



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2016 – 02:06 PM EST

PDB ID : 2X3T  
Title : Glutaraldehyde-crosslinked wheat germ agglutinin isolectin 1 crystal soaked with a synthetic glycopeptide  
Authors : Schwefel, D.; Maierhofer, C.; Wittmann, V.; Diederichs, K.; Welte, W.  
Deposited on : 2010-01-26  
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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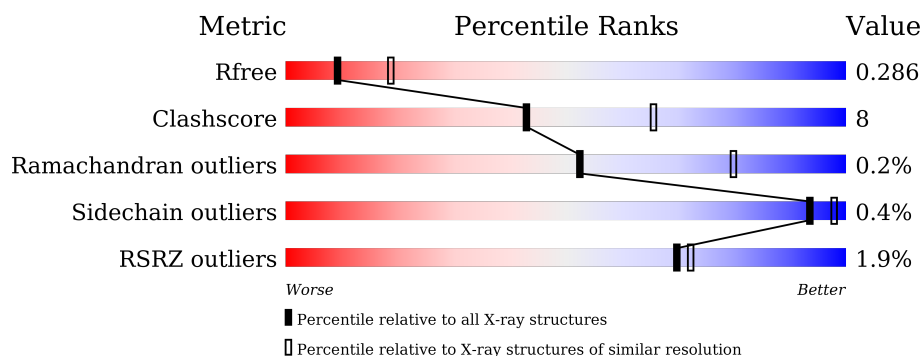
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

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## X-RAY DIFFRACTION

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.



<b>Metric</b>	<b>Whole archive (#Entries)</b>	<b>Similar resolution (#Entries, resolution range(Å))</b>
R <sub>free</sub>	91344	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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  $\geq 3$ , 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	171	<div> <div></div> <div>81%</div> <div>18%</div> <div>•</div> </div>
1	B	171	<div> <div></div> <div>82%</div> <div>15%</div> <div>••</div> </div>
1	C	171	<div> <div>3%</div> <div></div> <div>85%</div> <div>12%</div> <div>•</div> </div>
1	D	171	<div> <div>4%</div> <div></div> <div>88%</div> <div>12%</div> </div>
2	E	9	<div> <div>22%</div> <div></div> <div>78%</div> </div>
2	M	9	<div> <div>22%</div> <div></div> <div>78%</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
5	GOL	A	1174	-	-	-	X
5	GOL	B	1174	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4820 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.

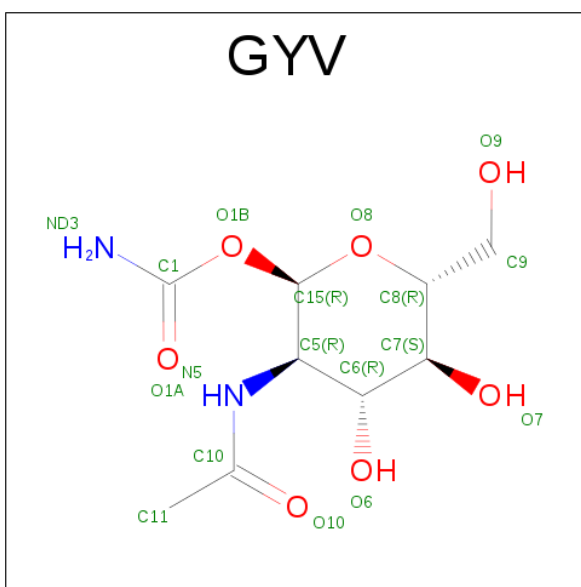
- Molecule 1 is a protein called AGGLUTININ ISOLECTIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1145	668	209	234	34			
1	B	167	Total	C	N	O	S	0	0	0
			1117	653	202	228	34			
1	C	166	Total	C	N	O	S	0	0	0
			1122	653	204	231	34			
1	D	171	Total	C	N	O	S	0	0	0
			1137	664	205	234	34			

- Molecule 2 is a protein called GLYCOPEPTIDE.

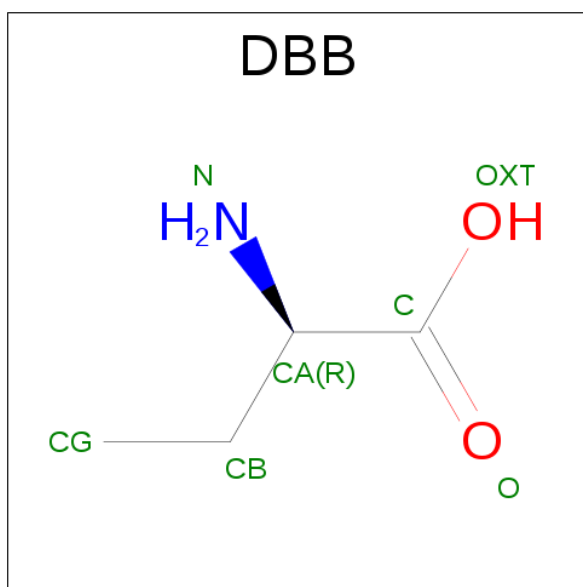
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			12	8	2	2			
2	M	2	Total	C	N	O	0	0	0
			12	8	2	2			

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-1-O-CARBAMOYL-2-DEOXY-ALPHA-D-G LUCOPYRANOSE) (three-letter code: GYV) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>2</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	9	2	7		
3	A	1	Total	C	N	O	0	0
			18	9	2	7		
3	B	1	Total	C	N	O	0	0
			18	9	2	7		
3	B	1	Total	C	N	O	0	0
			18	9	2	7		
3	C	1	Total	C	N	O	0	0
			18	9	2	7		
3	D	1	Total	C	N	O	0	0
			18	9	2	7		
3	D	1	Total	C	N	O	0	0
			18	9	2	7		
3	E	1	Total	C	N	O	0	0
			18	9	2	7		
3	E	1	Total	C	N	O	0	0
			18	9	2	7		
3	M	1	Total	C	N	O	0	0
			18	9	2	7		
3	M	1	Total	C	N	O	0	0
			18	9	2	7		

- Molecule 4 is D-ALPHA-AMINOBTYRIC ACID (three-letter code: DBB) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

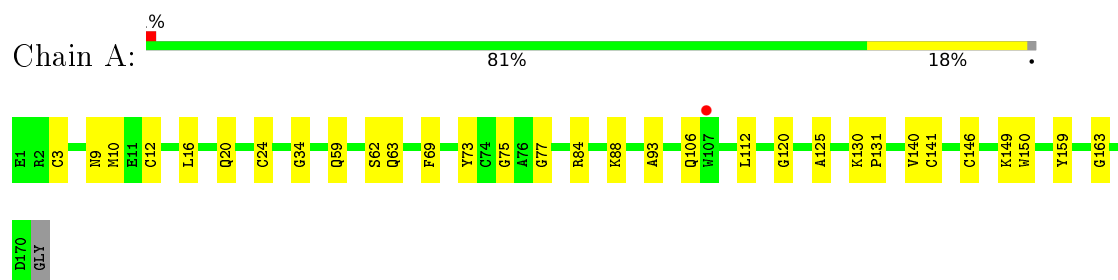
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		
6	B	9	Total	O	0	0
			9	9		
6	C	12	Total	O	0	0
			12	12		
6	D	6	Total	O	0	0
			6	6		

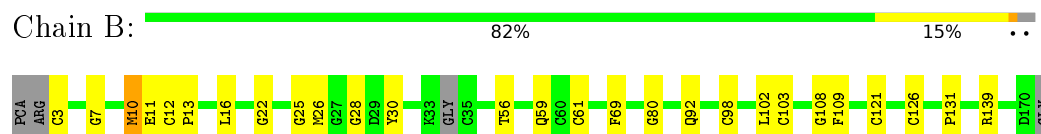
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

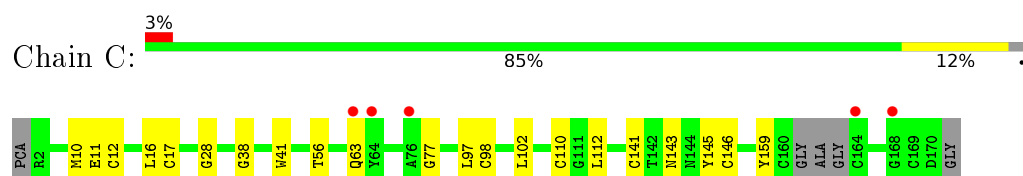
- Molecule 1: AGGLUTININ ISOLECTIN 1



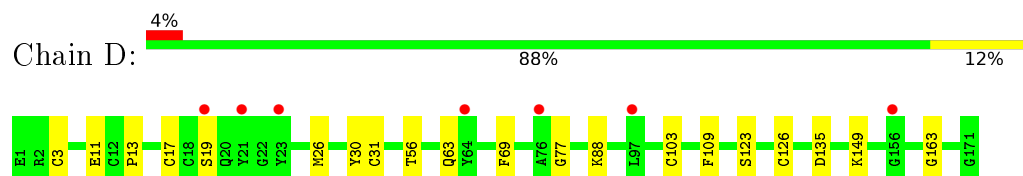
- Molecule 1: AGGLUTININ ISOLECTIN 1



- Molecule 1: AGGLUTININ ISOLECTIN 1



- Molecule 1: AGGLUTININ ISOLECTIN 1



- Molecule 2: GLYCOPEPTIDE



- Molecule 2: GLYCOPEPTIDE



Chain M:  22% 78%

LYS	DEB	DVA	T4	T5	DVA	DEB	GLU	BAL
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.64Å 93.21Å 92.50Å 90.00° 98.32° 90.00°	Depositor
Resolution (Å)	32.65 – 2.75 32.65 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (32.65-2.75) 99.6 (32.65-2.75)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.76Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.229 , 0.285 0.225 , 0.286	Depositor DCC
$R_{free}$ test set	1000 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	1.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	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 39.64 % 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 3.0784e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.24	0/1159	0.35	0/1557
1	B	0.24	0/1137	0.35	0/1525
1	C	0.23	0/1142	0.34	0/1533
1	D	0.24	0/1151	0.35	0/1546
All	All	0.24	0/4589	0.35	0/6161

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1145	0	954	29	0
1	B	1117	0	924	22	0
1	C	1122	0	924	14	0
1	D	1137	0	936	13	0
2	E	12	0	13	3	0
2	M	12	0	11	2	0
3	A	36	0	30	1	0
3	B	36	0	30	0	0
3	C	18	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	36	0	30	0	0
3	E	36	0	30	8	0
3	M	36	0	30	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	3	0	0	0	0
4	D	6	0	0	0	0
5	A	6	0	8	0	0
5	B	6	0	8	1	0
5	D	6	0	8	2	0
6	A	11	0	0	0	0
6	B	9	0	0	0	0
6	C	12	0	0	0	0
6	D	6	0	0	0	0
All	All	4820	0	3951	72	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 8.

All (72) 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:92:GLN:HG3	1:B:108:GLY:HA3	1.61	0.80
2:E:4:DBB:H1	3:E:1004:GYV:HD32	1.27	0.80
1:A:63:GLN:HB3	1:A:77:GLY:HA3	1.64	0.79
1:C:63:GLN:HB3	1:C:77:GLY:HA3	1.70	0.74
1:C:102:LEU:HD23	1:C:110:CYS:HB3	1.73	0.70
1:A:62:SER:CB	3:E:1005:GYV:H111	2.22	0.69
2:M:4:DBB:O	2:M:5:DBB:C	2.37	0.69
1:D:19:SER:HB2	1:D:30:TYR:HA	1.76	0.67
1:A:149:LYS:HB3	1:A:163:GLY:HA3	1.77	0.67
2:E:4:DBB:O	2:E:5:DBB:C	2.45	0.65
1:A:3:CYS:HB3	1:B:10:MET:HE3	1.79	0.64
1:A:3:CYS:HB3	1:B:10:MET:CE	2.28	0.62
1:A:9:ASN:O	1:B:13:PRO:HG3	2.01	0.60
1:C:10:MET:SD	1:D:3:CYS:HB3	2.42	0.59
1:B:126:CYS:O	5:B:1174:GOL:H31	2.03	0.59
1:D:88:LYS:HG2	1:D:109:PHE:CE1	2.39	0.57
2:E:4:DBB:N	3:E:1004:GYV:ND3	2.52	0.57
1:A:62:SER:HB3	3:E:1005:GYV:H111	1.87	0.56
1:C:146:CYS:HB3	1:C:159:TYR:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLU:OE2	1:B:56:THR:HB	2.06	0.55
1:C:10:MET:HA	1:D:13:PRO:HD3	1.89	0.54
1:B:61:CYS:HB3	1:B:80:GLY:H	1.73	0.54
1:B:3:CYS:HA	1:B:10:MET:HB3	1.88	0.54
1:A:159:TYR:CZ	3:A:1172:GYV:H113	2.45	0.52
1:A:149:LYS:HE3	1:A:150:TRP:CH2	2.44	0.52
1:D:63:GLN:HB3	1:D:77:GLY:O	2.09	0.52
1:A:106:GLN:HG2	1:A:120:GLY:CA	2.39	0.52
1:A:62:SER:HB2	3:E:1005:GYV:H111	1.91	0.51
1:B:12:CYS:HB3	1:B:16:LEU:HB2	1.92	0.51
1:D:103:CYS:HA	1:D:123:SER:O	2.11	0.51
1:A:73:TYR:CZ	3:E:1005:GYV:H113	2.46	0.50
1:A:24:CYS:SG	1:B:10:MET:HE1	2.51	0.50
1:C:98:CYS:HB3	1:C:102:LEU:HB3	1.94	0.50
1:B:7:GLY:O	1:B:10:MET:HB2	2.13	0.49
1:A:112:LEU:HD12	1:B:69:PHE:HD2	1.78	0.49
1:B:103:CYS:HB3	1:B:121:CYS:SG	2.52	0.49
1:D:26:MET:HE3	1:D:31:CYS:SG	2.53	0.48
2:M:4:DBB:O	2:M:5:DBB:O	2.30	0.48
1:A:112:LEU:HD12	1:B:69:PHE:CD2	2.49	0.48
1:A:12:CYS:HB2	1:A:16:LEU:O	2.14	0.48
1:D:149:LYS:HB3	1:D:163:GLY:HA3	1.96	0.47
1:D:11:GLU:OE2	1:D:56:THR:HB	2.13	0.47
1:C:11:GLU:OE2	1:C:56:THR:HB	2.14	0.47
1:C:17:CYS:HA	1:C:38:GLY:HA3	1.97	0.47
1:A:10:MET:SD	1:B:3:CYS:HB2	2.55	0.47
1:A:59:GLN:HG2	1:A:69:PHE:CE2	2.50	0.47
1:B:59:GLN:HG2	1:B:69:PHE:CE2	2.50	0.46
1:C:141:CYS:HB3	1:C:145:TYR:HB2	1.98	0.46
1:B:3:CYS:HB3	1:B:22:GLY:O	2.14	0.46
1:C:28:GLY:HA2	1:C:41:TRP:CH2	2.51	0.46
1:B:131:PRO:O	1:B:139:ARG:HD3	2.16	0.46
1:A:106:GLN:HG2	1:A:120:GLY:HA3	1.96	0.45
1:A:63:GLN:HB3	1:A:77:GLY:CA	2.42	0.45
1:D:126:CYS:O	5:D:1176:GOL:H11	2.16	0.45
1:A:59:GLN:HA	1:A:69:PHE:CZ	2.53	0.44
1:A:125:ALA:HA	1:B:26:MET:HE2	2.00	0.44
1:A:73:TYR:CE1	3:E:1005:GYV:H113	2.53	0.43
1:A:140:VAL:HG12	1:A:141:CYS:O	2.18	0.43
1:C:97:LEU:HD22	1:C:143:ASN:HD21	1.83	0.43
1:C:12:CYS:HB2	1:C:16:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:CYS:HB3	1:D:30:TYR:O	2.19	0.42
1:A:88:LYS:HB3	1:A:93:ALA:HB2	2.02	0.42
1:A:146:CYS:HB3	1:A:159:TYR:O	2.20	0.42
1:D:126:CYS:O	5:D:1176:GOL:H31	2.20	0.41
1:A:130:LYS:HA	1:A:131:PRO:HD3	1.89	0.41
1:C:112:LEU:HD12	1:D:69:PHE:HD2	1.85	0.41
1:C:102:LEU:HD12	1:C:112:LEU:HG	2.02	0.41
1:A:20:GLN:HB3	1:A:34:GLY:HA3	2.02	0.41
1:B:109:PHE:CD2	3:E:1004:GYV:H5	2.56	0.40
1:A:75:GLY:HA2	1:A:84:ARG:HD2	2.03	0.40
1:B:98:CYS:HB2	1:B:102:LEU:O	2.22	0.40
1:B:25:GLY:HA3	1:B:30:TYR:CD2	2.56	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	168/171 (98%)	151 (90%)	17 (10%)	0	100	100
1	B	163/171 (95%)	148 (91%)	14 (9%)	1 (1%)	30	57
1	C	162/171 (95%)	144 (89%)	18 (11%)	0	100	100
1	D	169/171 (99%)	148 (88%)	21 (12%)	0	100	100
All	All	662/684 (97%)	591 (89%)	70 (11%)	1 (0%)	52	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	114/119 (96%)	114 (100%)	0	100	100
1	B	112/119 (94%)	111 (99%)	1 (1%)	84	95
1	C	114/119 (96%)	114 (100%)	0	100	100
1	D	111/119 (93%)	110 (99%)	1 (1%)	84	95
All	All	451/476 (95%)	449 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	MET
1	D	135	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	C	14	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](#)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	PCA	A	1	1	7,8,9	1.65	1 (14%)	9,10,12	1.93	4 (44%)
1	PCA	D	1	1	7,8,9	1.65	1 (14%)	9,10,12	1.88	4 (44%)
2	DBB	E	4	3,2	3,5,6	0.39	0	3,5,7	1.25	0
2	DBB	E	5	3,2	3,5,6	0.39	0	3,5,7	1.25	0
2	DBB	M	4	3,2	3,5,6	0.34	0	3,5,7	1.82	1 (33%)
2	DBB	M	5	3,2	3,5,6	0.27	0	3,5,7	0.67	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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1
2	DBB	E	4	3,2	-	0/2/4/6	0/0/0/0
2	DBB	E	5	3,2	-	0/2/4/6	0/0/0/0
2	DBB	M	4	3,2	-	0/2/4/6	0/0/0/0
2	DBB	M	5	3,2	-	0/2/4/6	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	PCA	CD-N	4.26	1.46	1.33
1	A	1	PCA	CD-N	4.27	1.46	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	4	DBB	O-C-CA	-3.04	117.57	125.72
1	D	1	PCA	CA-N-CD	-3.04	102.72	113.53
1	A	1	PCA	CA-N-CD	-2.83	103.45	113.53
1	A	1	PCA	OE-CD-CG	-2.65	121.60	126.85
1	D	1	PCA	OE-CD-CG	-2.44	122.03	126.85
1	D	1	PCA	CB-CA-C	-2.17	109.58	112.80
1	D	1	PCA	CB-CA-N	2.03	109.51	103.34
1	A	1	PCA	CG-CD-N	2.09	114.63	108.28
1	A	1	PCA	CB-CA-N	2.46	110.81	103.34



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4	DBB	3	0
2	E	5	DBB	1	0
2	M	4	DBB	2	0
2	M	5	DBB	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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	GYV	A	1170	4	17,18,18	1.30	2 (11%)	21,25,25	2.11	9 (42%)
4	DBB	A	1171	3	2,2,6	0.27	0	0,1,7	0.00	-
3	GYV	A	1172	4	17,18,18	0.40	0	21,25,25	1.73	5 (23%)
4	DBB	A	1173	3	2,2,6	0.31	0	0,1,7	0.00	-
5	GOL	A	1174	-	5,5,5	0.36	0	5,5,5	0.21	0
3	GYV	B	1170	4	17,18,18	0.34	0	21,25,25	1.56	2 (9%)
4	DBB	B	1171	3	2,2,6	0.30	0	0,1,7	0.00	-
3	GYV	B	1172	4	17,18,18	0.31	0	21,25,25	1.37	3 (14%)
4	DBB	B	1173	3	2,2,6	0.31	0	0,1,7	0.00	-
5	GOL	B	1174	-	5,5,5	0.37	0	5,5,5	0.19	0
3	GYV	C	1172	4	17,18,18	0.34	0	21,25,25	1.35	5 (23%)
4	DBB	C	1173	3	2,2,6	0.32	0	0,1,7	0.00	-
3	GYV	D	1170	4	17,18,18	0.34	0	21,25,25	1.54	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DBB	D	1171	3	2,2,6	0.30	0	0,1,7	0.00	-
3	GYV	D	1172	4	17,18,18	0.30	0	21,25,25	1.50	4 (19%)
4	DBB	D	1173	3	2,2,6	0.31	0	0,1,7	0.00	-
5	GOL	D	1176	-	5,5,5	0.37	0	5,5,5	0.21	0
3	GYV	E	1004	2	17,18,18	0.47	0	21,25,25	1.37	3 (14%)
3	GYV	E	1005	2	17,18,18	0.33	0	21,25,25	1.13	2 (9%)
3	GYV	M	1004	2	17,18,18	0.81	0	21,25,25	1.62	6 (28%)
3	GYV	M	1005	2	17,18,18	1.21	1 (5%)	21,25,25	2.22	8 (38%)

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	GYV	A	1170	4	-	2/10/30/30	0/1/1/1
4	DBB	A	1171	3	-	0/0/0/6	0/0/0/0
3	GYV	A	1172	4	-	0/10/30/30	0/1/1/1
4	DBB	A	1173	3	-	0/0/0/6	0/0/0/0
5	GOL	A	1174	-	-	0/4/4/4	0/0/0/0
3	GYV	B	1170	4	-	2/10/30/30	0/1/1/1
4	DBB	B	1171	3	-	0/0/0/6	0/0/0/0
3	GYV	B	1172	4	-	0/10/30/30	0/1/1/1
4	DBB	B	1173	3	-	0/0/0/6	0/0/0/0
5	GOL	B	1174	-	-	0/4/4/4	0/0/0/0
3	GYV	C	1172	4	-	0/10/30/30	0/1/1/1
4	DBB	C	1173	3	-	0/0/0/6	0/0/0/0
3	GYV	D	1170	4	-	2/10/30/30	0/1/1/1
4	DBB	D	1171	3	-	0/0/0/6	0/0/0/0
3	GYV	D	1172	4	-	0/10/30/30	0/1/1/1
4	DBB	D	1173	3	-	0/0/0/6	0/0/0/0
5	GOL	D	1176	-	-	0/4/4/4	0/0/0/0
3	GYV	E	1004	2	-	0/10/30/30	0/1/1/1
3	GYV	E	1005	2	-	0/10/30/30	0/1/1/1
3	GYV	M	1004	2	-	0/10/30/30	0/1/1/1
3	GYV	M	1005	2	-	0/10/30/30	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1170	GYV	O1B-C15	-2.53	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1170	GYV	C6-C5	-2.53	1.47	1.53
3	M	1005	GYV	O1A-C1	-2.34	1.18	1.21

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1005	GYV	C7-C6-C5	-5.80	101.56	110.37
3	A	1170	GYV	C7-C6-C5	-4.97	102.83	110.37
3	B	1170	GYV	C15-O1B-C1	-4.84	109.61	116.53
3	D	1170	GYV	C15-O1B-C1	-4.26	110.44	116.53
3	A	1170	GYV	C6-C5-N5	-4.23	101.88	110.67
3	B	1172	GYV	C15-C5-N5	-3.91	103.65	111.01
3	A	1172	GYV	C7-C6-C5	-3.88	104.48	110.37
3	D	1172	GYV	C15-C5-N5	-3.79	103.87	111.01
3	D	1170	GYV	C15-C5-N5	-3.53	104.38	111.01
3	B	1170	GYV	C15-C5-N5	-3.47	104.48	111.01
3	A	1170	GYV	O1A-C1-ND3	-3.33	119.37	125.50
3	C	1172	GYV	C15-C5-N5	-3.07	105.23	111.01
3	M	1004	GYV	O7-C7-C6	-3.01	103.57	110.36
3	M	1004	GYV	C15-C5-N5	-2.98	105.40	111.01
3	E	1004	GYV	C15-C5-N5	-2.89	105.58	111.01
3	M	1005	GYV	O7-C7-C6	-2.64	104.40	110.36
3	D	1172	GYV	C6-C5-N5	-2.59	105.30	110.67
3	D	1172	GYV	C15-O1B-C1	-2.56	112.87	116.53
3	M	1004	GYV	C5-N5-C10	-2.56	116.49	123.21
3	M	1004	GYV	C6-C5-N5	-2.51	105.46	110.67
3	C	1172	GYV	C6-C5-N5	-2.48	105.52	110.67
3	M	1005	GYV	O6-C6-C7	-2.47	104.80	110.36
3	B	1172	GYV	C6-C5-N5	-2.45	105.58	110.67
3	A	1170	GYV	O8-C15-O1B	-2.40	101.71	108.39
3	M	1005	GYV	C6-C5-N5	-2.35	105.80	110.67
3	A	1170	GYV	C6-C7-C8	-2.32	106.08	110.23
3	A	1170	GYV	C9-C8-C7	-2.23	107.40	112.99
3	E	1005	GYV	C6-C5-N5	-2.22	106.07	110.67
3	A	1172	GYV	C15-C5-N5	-2.21	106.85	111.01
3	D	1170	GYV	C6-C5-N5	-2.20	106.11	110.67
3	C	1172	GYV	C7-C6-C5	-2.15	107.11	110.37
3	M	1005	GYV	C6-C7-C8	-2.15	106.40	110.23
3	A	1172	GYV	C6-C5-N5	-2.12	106.28	110.67
3	B	1172	GYV	O8-C8-C7	2.08	113.63	109.67
3	C	1172	GYV	C15-O8-C8	2.08	117.83	113.74
3	A	1170	GYV	O8-C8-C9	2.09	111.79	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1005	GYV	O6-C6-C5	2.12	113.95	109.57
3	A	1170	GYV	C15-C5-N5	2.14	115.05	111.01
3	M	1004	GYV	C15-O8-C8	2.20	118.06	113.74
3	E	1005	GYV	O8-C8-C7	2.30	114.05	109.67
3	A	1170	GYV	C15-O8-C8	2.35	118.35	113.74
3	M	1004	GYV	O8-C8-C7	2.38	114.21	109.67
3	C	1172	GYV	O8-C8-C7	2.42	114.28	109.67
3	D	1172	GYV	O8-C8-C7	2.49	114.42	109.67
3	E	1004	GYV	O8-C8-C7	2.72	114.85	109.67
3	E	1004	GYV	C6-C7-C8	2.74	115.11	110.23
3	M	1005	GYV	O8-C8-C7	3.03	115.44	109.67
3	A	1172	GYV	O8-C8-C7	3.42	116.19	109.67
3	A	1172	GYV	C15-O8-C8	4.00	121.59	113.74
3	M	1005	GYV	C15-O8-C8	4.34	122.27	113.74

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1170	GYV	C15-O1B-C1-ND3
3	D	1170	GYV	C15-O1B-C1-ND3
3	D	1170	GYV	C15-O1B-C1-O1A
3	A	1170	GYV	C15-O1B-C1-O1A
3	B	1170	GYV	C15-O1B-C1-ND3
3	B	1170	GYV	C15-O1B-C1-O1A

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1172	GYV	1	0
5	B	1174	GOL	1	0
5	D	1176	GOL	2	0
3	E	1004	GYV	3	0
3	E	1005	GYV	5	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 [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	169/171 (98%)	-0.03	1 (0%) 90 92	31, 47, 73, 105	2 (1%)
1	B	167/171 (97%)	0.17	0 100 100	32, 49, 76, 102	0
1	C	166/171 (97%)	0.22	5 (3%) 54 56	38, 52, 91, 130	2 (1%)
1	D	170/171 (99%)	0.32	7 (4%) 41 42	37, 56, 86, 117	0
2	E	0/9	-	-	-	-
2	M	0/9	-	-	-	-
All	All	672/702 (95%)	0.17	13 (1%) 70 72	31, 51, 84, 130	4 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	23	TYR	4.2
1	D	21	TYR	3.4
1	D	19	SER	2.8
1	C	64	TYR	2.7
1	D	76	ALA	2.7
1	A	107	TRP	2.7
1	D	97	LEU	2.6
1	D	64	TYR	2.3
1	C	168	GLY	2.3
1	C	76	ALA	2.3
1	C	164	CYS	2.3
1	C	63	GLN	2.0
1	D	156	GLY	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DBB	E	4	6/7	0.74	0.32	-	53,53,53,53	0
2	DBB	E	5	6/7	0.71	0.41	-	53,54,54,54	0
1	PCA	D	1	8/9	0.76	0.28	-	82,84,86,86	0
2	DBB	M	4	6/7	0.68	0.37	-	72,73,74,75	0
2	DBB	M	5	6/7	0.80	0.21	-	64,68,69,71	0
1	PCA	A	1	8/9	0.80	0.24	-	94,94,95,95	0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	1174	6/6	0.87	0.34	3.56	73,76,77,78	0
5	GOL	B	1174	6/6	0.89	0.26	2.01	52,53,53,54	0
5	GOL	D	1176	6/6	0.94	0.24	1.74	60,60,61,62	0
3	GYV	E	1004	18/18	0.89	0.20	1.27	52,52,53,53	0
3	GYV	B	1170	18/18	0.85	0.25	0.84	74,78,83,84	0
3	GYV	A	1172	18/18	0.88	0.22	0.53	71,82,90,91	0
3	GYV	M	1004	18/18	0.87	0.23	0.31	74,77,78,78	0
3	GYV	A	1170	18/18	0.88	0.20	-0.16	48,49,51,52	0
3	GYV	E	1005	18/18	0.90	0.18	-0.26	53,53,54,54	0
3	GYV	D	1170	18/18	0.88	0.28	-0.26	63,66,72,73	0
3	GYV	C	1172	18/18	0.94	0.17	-0.40	50,51,54,54	0
3	GYV	D	1172	18/18	0.92	0.16	-0.41	75,76,78,79	0
3	GYV	M	1005	18/18	0.91	0.15	-0.87	43,55,59,62	0
3	GYV	B	1172	18/18	0.88	0.18	-0.90	70,80,84,86	0
4	DBB	B	1173	3/7	0.63	0.37	-	58,58,62,66	0
4	DBB	A	1171	3/7	0.64	0.40	-	47,47,48,48	0
4	DBB	C	1173	3/7	0.71	0.39	-	51,51,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DBB	D	1173	3/7	0.17	0.42	-	75,75,75,76	0
4	DBB	B	1171	3/7	0.57	0.35	-	84,84,84,84	0
4	DBB	A	1173	3/7	0.77	0.33	-	92,92,92,93	0
4	DBB	D	1171	3/7	0.84	0.24	-	70,70,70,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.