



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:58 am BST

PDB ID : 3MUE  
Title : Crystal Structure of Pantoate-beta-Alanine Ligase from Salmonella typhimurium  
Authors : Kim, Y.; Makowska-Grzyska, M.; Maltseva, N.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CS-GID)  
Deposited on : 2010-05-03  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (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

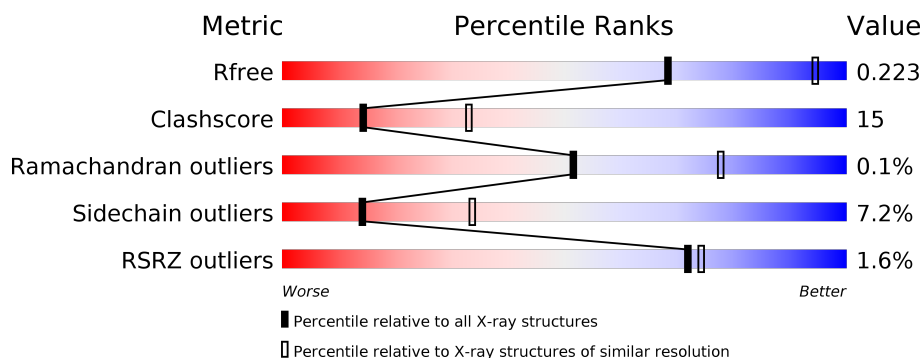
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	287	<div> <div>75%</div> <div>21%</div> <div>• •</div> </div>
1	B	287	<div> <div>70%</div> <div>24%</div> <div>5%</div> <div>•</div> </div>
1	C	287	<div> <div>4%</div> <div>64%</div> <div>30%</div> <div>5%</div> <div>•</div> </div>
1	D	287	<div> <div>4%</div> <div>67%</div> <div>31%</div> <div>• •</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	295	-	-	-	X
2	GOL	C	294	-	-	X	X
2	GOL	D	285	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9523 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 Pantothenate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	1	0
			2253	1423	402	418	10			
1	B	285	Total	C	N	O	S	0	2	0
			2260	1426	403	421	10			
1	C	283	Total	C	N	O	S	0	3	0
			2258	1427	404	417	10			
1	D	284	Total	C	N	O	S	0	5	0
			2288	1443	414	421	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q8ZRR1
A	-1	ASN	-	EXPRESSION TAG	UNP Q8ZRR1
A	0	ALA	-	EXPRESSION TAG	UNP Q8ZRR1
B	-2	SER	-	EXPRESSION TAG	UNP Q8ZRR1
B	-1	ASN	-	EXPRESSION TAG	UNP Q8ZRR1
B	0	ALA	-	EXPRESSION TAG	UNP Q8ZRR1
C	-2	SER	-	EXPRESSION TAG	UNP Q8ZRR1
C	-1	ASN	-	EXPRESSION TAG	UNP Q8ZRR1
C	0	ALA	-	EXPRESSION TAG	UNP Q8ZRR1
D	-2	SER	-	EXPRESSION TAG	UNP Q8ZRR1
D	-1	ASN	-	EXPRESSION TAG	UNP Q8ZRR1
D	0	ALA	-	EXPRESSION TAG	UNP Q8ZRR1

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



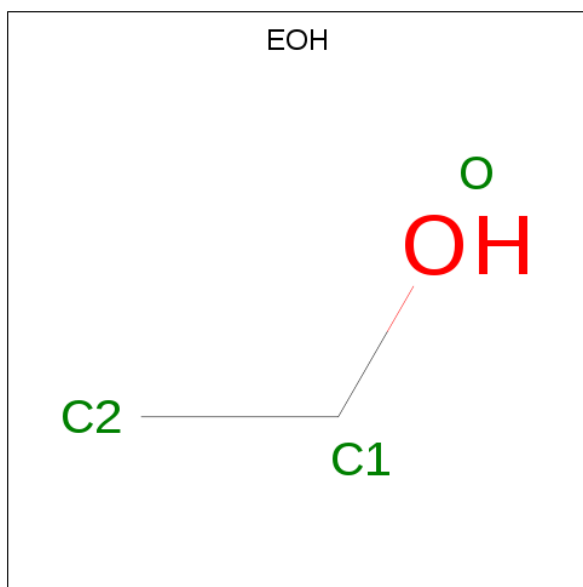
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total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

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

- Molecule 3 is ETHANOL (three-letter code: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).



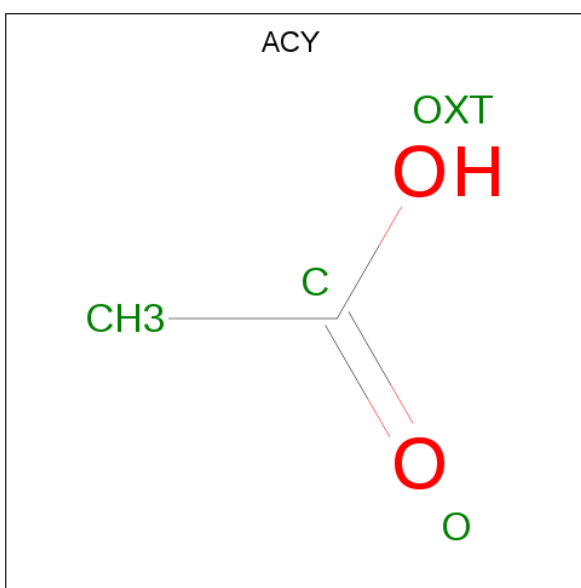
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	2	1		
3	A	1	Total	C	O	0	0
			3	2	1		
3	A	1	Total	C	O	0	0
			3	2	1		
3	B	1	Total	C	O	0	0
			3	2	1		
3	C	1	Total	C	O	0	0
			3	2	1		

- Molecule 4 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

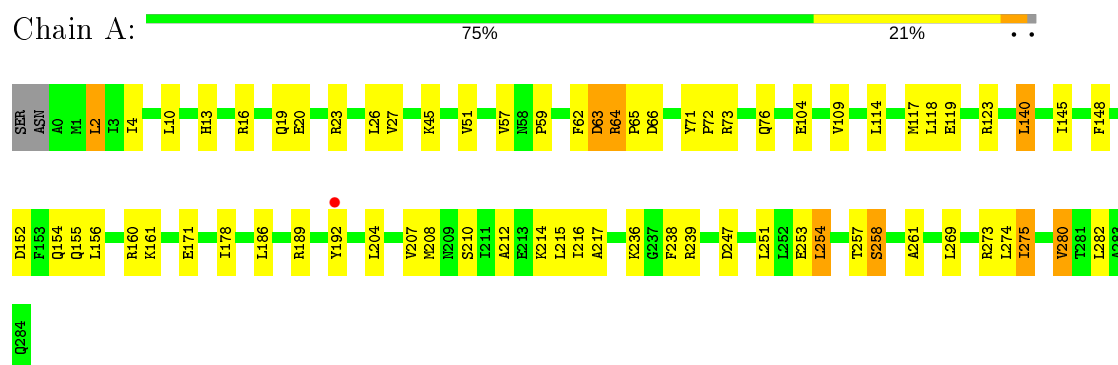
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	125	Total 125	O 125	0	0
6	B	114	Total 114	O 114	0	0
6	C	49	Total 49	O 49	0	0
6	D	51	Total 51	O 51	0	0



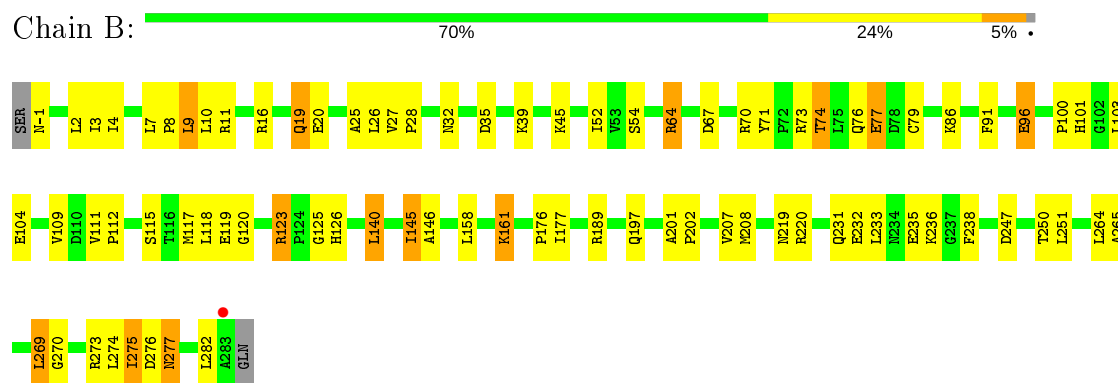
### 3 Residue-property plots [i](#)

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.

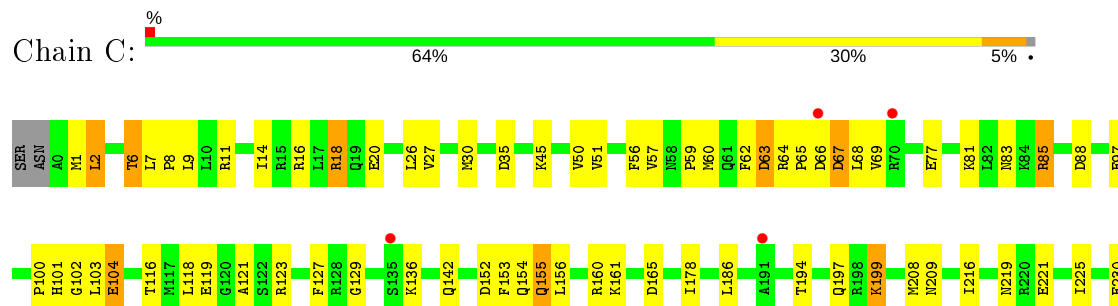
#### • Molecule 1: Pantothenate synthetase



#### • Molecule 1: Pantothenate synthetase

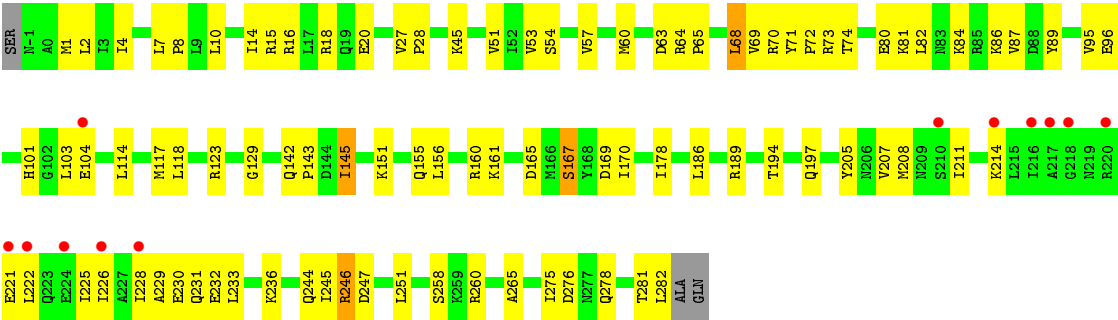


#### • Molecule 1: Pantothenate synthetase





● Molecule 1: Pantothenate synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.23Å 134.92Å 93.92Å 90.00° 93.96° 90.00°	Depositor
Resolution (Å)	35.39 – 2.70 35.39 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.39-2.70) 98.9 (35.39-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.15 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, $R_{free}$	0.178 , 0.229 0.171 , 0.223	Depositor DCC
$R_{free}$ test set	2713 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 71.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9523	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, ACY, EOH, SO4

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	0.59	0/2286	0.73	0/3090
1	B	0.55	0/2293	0.70	0/3100
1	C	0.47	0/2291	0.63	1/3096 (0.0%)
1	D	0.44	0/2321	0.59	0/3135
All	All	0.51	0/9191	0.66	1/12421 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	ASP	CB-CG-OD2	5.17	122.95	118.30

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	2253	0	2316	55	0
1	B	2260	0	2317	72	0
1	C	2258	0	2325	90	0
1	D	2288	0	2355	79	0
2	A	12	0	16	0	0
2	B	36	0	48	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	0	32	11	0
2	D	24	0	32	5	0
3	A	9	0	18	1	0
3	B	3	0	6	0	0
3	C	3	0	6	0	0
4	A	10	0	0	0	0
5	A	4	0	3	0	0
6	A	125	0	0	1	0
6	B	114	0	0	6	0
6	C	49	0	0	3	0
6	D	51	0	0	2	0
All	All	9523	0	9474	289	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 15.

All (289) 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:208:MET:HE3	1:B:276:ASP:HB3	1.14	1.09
1:B:74:THR:HG22	1:B:77:GLU:H	1.24	1.03
1:B:101:HIS:HB2	2:B:294:GOL:H32	1.40	1.02
1:D:73[B]:ARG:HH21	1:D:73[B]:ARG:HG2	1.27	1.00
1:C:161:LYS:HE3	1:C:165:ASP:OD2	1.69	0.92
1:B:74:THR:CG2	1:B:77:GLU:H	1.84	0.91
1:D:60:MET:HG3	1:D:103:LEU:HD22	1.52	0.91
1:C:250:THR:HG22	1:C:252:LEU:H	1.36	0.89
1:B:35:ASP:HB2	2:B:291:GOL:H12	1.55	0.88
1:C:268:TRP:CZ2	1:C:273:ARG:HD2	2.08	0.88
1:D:60:MET:HE2	1:D:129:GLY:HA2	1.57	0.86
1:D:101:HIS:HB2	2:D:292:GOL:H31	1.58	0.86
1:C:269:LEU:HB3	1:C:272:ALA:HB3	1.55	0.86
1:D:247:ASP:OD2	1:D:258:SER:HB3	1.76	0.85
1:D:143:PRO:HG2	1:D:170:ILE:HD13	1.59	0.84
1:A:192:TYR:CD2	1:A:192:TYR:O	2.30	0.84
1:A:16:ARG:HD2	1:A:20:GLU:OE2	1.79	0.83
1:A:178:ILE:HG22	1:A:186:LEU:HD12	1.60	0.81
1:C:119:GLU:OE1	2:C:294:GOL:H12	1.80	0.80
1:D:104:GLU:HB2	6:D:307:HOH:O	1.81	0.79
1:D:189:ARG:HH11	1:D:189:ARG:HG3	1.45	0.79
1:A:216:ILE:HD11	1:A:280:VAL:HG22	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ASP:O	1:C:65:PRO:HD3	1.83	0.78
1:B:125:GLY:N	2:B:295:GOL:H11	1.98	0.77
1:A:13:HIS:ND1	1:A:16:ARG:NH2	2.33	0.75
1:C:127:PHE:CZ	1:C:154:GLN:HG2	2.23	0.74
1:D:117:MET:HG3	1:D:118:LEU:HG	1.70	0.74
1:C:208:MET:HE3	1:C:278:GLN:HB2	1.69	0.73
1:C:194:THR:OG1	1:C:197:GLN:HG3	1.89	0.73
1:D:189:ARG:HG3	1:D:189:ARG:NH1	2.02	0.73
1:D:18[B]:ARG:O	1:D:18[B]:ARG:HD3	1.89	0.73
1:B:74:THR:HG22	1:B:77:GLU:HB2	1.71	0.73
1:C:152:ASP:HB3	2:C:294:GOL:H2	1.69	0.73
1:B:9:LEU:HD12	1:B:9:LEU:O	1.88	0.72
1:B:208:MET:HE3	1:B:276:ASP:CB	2.08	0.72
1:D:60:MET:CE	1:D:129:GLY:HA2	2.20	0.72
1:D:10:LEU:O	1:D:14:ILE:HG12	1.90	0.71
1:B:208:MET:CE	1:B:265:ALA:HB3	2.19	0.71
1:B:7:LEU:HD23	1:B:140:LEU:HD11	1.71	0.71
1:B:74:THR:HG22	1:B:77:GLU:N	2.03	0.71
1:B:117:MET:HG3	1:B:118:LEU:HG	1.72	0.70
1:A:23[B]:ARG:HH12	1:A:145:ILE:HD11	1.57	0.70
1:D:73[B]:ARG:NH2	1:D:73[B]:ARG:HG2	1.99	0.69
1:D:2[A]:LEU:HD21	1:D:89:TYR:CE1	2.28	0.69
1:A:10:LEU:HD23	1:A:140:LEU:HD13	1.75	0.68
1:B:101:HIS:CB	2:B:294:GOL:H32	2.22	0.68
1:D:18[B]:ARG:C	1:D:18[B]:ARG:HD3	2.14	0.68
1:A:192:TYR:O	1:A:192:TYR:CG	2.46	0.68
1:C:155:GLN:HE22	2:C:292:GOL:H32	1.57	0.68
1:D:27:VAL:HB	1:D:53:VAL:HG22	1.76	0.67
1:C:18:ARG:NH1	1:D:18[A]:ARG:CZ	2.57	0.67
1:A:178:ILE:CG2	1:A:186:LEU:HD12	2.23	0.67
1:C:64:ARG:O	1:C:67:ASP:HB2	1.96	0.66
1:D:2[B]:LEU:HD23	1:D:4:ILE:HD11	1.79	0.65
1:B:208:MET:HE1	1:B:265:ALA:HB3	1.77	0.65
1:B:10:LEU:HD22	1:B:91:PHE:CD1	2.32	0.65
1:C:250:THR:HG22	1:C:252:LEU:N	2.08	0.64
1:A:152:ASP:HB3	6:A:392:HOH:O	1.96	0.64
1:B:115:SER:HB2	2:B:295:GOL:H2	1.78	0.64
1:B:104:GLU:HA	1:B:104:GLU:OE1	1.98	0.64
1:C:11[B]:ARG:HD2	1:D:169:ASP:OD2	1.97	0.63
1:D:68:LEU:HD21	1:D:95:VAL:HG21	1.81	0.63
1:C:118:LEU:HD23	1:C:118:LEU:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ILE:C	1:D:145:ILE:HD13	2.18	0.63
1:D:208:MET:HE1	1:D:265:ALA:HB3	1.80	0.62
1:A:23[B]:ARG:NH1	1:A:145:ILE:HD11	2.14	0.62
1:B:64:ARG:NH2	6:B:369:HOH:O	2.32	0.62
1:D:232:GLU:O	1:D:236:LYS:HG3	1.99	0.62
1:C:268:TRP:CZ3	1:C:273:ARG:HB2	2.34	0.62
1:D:45:LYS:HG2	1:D:51:VAL:HG21	1.81	0.61
1:B:231:GLN:O	1:B:235:GLU:HG3	2.01	0.61
1:C:62:PHE:CD1	1:C:68:LEU:HD13	2.36	0.60
1:A:189:ARG:HH12	1:A:275:ILE:HG23	1.66	0.60
1:C:16:ARG:HD2	6:C:317:HOH:O	2.01	0.59
1:C:14:ILE:O	1:C:18:ARG:HG2	2.02	0.59
1:D:207:VAL:HG21	1:D:233:LEU:HD23	1.83	0.59
1:A:215:LEU:O	1:A:217:ALA:O	2.21	0.59
1:B:120:GLY:HA2	6:B:340:HOH:O	2.01	0.59
1:D:226:ILE:HD11	1:D:245:ILE:CD1	2.33	0.59
1:C:127:PHE:CE2	2:C:294:GOL:H11	2.38	0.59
1:B:220:ARG:NH1	1:B:282:LEU:HD22	2.18	0.59
1:B:125:GLY:H	2:B:295:GOL:H11	1.68	0.59
1:C:77:GLU:O	1:C:81:LYS:HG3	2.03	0.58
1:C:152:ASP:HB3	2:C:294:GOL:C2	2.34	0.58
1:C:30:MET:HG2	1:C:57:VAL:HA	1.86	0.58
1:C:250:THR:CG2	1:C:252:LEU:HB2	2.33	0.58
1:C:127:PHE:HE2	2:C:294:GOL:H11	1.68	0.58
1:A:216:ILE:HD11	1:A:280:VAL:CG2	2.34	0.57
1:C:16:ARG:O	1:C:20:GLU:HG3	2.04	0.57
1:A:63:ASP:OD2	1:A:123:ARG:HB3	2.03	0.57
1:B:126:HIS:HB3	6:B:340:HOH:O	2.04	0.57
1:C:11[B]:ARG:HH22	1:C:142:GLN:HE21	1.52	0.57
1:B:208:MET:HE2	1:B:265:ALA:HB3	1.86	0.56
1:C:18:ARG:HH12	1:D:18[A]:ARG:CZ	2.19	0.56
1:B:25:ALA:HB2	1:B:145:ILE:HD13	1.88	0.56
1:D:1:MET:HB2	1:D:87:VAL:O	2.06	0.56
1:C:136:LYS:HG3	1:D:167:SER:HB2	1.87	0.55
1:C:259:LYS:HG3	1:C:260:ARG:HG3	1.88	0.55
1:D:81:LYS:HE3	6:D:330:HOH:O	2.07	0.55
1:A:109:VAL:HG22	1:B:109:VAL:HG22	1.90	0.54
1:D:161:LYS:HE2	1:D:165:ASP:OD2	2.06	0.54
1:A:204:LEU:O	1:A:208:MET:HG3	2.07	0.54
1:D:189:ARG:HH11	1:D:189:ARG:CG	2.17	0.53
1:D:2[B]:LEU:CD2	1:D:4:ILE:HD11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:PRO:HG2	1:D:170:ILE:CD1	2.34	0.53
1:D:221:GLU:O	1:D:225:ILE:HG12	2.08	0.53
1:A:156:LEU:O	1:A:160:ARG:HG3	2.09	0.53
1:B:4:ILE:HD13	1:B:4:ILE:N	2.24	0.52
1:B:70:ARG:HB2	1:B:71:TYR:CE2	2.44	0.52
1:C:269:LEU:N	1:C:272:ALA:O	2.37	0.52
1:D:226:ILE:HD11	1:D:245:ILE:HD13	1.92	0.52
1:C:62:PHE:CG	1:C:68:LEU:HD13	2.45	0.52
1:A:247:ASP:OD2	1:A:258:SER:HB3	2.10	0.51
1:C:118:LEU:H	1:C:118:LEU:HD23	1.73	0.51
1:B:25:ALA:CB	1:B:145:ILE:HD13	2.41	0.51
1:C:104:GLU:HB2	6:C:291:HOH:O	2.10	0.51
1:B:96:GLU:H	1:B:96:GLU:CD	2.14	0.51
1:A:189:ARG:NH1	1:A:275:ILE:HG23	2.26	0.51
1:C:250:THR:HG21	1:C:252:LEU:HB2	1.93	0.51
1:D:60:MET:CG	1:D:103:LEU:HD22	2.35	0.51
1:C:63:ASP:OD2	1:C:63:ASP:N	2.30	0.50
1:A:19:GLN:HB3	1:C:199:LYS:HE2	1.93	0.50
1:A:73:ARG:HG3	1:A:73:ARG:HH21	1.76	0.50
1:C:119:GLU:O	1:C:123:ARG:HG3	2.11	0.50
1:C:155:GLN:NE2	2:C:292:GOL:H32	2.26	0.50
1:C:264:LEU:HD23	1:C:277:ASN:HB2	1.92	0.50
1:B:264:LEU:HD23	1:B:277:ASN:HB2	1.94	0.49
1:B:32:ASN:HA	1:B:73:ARG:HD3	1.94	0.49
1:D:156:LEU:HD21	1:D:160:ARG:HH21	1.77	0.49
1:D:208:MET:CE	1:D:265:ALA:HB3	2.42	0.49
1:D:281:THR:HG22	1:D:282:LEU:N	2.27	0.49
1:C:156:LEU:O	1:C:160:ARG:HG3	2.13	0.49
1:C:245:ILE:C	1:C:246[B]:ARG:HG2	2.32	0.49
1:B:39:LYS:NZ	1:B:176:PRO:O	2.45	0.49
1:C:153:PHE:H	1:C:153:PHE:HD2	1.58	0.49
1:D:207:VAL:CG1	1:D:229:ALA:HB1	2.43	0.49
1:C:230:GLU:HG2	1:C:240:ALA:HB1	1.94	0.48
1:D:228:ILE:O	1:D:232:GLU:HB2	2.13	0.48
1:B:9:LEU:HD12	1:B:9:LEU:C	2.31	0.48
1:D:7:LEU:HB2	1:D:8:PRO:HD3	1.94	0.48
1:C:153:PHE:CD2	1:C:153:PHE:N	2.81	0.48
1:C:247:ASP:OD1	1:C:250:THR:HB	2.13	0.48
1:C:234:ASN:HA	1:C:238:PHE:O	2.12	0.48
1:C:30:MET:HG2	1:C:56:PHE:O	2.14	0.48
1:D:178:ILE:CG2	1:D:186:LEU:HD12	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2[A]:LEU:H	1:D:2[A]:LEU:HD23	1.78	0.48
1:C:219:ASN:CG	1:C:225:ILE:HD11	2.34	0.47
1:D:275:ILE:HG22	1:D:276:ASP:N	2.29	0.47
1:C:1:MET:HG2	1:C:2:LEU:N	2.29	0.47
1:C:102:GLY:HA3	6:C:291:HOH:O	2.12	0.47
1:C:259:LYS:HG3	1:C:260:ARG:N	2.29	0.47
1:D:178:ILE:HG22	1:D:186:LEU:HD12	1.96	0.47
1:A:261:ALA:HB2	1:A:282:LEU:HD11	1.96	0.47
1:C:262:VAL:O	1:C:262:VAL:HG13	2.14	0.47
1:B:3:ILE:C	1:B:4:ILE:HD13	2.35	0.47
1:B:74:THR:HG23	1:B:76:GLN:N	2.30	0.47
1:C:244:GLN:HG2	1:C:246[B]:ARG:CZ	2.45	0.47
1:C:209:ASN:HD22	1:C:278:GLN:HE22	1.62	0.47
1:D:142:GLN:HB3	2:D:285:GOL:H32	1.97	0.47
1:A:2:LEU:HD13	1:A:4:ILE:HD11	1.97	0.47
1:B:273:ARG:NH1	1:B:275:ILE:HD11	2.30	0.47
1:C:116:THR:O	1:C:121:ALA:HA	2.14	0.46
1:C:60:MET:HG2	1:C:129:GLY:HA2	1.96	0.46
1:C:250:THR:HG22	1:C:252:LEU:CB	2.44	0.46
1:D:205:TYR:O	1:D:208:MET:HB3	2.15	0.46
1:D:73[B]:ARG:CG	1:D:73[B]:ARG:NH2	2.70	0.46
1:A:62:PHE:CE2	3:A:298:EOH:H22	2.51	0.46
1:D:101:HIS:HB2	2:D:292:GOL:C3	2.39	0.46
1:D:225:ILE:O	1:D:228:ILE:HG22	2.16	0.46
1:D:226:ILE:O	1:D:230:GLU:HB2	2.14	0.46
1:B:11[A]:ARG:CD	6:B:383:HOH:O	2.63	0.46
1:B:201:ALA:N	1:B:202:PRO:CD	2.79	0.46
1:D:208:MET:HG2	1:D:278:GLN:NE2	2.30	0.46
1:A:10:LEU:CD2	1:A:140:LEU:HD13	2.43	0.46
1:B:3:ILE:HD13	1:B:79:CYS:SG	2.56	0.46
1:C:9[B]:LEU:HD12	1:C:9[B]:LEU:O	2.16	0.46
1:A:104:GLU:CD	1:A:104:GLU:H	2.19	0.45
1:A:119:GLU:O	1:A:123:ARG:HG3	2.16	0.45
1:B:232:GLU:O	1:B:236:LYS:HG3	2.16	0.45
1:A:57:VAL:O	1:A:59:PRO:HD3	2.16	0.45
1:C:178:ILE:HG22	1:C:186:LEU:HD12	1.98	0.45
1:C:208:MET:HE3	1:C:278:GLN:HE21	1.81	0.45
1:C:257:THR:O	1:C:257:THR:HG22	2.16	0.45
1:C:50:VAL:HG13	1:C:88:ASP:CB	2.45	0.45
1:C:209:ASN:HD22	1:C:278:GLN:NE2	2.15	0.45
1:C:246[A]:ARG:HD2	1:C:251:LEU:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:LEU:HD22	1:B:91:PHE:CE1	2.51	0.45
1:C:14:ILE:O	1:C:18:ARG:CG	2.63	0.45
1:D:208:MET:HG2	1:D:278:GLN:HE21	1.82	0.45
1:D:211:ILE:HG23	1:D:225:ILE:HG21	1.97	0.45
1:C:45:LYS:HG2	1:C:51:VAL:HG21	1.99	0.45
1:B:74:THR:HG22	1:B:77:GLU:CB	2.43	0.45
1:C:259:LYS:O	1:C:282:LEU:N	2.47	0.45
1:D:63:ASP:C	1:D:65:PRO:HD3	2.38	0.45
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.76	0.44
1:B:16:ARG:O	1:B:20:GLU:HG3	2.17	0.44
1:C:83:ASN:C	1:C:85:ARG:H	2.20	0.44
1:B:119:GLU:O	1:B:123:ARG:HG3	2.18	0.44
1:C:30:MET:HE1	2:C:293:GOL:H32	1.98	0.44
1:A:238:PHE:CE2	1:A:269:LEU:HD22	2.52	0.44
1:B:247:ASP:HB3	1:B:250:THR:OG1	2.18	0.44
1:D:71:TYR:HA	1:D:72:PRO:HD3	1.78	0.44
1:D:16[B]:ARG:HD2	1:D:20:GLU:OE2	2.18	0.44
1:D:117:MET:HE1	1:D:251:LEU:O	2.17	0.44
1:A:254:LEU:HA	1:A:254:LEU:HD12	1.82	0.44
1:B:28:PRO:HA	1:B:54:SER:OG	2.18	0.44
1:D:2[A]:LEU:N	1:D:2[A]:LEU:HD23	2.33	0.44
1:D:7:LEU:N	1:D:8:PRO:CD	2.81	0.44
1:D:101:HIS:CB	2:D:292:GOL:H31	2.41	0.43
1:A:71:TYR:HA	1:A:72:PRO:HD3	1.91	0.43
1:C:6:THR:OG1	1:C:8:PRO:HD2	2.17	0.43
1:A:26:LEU:HD12	1:A:27:VAL:N	2.33	0.43
1:C:100:PRO:HB2	1:C:101:HIS:CE1	2.53	0.43
1:C:11[B]:ARG:CD	1:D:169:ASP:OD2	2.66	0.43
1:A:207:VAL:HG23	1:A:236:LYS:HE3	2.01	0.43
1:B:7:LEU:CD2	1:B:140:LEU:HD11	2.43	0.43
1:B:96:GLU:O	1:B:100:PRO:HA	2.19	0.43
1:D:80:GLU:O	1:D:84:LYS:HD3	2.18	0.43
1:A:45:LYS:HG3	1:A:51:VAL:HG21	2.00	0.43
1:B:2:LEU:HD23	1:B:2:LEU:HA	1.69	0.43
1:C:152:ASP:CB	2:C:294:GOL:H2	2.42	0.43
1:A:119:GLU:HG2	1:A:123:ARG:HD3	2.00	0.43
1:B:86:LYS:HD3	1:B:86:LYS:HA	1.83	0.43
1:C:208:MET:CE	1:C:278:GLN:HB2	2.44	0.43
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.62	0.43
1:B:238:PHE:HE2	1:B:274:LEU:HD12	1.84	0.43
1:C:57:VAL:O	1:C:59:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HD13	1:A:171:GLU:HB3	2.01	0.43
1:A:275:ILE:HG12	1:A:275:ILE:O	2.11	0.43
1:B:111:VAL:HG13	1:B:161:LYS:HD2	2.01	0.43
1:A:117:MET:HG3	1:A:118:LEU:HG	2.00	0.43
1:B:74:THR:CG2	1:B:77:GLU:N	2.66	0.43
1:C:186:LEU:HA	1:C:186:LEU:HD23	1.72	0.43
1:A:210:SER:O	1:A:214:LYS:HG3	2.19	0.42
1:A:269:LEU:HD12	1:A:269:LEU:HA	1.73	0.42
1:B:189:ARG:HD3	1:B:189:ARG:HA	1.67	0.42
1:D:123:ARG:HH21	1:D:123:ARG:HG2	1.84	0.42
1:A:45:LYS:CG	1:A:51:VAL:HG21	2.49	0.42
1:B:117:MET:CE	1:B:251:LEU:HB2	2.49	0.42
1:D:245:ILE:HD12	1:D:245:ILE:N	2.34	0.42
1:D:226:ILE:CG1	1:D:245:ILE:CD1	2.97	0.42
1:D:7:LEU:HA	1:D:7:LEU:HD23	1.83	0.42
1:B:197:GLN:NE2	1:B:270:GLY:HA3	2.35	0.42
1:C:282:LEU:HA	1:C:282:LEU:HD12	1.79	0.42
1:A:148:PHE:HB2	1:A:156:LEU:HD13	2.02	0.42
1:C:266:ALA:HA	1:C:274:LEU:O	2.20	0.42
1:B:11[A]:ARG:HD2	6:B:383:HOH:O	2.19	0.41
1:B:7:LEU:HB2	1:B:8:PRO:HD3	2.01	0.41
1:C:119:GLU:OE1	2:C:294:GOL:H31	2.21	0.41
1:A:238:PHE:HE2	1:A:274:LEU:HD12	1.85	0.41
1:D:118:LEU:HD21	1:D:246:ARG:NH2	2.35	0.41
1:A:13:HIS:CE1	1:A:16:ARG:HH21	2.37	0.41
1:A:273:ARG:O	1:A:273:ARG:HG2	2.21	0.41
1:B:111:VAL:HA	1:B:112:PRO:HD3	1.85	0.41
1:B:26:LEU:HD12	1:B:27:VAL:H	1.86	0.41
1:C:26:LEU:HD12	1:C:27:VAL:H	1.84	0.41
1:D:28:PRO:HA	1:D:54:SER:OG	2.21	0.41
1:A:2:LEU:HD23	1:A:2:LEU:HA	1.70	0.41
1:D:82:LEU:HD23	1:D:82:LEU:HA	1.89	0.41
1:A:119:GLU:OE2	1:A:123:ARG:NH1	2.44	0.41
1:C:7:LEU:HG	1:C:97:GLU:OE2	2.19	0.41
1:D:194:THR:OG1	1:D:197:GLN:HB2	2.20	0.41
1:B:19:GLN:NE2	2:C:296:GOL:H31	2.35	0.41
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.94	0.41
1:D:260[B]:ARG:HB2	1:D:260[B]:ARG:HE	1.69	0.41
1:B:177:ILE:HD12	6:B:300:HOH:O	2.20	0.41
1:A:154:GLN:HG3	1:A:251:LEU:CD1	2.51	0.41
1:A:16:ARG:CD	1:A:20:GLU:OE2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:HA	1:A:65:PRO:HD3	1.86	0.41
1:B:118:LEU:N	1:B:118:LEU:HD23	2.36	0.41
1:B:197:GLN:HE22	1:B:270:GLY:HA3	1.84	0.41
1:C:103:LEU:HD23	1:C:103:LEU:N	2.36	0.41
1:D:114:LEU:HD23	1:D:114:LEU:HA	1.89	0.41
1:D:64:ARG:N	1:D:65:PRO:HD3	2.35	0.41
1:C:11[B]:ARG:HH22	1:C:142:GLN:NE2	2.17	0.41
1:C:26:LEU:HD12	1:C:27:VAL:N	2.36	0.41
1:B:207:VAL:HG21	1:B:233:LEU:HG	2.03	0.40
1:C:250:THR:HG22	1:C:252:LEU:HB2	2.01	0.40
1:A:251:LEU:HA	1:A:251:LEU:HD23	1.88	0.40
1:A:161:LYS:HE2	2:B:294:GOL:H12	2.02	0.40
1:D:2[B]:LEU:CD2	1:D:4:ILE:CD1	2.99	0.40
1:D:60:MET:HG3	1:D:103:LEU:CD2	2.37	0.40
1:B:219:ASN:C	1:B:219:ASN:OD1	2.60	0.40
1:C:83:ASN:C	1:C:85:ARG:N	2.74	0.40
1:A:212:ALA:HB1	1:A:280:VAL:HG21	2.03	0.40
1:B:145:ILE:HG12	1:B:146:ALA:N	2.28	0.40
1:B:70:ARG:HB2	1:B:71:TYR:CD2	2.56	0.40
1:C:142:GLN:HE22	2:D:285:GOL:H31	1.86	0.40
1:C:259:LYS:HE3	1:C:260:ARG:HH21	1.85	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	284/287 (99%)	274 (96%)	10 (4%)	0	100	100
1	B	285/287 (99%)	276 (97%)	9 (3%)	0	100	100
1	C	284/287 (99%)	266 (94%)	17 (6%)	1 (0%)	34	60
1	D	287/287 (100%)	273 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1140/1148 (99%)	1089 (96%)	50 (4%)	1 (0%)	51 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	270	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	242/243 (100%)	228 (94%)	14 (6%)	20 43
1	B	243/243 (100%)	225 (93%)	18 (7%)	13 32
1	C	243/243 (100%)	223 (92%)	20 (8%)	11 26
1	D	246/243 (101%)	229 (93%)	17 (7%)	15 35
All	All	974/972 (100%)	905 (93%)	69 (7%)	14 34

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	63	ASP
1	A	64	ARG
1	A	66	ASP
1	A	76	GLN
1	A	140	LEU
1	A	155	GLN
1	A	239	ARG
1	A	253	GLU
1	A	254	LEU
1	A	257	THR
1	A	258	SER
1	A	275	ILE
1	A	280	VAL

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Mol	Chain	Res	Type
1	B	-1	ASN
1	B	9	LEU
1	B	19	GLN
1	B	45	LYS
1	B	52	ILE
1	B	64	ARG
1	B	67	ASP
1	B	74	THR
1	B	77	GLU
1	B	96	GLU
1	B	123	ARG
1	B	140	LEU
1	B	145	ILE
1	B	158	LEU
1	B	161	LYS
1	B	269	LEU
1	B	275	ILE
1	B	277	ASN
1	C	2	LEU
1	C	6	THR
1	C	18	ARG
1	C	35	ASP
1	C	63	ASP
1	C	67	ASP
1	C	69	VAL
1	C	85	ARG
1	C	104	GLU
1	C	155	GLN
1	C	199	LYS
1	C	216	ILE
1	C	221	GLU
1	C	235	GLU
1	C	244	GLN
1	C	259	LYS
1	C	269	LEU
1	C	271	GLN
1	C	281	THR
1	C	282	LEU
1	D	15	ARG
1	D	57	VAL
1	D	68	LEU
1	D	69	VAL

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Mol	Chain	Res	Type
1	D	70	ARG
1	D	74	THR
1	D	86	LYS
1	D	96	GLU
1	D	145	ILE
1	D	151	LYS
1	D	155	GLN
1	D	167	SER
1	D	214	LYS
1	D	222	LEU
1	D	231	GLN
1	D	244	GLN
1	D	246	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	278	GLN
1	B	13	HIS
1	B	19	GLN
1	B	83	ASN
1	B	106	GLN
1	B	155	GLN
1	B	271	GLN
1	B	278	GLN
1	C	12	GLN
1	C	13	HIS
1	C	83	ASN
1	C	126	HIS
1	C	142	GLN
1	C	155	GLN
1	C	209	ASN
1	C	271	GLN
1	C	278	GLN
1	D	190	ASN
1	D	278	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

24 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	$\# Z  > 2$
2	GOL	A	291	-	5,5,5	0.35	0	5,5,5	0.40	0
4	SO4	A	297	-	4,4,4	0.14	0	6,6,6	0.06	0
2	GOL	B	296	-	5,5,5	0.37	0	5,5,5	0.25	0
2	GOL	D	292	-	5,5,5	0.37	0	5,5,5	0.33	0
2	GOL	A	294	-	5,5,5	0.31	0	5,5,5	0.37	0
2	GOL	B	294	-	5,5,5	0.40	0	5,5,5	0.30	0
3	EOH	A	298	-	2,2,2	0.43	0	1,1,1	0.19	0
2	GOL	B	291	-	5,5,5	0.38	0	5,5,5	0.47	0
3	EOH	C	295	-	2,2,2	0.46	0	1,1,1	0.17	0
3	EOH	A	292	-	2,2,2	0.48	0	1,1,1	0.05	0
2	GOL	C	296	-	5,5,5	0.35	0	5,5,5	0.36	0
2	GOL	C	292	-	5,5,5	0.37	0	5,5,5	0.37	0
3	EOH	A	296	-	2,2,2	0.49	0	1,1,1	0.03	0
4	SO4	A	293	-	4,4,4	0.14	0	6,6,6	0.11	0
2	GOL	D	291	-	5,5,5	0.36	0	5,5,5	0.29	0
2	GOL	D	285	-	5,5,5	0.43	0	5,5,5	0.20	0
2	GOL	B	292	-	5,5,5	0.42	0	5,5,5	0.44	0
2	GOL	C	294	-	5,5,5	0.38	0	5,5,5	0.12	0
2	GOL	D	293	-	5,5,5	0.37	0	5,5,5	0.30	0
2	GOL	B	295	-	5,5,5	0.40	0	5,5,5	0.39	0
5	ACY	A	295	-	1,3,3	1.73	0	0,3,3	0.00	-
2	GOL	C	293	-	5,5,5	0.36	0	5,5,5	0.23	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	B	293	-	5,5,5	0.33	0	5,5,5	0.29	0
3	EOH	B	297	-	2,2,2	0.47	0	1,1,1	0.09	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	D	291	-	-	2/4/4/4	-
2	GOL	A	291	-	-	2/4/4/4	-
2	GOL	B	295	-	-	3/4/4/4	-
2	GOL	B	296	-	-	2/4/4/4	-
2	GOL	B	291	-	-	2/4/4/4	-
2	GOL	D	292	-	-	2/4/4/4	-
2	GOL	A	294	-	-	4/4/4/4	-
2	GOL	B	292	-	-	4/4/4/4	-
2	GOL	C	294	-	-	4/4/4/4	-
2	GOL	D	285	-	-	2/4/4/4	-
2	GOL	C	293	-	-	2/4/4/4	-
2	GOL	D	293	-	-	2/4/4/4	-
2	GOL	B	293	-	-	2/4/4/4	-
2	GOL	B	294	-	-	0/4/4/4	-
2	GOL	C	296	-	-	2/4/4/4	-
2	GOL	C	292	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	291	GOL	O1-C1-C2-O2
2	A	291	GOL	O1-C1-C2-C3
2	B	296	GOL	O1-C1-C2-C3
2	B	291	GOL	O1-C1-C2-C3
2	C	292	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	D	291	GOL	O1-C1-C2-C3
2	B	292	GOL	O1-C1-C2-C3
2	B	292	GOL	C1-C2-C3-O3
2	C	294	GOL	O1-C1-C2-O2
2	C	294	GOL	O1-C1-C2-C3
2	C	293	GOL	O1-C1-C2-C3
2	B	293	GOL	O1-C1-C2-C3
2	D	292	GOL	O1-C1-C2-C3
2	A	294	GOL	O1-C1-C2-C3
2	A	294	GOL	C1-C2-C3-O3
2	D	285	GOL	O1-C1-C2-C3
2	C	294	GOL	C1-C2-C3-O3
2	D	293	GOL	O1-C1-C2-C3
2	B	295	GOL	C1-C2-C3-O3
2	D	285	GOL	O1-C1-C2-O2
2	B	292	GOL	O1-C1-C2-O2
2	B	292	GOL	O2-C2-C3-O3
2	B	293	GOL	O1-C1-C2-O2
2	B	296	GOL	O1-C1-C2-O2
2	A	294	GOL	O1-C1-C2-O2
2	A	294	GOL	O2-C2-C3-O3
2	B	291	GOL	O1-C1-C2-O2
2	C	293	GOL	O1-C1-C2-O2
2	C	296	GOL	O1-C1-C2-O2
2	C	292	GOL	O1-C1-C2-O2
2	D	293	GOL	O1-C1-C2-O2
2	D	292	GOL	O1-C1-C2-O2
2	D	291	GOL	O1-C1-C2-O2
2	C	294	GOL	O2-C2-C3-O3
2	B	295	GOL	O2-C2-C3-O3
2	C	296	GOL	O1-C1-C2-C3
2	B	295	GOL	O1-C1-C2-C3

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	292	GOL	3	0
2	B	294	GOL	3	0
3	A	298	EOH	1	0
2	B	291	GOL	1	0
2	C	296	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	292	GOL	2	0
2	D	285	GOL	2	0
2	C	294	GOL	7	0
2	B	295	GOL	3	0
2	C	293	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<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	285/287 (99%)	-0.54	1 (0%) 92 93	28, 46, 82, 150	0
1	B	285/287 (99%)	-0.40	1 (0%) 92 93	29, 53, 90, 120	0
1	C	283/287 (98%)	-0.18	4 (1%) 75 77	39, 70, 111, 159	0
1	D	284/287 (98%)	-0.10	12 (4%) 36 35	49, 70, 121, 147	0
All	All	1137/1148 (99%)	-0.31	18 (1%) 72 74	28, 61, 107, 159	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	217	ALA	4.1
1	B	283	ALA	3.9
1	D	218	GLY	3.6
1	C	191	ALA	3.5
1	D	222	LEU	3.4
1	D	214	LYS	3.2
1	C	70	ARG	3.1
1	C	66	ASP	2.5
1	A	192	TYR	2.4
1	D	210	SER	2.2
1	D	104	GLU	2.2
1	D	224	GLU	2.1
1	D	221	GLU	2.1
1	D	228	ILE	2.1
1	C	135	SER	2.1
1	D	226	ILE	2.1
1	D	220	ARG	2.0
1	D	216	ILE	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 ⓘ

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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	294	6/6	0.37	0.64	113,116,122,123	0
2	GOL	D	285	6/6	0.56	0.43	93,102,107,110	0
3	EOH	A	292	3/3	0.67	0.29	63,63,65,76	0
2	GOL	B	293	6/6	0.70	0.23	102,106,109,110	0
2	GOL	B	296	6/6	0.76	0.35	98,107,114,115	0
2	GOL	B	295	6/6	0.78	0.49	50,79,82,85	0
2	GOL	C	296	6/6	0.82	0.37	97,100,113,118	0
2	GOL	A	294	6/6	0.84	0.31	64,78,94,101	0
2	GOL	C	293	6/6	0.85	0.24	110,112,114,115	0
4	SO4	A	293	5/5	0.87	0.26	111,127,128,132	0
2	GOL	D	291	6/6	0.88	0.38	107,113,116,118	0
4	SO4	A	297	5/5	0.88	0.17	134,140,144,150	0
3	EOH	B	297	3/3	0.88	0.44	72,72,76,76	0
3	EOH	C	295	3/3	0.90	0.49	78,78,84,88	0
2	GOL	B	294	6/6	0.92	0.31	55,74,76,77	0
2	GOL	D	293	6/6	0.92	0.23	64,71,92,104	0
2	GOL	D	292	6/6	0.93	0.20	71,78,78,81	0
3	EOH	A	298	3/3	0.94	0.37	63,63,68,69	0
2	GOL	B	291	6/6	0.94	0.27	79,90,94,100	0
3	EOH	A	296	3/3	0.95	0.13	54,54,61,67	0
5	ACY	A	295	4/4	0.96	0.22	65,66,75,76	0
2	GOL	C	292	6/6	0.96	0.27	66,81,87,95	0
2	GOL	B	292	6/6	0.97	0.17	37,50,60,62	0
2	GOL	A	291	6/6	0.97	0.28	42,52,55,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.