
5	B	323	Total O 323 323	0	0
5	C	2	Total O 2 2	0	0
5	D	4	Total O 4 4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

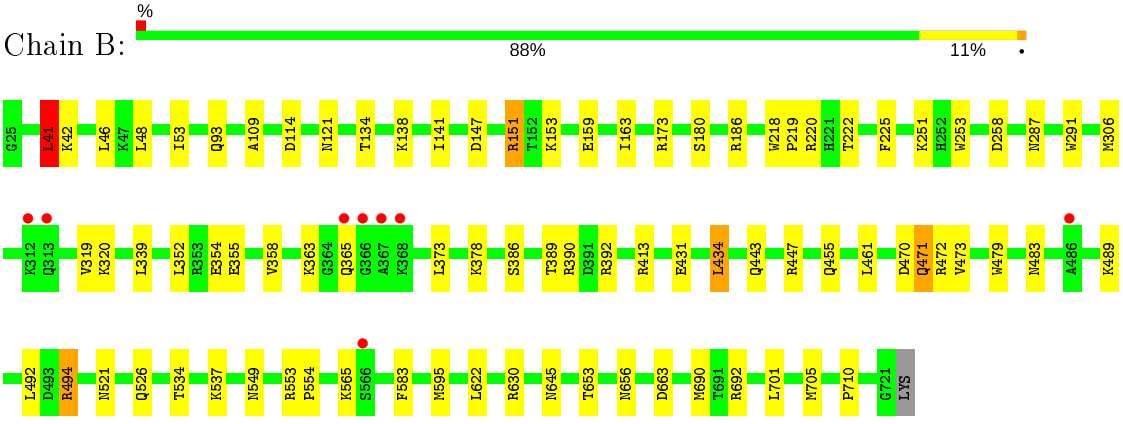
- Molecule 1: dipeptidyl aminopeptidase BII

Chain A:



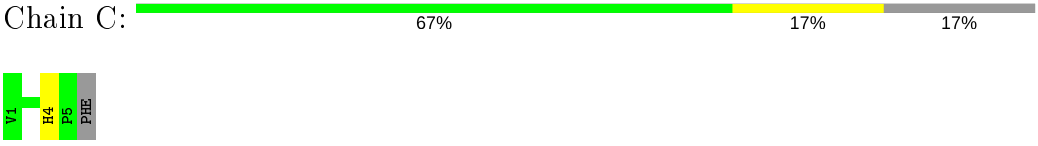
- Molecule 1: dipeptidyl aminopeptidase BII

Chain B:



- Molecule 2: Angiotensin IV

Chain C:



- Molecule 2: Angiotensin IV

Chain D:


V1
H4
P5
PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	120.96Å 120.96Å 219.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.87 – 1.95 39.84 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.87-1.95) 98.2 (39.84-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.93 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.187 , 0.244 0.196 , 0.250	Depositor DCC
R_{free} test set	5834 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11619	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.58 % 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 5.5409e-03.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.90	2/5483 (0.0%)	1.04	23/7432 (0.3%)
1	B	0.85	1/5483 (0.0%)	0.97	14/7432 (0.2%)
2	C	1.15	0/46	1.04	0/63
2	D	1.13	0/46	1.13	0/63
All	All	0.88	3/11058 (0.0%)	1.01	37/14990 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	220	ARG	CD-NE	-5.61	1.36	1.46
1	A	220	ARG	CD-NE	-5.34	1.37	1.46
1	A	504	GLU	CD-OE1	5.18	1.31	1.25

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220	ARG	NE-CZ-NH1	-24.68	107.96	120.30
1	B	220	ARG	NE-CZ-NH1	-22.23	109.19	120.30
1	A	220	ARG	NE-CZ-NH2	19.58	130.09	120.30
1	B	220	ARG	NE-CZ-NH2	16.99	128.80	120.30
1	A	325	MET	CG-SD-CE	-9.62	84.80	100.20
1	A	446	ARG	NE-CZ-NH1	9.50	125.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	344	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	B	220	ARG	CG-CD-NE	-8.14	94.71	111.80
1	B	220	ARG	CD-NE-CZ	7.45	134.03	123.60
1	B	173	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	220	ARG	CG-CD-NE	-7.03	97.04	111.80
1	A	344	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	220	ARG	CD-NE-CZ	6.69	132.97	123.60
1	A	718	MET	N-CA-C	6.49	128.53	111.00
1	A	34	LEU	CA-CB-CG	-6.40	100.59	115.30
1	A	41	LEU	CA-CB-CG	6.21	129.59	115.30
1	A	425	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	B	413	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	663	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	41	LEU	CA-CB-CG	5.87	128.79	115.30
1	A	446	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	624	ASP	CB-CG-OD1	5.82	123.54	118.30
1	B	494	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	514	ARG	CG-CD-NE	-5.68	99.87	111.80
1	B	692	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	186	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	470	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	453	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	A	453	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	67	LEU	CA-C-N	5.27	126.75	116.20
1	A	151	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	151	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	186	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	258	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	147	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	286	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	580	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	ARG	Sidechain
1	A	68	GLY	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	5366	0	5282	42	0
1	B	5366	0	5282	47	0
2	C	44	0	45	0	0
2	D	44	0	45	5	0
3	A	24	0	32	2	0
3	B	30	0	40	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	412	0	0	7	0
5	B	323	0	0	0	0
5	C	2	0	0	0	0
5	D	4	0	0	4	0
All	All	11619	0	10726	92	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 (92) 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:470:ASP:O	1:B:471:GLN:HB2	1.68	0.93
1:B:287:ASN:HD21	1:B:390:ARG:HH11	1.22	0.87
2:D:4:HIS:HB3	5:D:103:HOH:O	1.76	0.85
1:B:287:ASN:HD21	1:B:390:ARG:NH1	1.77	0.82
1:A:252:HIS:ND1	3:A:802:GOL:O1	2.15	0.78
1:A:50:PRO:HD3	5:A:1145:HOH:O	1.86	0.76
2:D:4:HIS:NE2	5:D:104:HOH:O	2.12	0.72
1:A:287:ASN:HB3	5:A:1259:HOH:O	1.89	0.72
1:A:665:HIS:HE1	5:A:1263:HOH:O	1.73	0.70
1:A:222:THR:H	1:A:645:ASN:HD21	1.38	0.69
1:A:281:LEU:HD23	1:A:380:LEU:HD13	1.75	0.69
1:B:473:VAL:HG11	1:B:534:THR:HG21	1.76	0.67
1:B:470:ASP:O	1:B:471:GLN:CB	2.40	0.66
1:B:653:THR:H	1:B:656:ASN:HD22	1.44	0.66
2:D:4:HIS:CB	5:D:103:HOH:O	2.38	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLN:HE21	3:A:803:GOL:H12	1.62	0.64
1:B:109:ALA:HB1	1:B:114:ASP:HB2	1.80	0.64
1:B:287:ASN:ND2	1:B:390:ARG:NH1	2.45	0.63
1:A:595:MET:HE3	1:B:595:MET:HE3	1.82	0.62
1:B:392:ARG:H	1:B:471:GLN:HE21	1.47	0.61
1:B:222:THR:H	1:B:645:ASN:HD21	1.47	0.60
1:A:100:ASN:ND2	5:A:1110:HOH:O	2.34	0.60
1:B:472:ARG:HH22	1:B:483:ASN:ND2	2.02	0.58
1:A:556:TYR:CE2	1:A:560:LEU:HD11	2.40	0.57
1:B:134:THR:HG22	1:B:138:LYS:HD3	1.87	0.56
1:A:719:ASN:O	1:A:719:ASN:ND2	2.39	0.56
1:B:93:GLN:NE2	1:B:447:ARG:HE	2.03	0.56
1:B:306:MET:CE	1:B:455:GLN:HB3	2.36	0.55
1:A:68:GLY:CA	5:A:952:HOH:O	2.55	0.55
1:A:25:GLY:N	5:A:1182:HOH:O	2.39	0.54
1:B:218:TRP:CG	1:B:219:PRO:HA	2.44	0.53
1:B:431:GLU:HA	1:B:434:LEU:HD22	1.90	0.53
1:B:472:ARG:HH22	1:B:483:ASN:HD21	1.55	0.53
1:B:472:ARG:HH22	1:B:483:ASN:CG	2.13	0.52
1:B:473:VAL:CG1	1:B:534:THR:HG21	2.40	0.52
1:B:253:TRP:CE2	3:B:804:GOL:H32	2.44	0.52
1:B:354:GLU:O	1:B:358:VAL:HG23	2.10	0.51
1:A:276:THR:HA	1:A:683:ASN:OD1	2.10	0.51
1:B:553:ARG:N	1:B:554:PRO:CD	2.74	0.51
1:B:41:LEU:HG	1:B:46:LEU:HD22	1.93	0.50
1:B:705:MET:O	1:B:710:PRO:HA	2.11	0.50
1:B:389:THR:HA	1:B:471:GLN:HE22	1.76	0.50
1:B:622:LEU:HD23	1:B:622:LEU:C	2.32	0.49
1:B:93:GLN:HE22	1:B:447:ARG:HE	1.57	0.49
1:A:446:ARG:HD2	5:A:1258:HOH:O	2.12	0.49
1:B:134:THR:HG22	1:B:138:LYS:CD	2.42	0.49
1:A:281:LEU:HD23	1:A:380:LEU:CD1	2.42	0.48
1:A:37:ILE:O	1:A:41:LEU:HB2	2.14	0.48
1:B:363:LYS:C	1:B:365:GLN:H	2.15	0.48
1:A:595:MET:CE	1:B:595:MET:HE3	2.42	0.48
1:B:121:ASN:H	1:B:443:GLN:NE2	2.12	0.48
1:A:38:ALA:HB1	1:A:50:PRO:HG3	1.95	0.47
2:D:4:HIS:CD2	2:D:5:PRO:HD2	2.50	0.47
1:B:41:LEU:HD13	1:B:583:PHE:CG	2.50	0.46
1:A:653:THR:H	1:A:656:ASN:HD22	1.64	0.46
1:B:159:GLU:HG2	1:B:163:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:ARG:NH2	1:B:483:ASN:HD21	2.13	0.45
1:B:479:TRP:O	1:B:494:ARG:NH2	2.50	0.45
1:A:366:GLY:O	1:A:367:ALA:C	2.55	0.45
1:A:93:GLN:NE2	1:A:447:ARG:HE	2.15	0.45
1:A:220:ARG:HD2	1:A:222:THR:OG1	2.17	0.44
1:A:306:MET:CE	1:A:456:LEU:HD23	2.47	0.44
1:A:41:LEU:HD13	1:A:583:PHE:CG	2.52	0.44
1:B:134:THR:O	1:B:138:LYS:HG2	2.18	0.44
1:A:43:LYS:HD3	1:A:43:LYS:O	2.18	0.44
1:A:321:TYR:O	1:A:325:MET:HB2	2.16	0.44
2:D:4:HIS:C	5:D:103:HOH:O	2.55	0.44
1:B:291:TRP:CZ2	1:B:390:ARG:HG3	2.53	0.43
1:B:218:TRP:HA	1:B:219:PRO:C	2.39	0.43
1:A:306:MET:HE2	1:A:456:LEU:HD23	2.01	0.43
1:B:141:ILE:HG23	1:B:151:ARG:HG2	2.00	0.43
1:A:93:GLN:HE22	1:A:447:ARG:HE	1.66	0.43
1:A:344:ARG:NH2	1:A:678:GLU:O	2.52	0.42
1:A:465:ILE:CG2	1:A:465:ILE:O	2.67	0.42
1:A:365:GLN:HB3	1:A:368:LYS:HE3	2.01	0.42
1:A:222:THR:H	1:A:645:ASN:ND2	2.11	0.42
1:A:370:GLN:N	1:A:371:PRO:CD	2.82	0.42
1:B:549:ASN:HD21	1:B:553:ARG:HH21	1.67	0.42
1:A:622:LEU:C	1:A:622:LEU:HD23	2.40	0.41
1:B:218:TRP:CD2	1:B:219:PRO:HA	2.55	0.41
1:B:225:PHE:CG	1:B:701:LEU:HG	2.56	0.41
1:A:319:VAL:HG13	1:A:320:LYS:N	2.35	0.41
1:A:567:GLN:OE1	1:A:567:GLN:HA	2.21	0.41
1:A:274:GLY:HA2	1:A:577:LEU:HG	2.03	0.41
1:B:320:LYS:O	1:B:447:ARG:HA	2.20	0.41
1:A:495:LEU:HA	1:A:495:LEU:HD23	1.92	0.41
1:A:396:LEU:HA	1:A:396:LEU:HD12	1.94	0.40
1:A:494:ARG:HH21	1:A:494:ARG:HB2	1.86	0.40
1:A:61:MET:HE1	1:A:581:ILE:HD13	2.03	0.40
1:B:521:ASN:HA	1:B:526:GLN:NE2	2.36	0.40
1:B:41:LEU:HD13	1:B:583:PHE:CD1	2.57	0.40
1:B:48:LEU:HD12	1:B:53:ILE:HD11	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	695/698 (100%)	672 (97%)	22 (3%)	1 (0%)	51 43
1	B	695/698 (100%)	670 (96%)	25 (4%)	0	100 100
2	C	3/6 (50%)	1 (33%)	2 (67%)	0	100 100
2	D	3/6 (50%)	1 (33%)	2 (67%)	0	100 100
All	All	1396/1408 (99%)	1344 (96%)	51 (4%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	569	GLU

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	540/541 (100%)	519 (96%)	21 (4%)	32 19
1	B	540/541 (100%)	519 (96%)	21 (4%)	32 19
2	C	5/6 (83%)	4 (80%)	1 (20%)	1 0
2	D	5/6 (83%)	5 (100%)	0	100 100
All	All	1090/1094 (100%)	1047 (96%)	43 (4%)	32 19

All (43) 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	43	LYS
1	A	51	GLN
1	A	76	SER
1	A	93	GLN
1	A	135	LYS
1	A	180	SER
1	A	242	SER
1	A	312	LYS
1	A	368	LYS
1	A	380	LEU
1	A	401	ASN
1	A	434	LEU
1	A	446	ARG
1	A	461	LEU
1	A	507	LEU
1	A	557	LEU
1	A	613	GLN
1	A	719	ASN
1	B	41	LEU
1	B	42	LYS
1	B	153	LYS
1	B	180	SER
1	B	251	LYS
1	B	319	VAL
1	B	339	LEU
1	B	352	LEU
1	B	355	GLU
1	B	373	LEU
1	B	378	LYS
1	B	386	SER
1	B	434	LEU
1	B	461	LEU
1	B	471	GLN
1	B	489	LYS
1	B	492	LEU
1	B	537	LYS
1	B	565	LYS
1	B	630	ARG
1	B	690	MET
2	C	4	HIS

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

Mol	Chain	Res	Type
1	A	84	ASN
1	A	93	GLN
1	A	190	ASN
1	A	249	GLN
1	A	290	GLN
1	A	303	GLN
1	A	318	GLN
1	A	334	ASN
1	A	338	GLN
1	A	443	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	249	GLN
1	B	277	ASN
1	B	287	ASN
1	B	299	HIS
1	B	303	GLN
1	B	334	ASN
1	B	338	GLN
1	B	370	GLN
1	B	443	GLN
1	B	471	GLN
1	B	645	ASN
1	B	656	ASN
1	B	665	HIS
2	C	4	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
3	GOL	B	802	-	5,5,5	0.23	0	5,5,5	0.54	0
3	GOL	A	802	-	5,5,5	0.34	0	5,5,5	0.79	0
3	GOL	A	801	-	5,5,5	0.53	0	5,5,5	1.40	1 (20%)
3	GOL	B	803	-	5,5,5	0.28	0	5,5,5	0.47	0
3	GOL	B	804	-	5,5,5	0.36	0	5,5,5	0.50	0
3	GOL	A	804	-	5,5,5	0.25	0	5,5,5	0.84	0
3	GOL	B	805	-	5,5,5	0.35	0	5,5,5	0.38	0
3	GOL	A	803	-	5,5,5	0.24	0	5,5,5	0.48	0
3	GOL	B	801	-	5,5,5	0.93	0	5,5,5	1.35	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
3	GOL	B	802	-	-	2/4/4/4	-
3	GOL	A	802	-	-	2/4/4/4	-
3	GOL	A	801	-	-	0/4/4/4	-
3	GOL	B	803	-	-	2/4/4/4	-
3	GOL	B	804	-	-	0/4/4/4	-
3	GOL	A	804	-	-	2/4/4/4	-
3	GOL	B	805	-	-	0/4/4/4	-
3	GOL	A	803	-	-	2/4/4/4	-
3	GOL	B	801	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	801	GOL	C3-C2-C1	-2.06	103.71	111.70
3	A	801	GOL	O3-C3-C2	-2.03	100.45	110.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	GOL	O1-C1-C2-C3
3	B	803	GOL	C1-C2-C3-O3
3	A	804	GOL	C1-C2-C3-O3
3	A	803	GOL	O1-C1-C2-C3
3	A	804	GOL	O2-C2-C3-O3
3	A	802	GOL	O1-C1-C2-C3
3	A	803	GOL	O1-C1-C2-O2
3	B	802	GOL	O1-C1-C2-O2
3	A	802	GOL	O1-C1-C2-O2
3	B	803	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	GOL	1	0
3	B	804	GOL	1	0
3	A	803	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	697/698 (99%)	-0.31	4 (0%) 89 93	8, 20, 37, 55	0
1	B	697/698 (99%)	-0.19	8 (1%) 80 85	7, 23, 43, 58	0
2	C	5/6 (83%)	0.95	0 100 100	11, 14, 33, 39	0
2	D	5/6 (83%)	1.06	0 100 100	12, 13, 37, 55	0
All	All	1404/1408 (99%)	-0.24	12 (0%) 84 89	7, 22, 40, 58	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	367	ALA	3.7
1	B	486	ALA	3.4
1	B	366	GLY	3.3
1	B	312	LYS	2.6
1	A	366	GLY	2.4
1	B	368	LYS	2.4
1	B	365	GLN	2.2
1	A	68	GLY	2.2
1	A	368	LYS	2.2
1	B	313	GLN	2.1
1	B	566	SER	2.0
1	A	568	GLY	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

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. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
3	GOL	B	805	6/6	0.84	0.24	49,53,55,58	0
3	GOL	A	804	6/6	0.90	0.14	30,36,38,43	0
3	GOL	B	804	6/6	0.91	0.16	38,44,46,46	0
3	GOL	A	803	6/6	0.91	0.14	47,49,49,55	0
3	GOL	B	802	6/6	0.93	0.11	27,34,36,39	0
3	GOL	A	802	6/6	0.94	0.12	28,32,33,36	0
3	GOL	B	803	6/6	0.95	0.10	40,42,43,48	0
3	GOL	B	801	6/6	0.96	0.10	14,19,20,25	0
3	GOL	A	801	6/6	0.97	0.06	15,17,18,20	0
4	ZN	B	807	1/1	0.98	0.06	41,41,41,41	0
4	ZN	A	805	1/1	0.99	0.03	38,38,38,38	0
4	ZN	A	806	1/1	0.99	0.04	35,35,35,35	0
4	ZN	B	806	1/1	0.99	0.04	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.