



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:32 pm BST

PDB ID : 6DWO  
Title : Crystal structure of alpha-1-2-mannosidase from Enterococcus faecalis V583  
Authors : Fisher, A.J.; Li, Y.  
Deposited on : 2018-06-26  
Resolution : 2.15 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

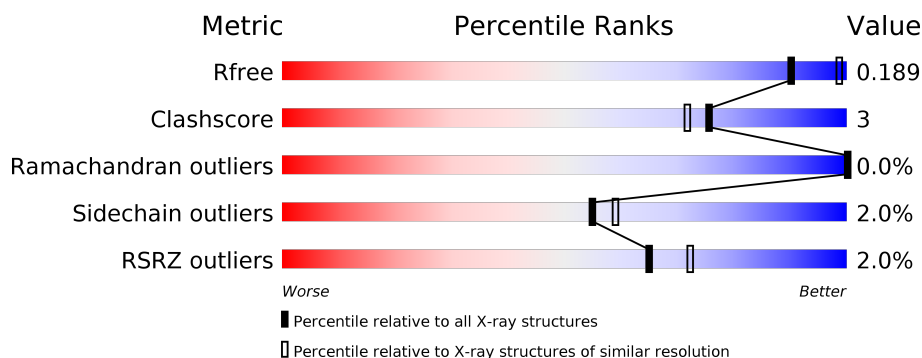
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	721	<div> <div>2%</div> <div>92%</div> <div>7%</div> </div>
1	B	721	<div> <div>2%</div> <div>92%</div> <div>6%</div> </div>
1	C	721	<div> <div>3%</div> <div>93%</div> <div>6%</div> </div>
1	D	721	<div> <div>2%</div> <div>92%</div> <div>6%</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	A	807	-	-	X	-
2	GOL	B	1006	-	-	X	-
2	GOL	B	1009	-	X	-	-
2	GOL	C	1005	-	-	X	-
2	GOL	C	1007	-	-	X	-
2	GOL	D	1006	-	-	X	-
2	GOL	D	1009	-	-	X	-
5	ACT	A	805	-	-	X	-
5	ACT	C	1003	-	-	X	-
5	ACT	D	1005	-	-	X	-
6	PO4	B	1011	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24774 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 Alpha-1,2-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	712	Total	C	N	O	S	0	3	0
			5781	3710	944	1106	21			
1	B	712	Total	C	N	O	S	0	0	0
			5766	3700	944	1101	21			
1	C	712	Total	C	N	O	S	0	0	0
			5766	3700	944	1101	21			
1	D	712	Total	C	N	O	S	0	0	0
			5766	3700	944	1101	21			

There are 32 discrepancies between the modelled and reference sequences:

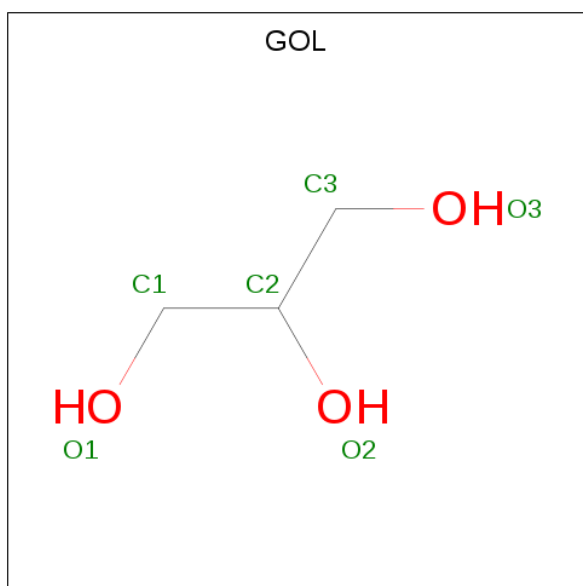
Chain	Residue	Modelled	Actual	Comment	Reference
A	714	LEU	-	expression tag	UNP Q832K9
A	715	GLU	-	expression tag	UNP Q832K9
A	716	HIS	-	expression tag	UNP Q832K9
A	717	HIS	-	expression tag	UNP Q832K9
A	718	HIS	-	expression tag	UNP Q832K9
A	719	HIS	-	expression tag	UNP Q832K9
A	720	HIS	-	expression tag	UNP Q832K9
A	721	HIS	-	expression tag	UNP Q832K9
B	714	LEU	-	expression tag	UNP Q832K9
B	715	GLU	-	expression tag	UNP Q832K9
B	716	HIS	-	expression tag	UNP Q832K9
B	717	HIS	-	expression tag	UNP Q832K9
B	718	HIS	-	expression tag	UNP Q832K9
B	719	HIS	-	expression tag	UNP Q832K9
B	720	HIS	-	expression tag	UNP Q832K9
B	721	HIS	-	expression tag	UNP Q832K9
C	714	LEU	-	expression tag	UNP Q832K9
C	715	GLU	-	expression tag	UNP Q832K9
C	716	HIS	-	expression tag	UNP Q832K9
C	717	HIS	-	expression tag	UNP Q832K9
C	718	HIS	-	expression tag	UNP Q832K9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	719	HIS	-	expression tag	UNP Q832K9
C	720	HIS	-	expression tag	UNP Q832K9
C	721	HIS	-	expression tag	UNP Q832K9
D	714	LEU	-	expression tag	UNP Q832K9
D	715	GLU	-	expression tag	UNP Q832K9
D	716	HIS	-	expression tag	UNP Q832K9
D	717	HIS	-	expression tag	UNP Q832K9
D	718	HIS	-	expression tag	UNP Q832K9
D	719	HIS	-	expression tag	UNP Q832K9
D	720	HIS	-	expression tag	UNP Q832K9
D	721	HIS	-	expression tag	UNP Q832K9

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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	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		

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

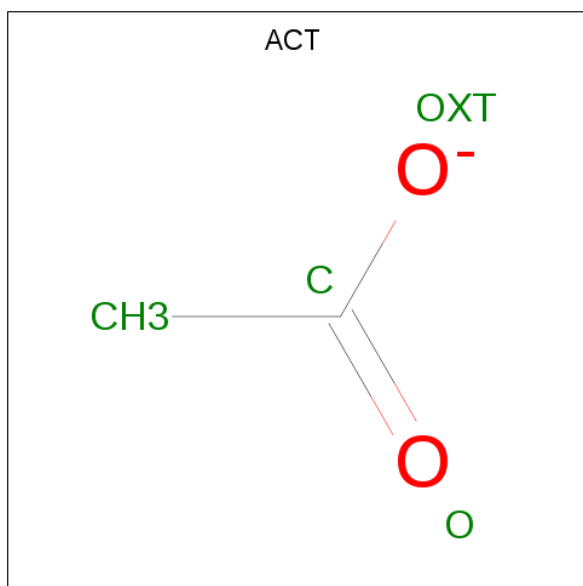
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total K 1 1	0	0
4	A	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total K 1 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



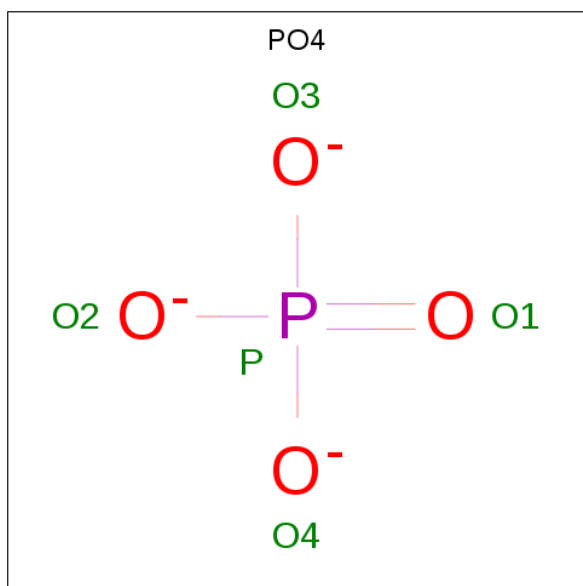
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



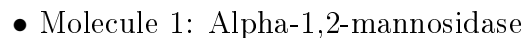
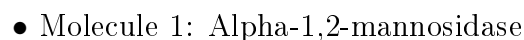
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

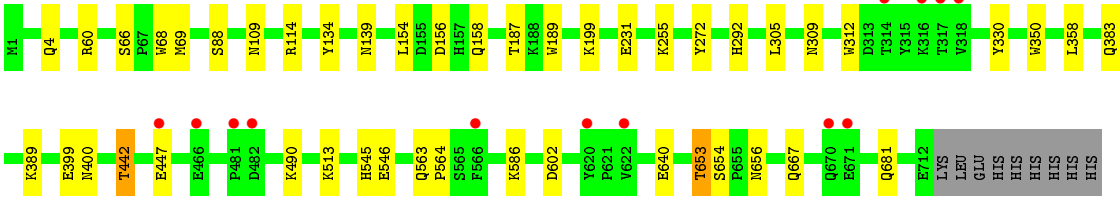
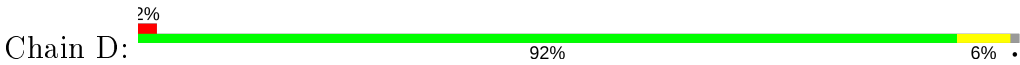
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	407	Total	O	0	0
			407	407		
7	B	415	Total	O	0	0
			415	415		
7	C	355	Total	O	0	0
			355	355		
7	D	360	Total	O	0	0
			360	360		



- Molecule 1: Alpha-1,2-mannosidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.35Å 168.99Å 258.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.18 – 2.15 39.15 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.18-2.15) 99.0 (39.15-2.15)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.155 , 0.189 0.155 , 0.189	Depositor DCC
$R_{free}$ test set	9643 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	24774	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, K, CA, PO4, ACT

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	0.47	0/5962	0.73	1/8106 (0.0%)
1	B	0.45	0/5938	0.72	0/8073
1	C	0.45	0/5938	0.73	2/8073 (0.0%)
1	D	0.44	0/5938	0.72	1/8073 (0.0%)
All	All	0.45	0/23776	0.72	4/32325 (0.0%)

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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	15	GLN	CB-CA-C	-7.76	94.88	110.40
1	C	231	GLU	CB-CA-C	-6.14	98.11	110.40
1	D	231	GLU	CB-CA-C	-6.10	98.20	110.40
1	A	453	ARG	NE-CZ-NH1	5.63	123.11	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	301	ARG	Sidechain
1	C	235	ARG	Sidechain

## 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	5781	0	5483	33	0
1	B	5766	0	5466	36	0
1	C	5766	0	5466	32	0
1	D	5766	0	5466	35	0
2	A	24	0	31	8	0
2	B	24	0	31	11	0
2	C	24	0	31	12	0
2	D	24	0	31	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	12	0	9	3	0
5	B	12	0	9	2	0
5	C	8	0	6	3	0
5	D	12	0	9	4	0
6	B	10	0	0	2	0
7	A	407	0	0	7	1
7	B	415	0	0	9	1
7	C	355	0	0	5	0
7	D	360	0	0	7	0
All	All	24774	0	22038	140	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 3.

All (140) 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:D:546:GLU:OE1	2:D:1006:GOL:H31	1.63	0.98
1:B:545:HIS:NE2	2:B:1006:GOL:H31	1.84	0.92
1:D:114:ARG:HE	5:D:1005:ACT:H3	1.37	0.89
1:B:17:SER:HB3	6:B:1011:PO4:O3	1.72	0.88
1:D:442:THR:CG2	7:D:1447:HOH:O	2.24	0.84
1:C:545:HIS:NE2	2:C:1005:GOL:H31	1.97	0.80
1:D:114:ARG:HE	5:D:1005:ACT:CH3	1.95	0.79
1:C:68:TRP:CD1	2:C:1005:GOL:H12	2.19	0.78
1:C:60:ARG:HH12	2:C:1007:GOL:H31	1.50	0.76
1:C:653:THR:HG23	1:C:654:SER:O	1.88	0.74
1:A:704:GLU:OE1	7:A:901:HOH:O	2.06	0.73
1:B:710:SER:HB3	7:B:1140:HOH:O	1.88	0.72
2:B:1006:GOL:H11	7:B:1429:HOH:O	1.89	0.72
1:B:602:ASP:OD2	2:B:1006:GOL:C1	2.38	0.72
1:A:653:THR:HG23	1:A:654:SER:O	1.90	0.70
1:B:653:THR:HG23	1:B:654:SER:O	1.90	0.70
1:D:60:ARG:HH12	2:D:1009:GOL:H12	1.56	0.70
1:D:653:THR:HG23	1:D:654:SER:O	1.91	0.70
1:D:60:ARG:HH22	2:D:1009:GOL:H32	1.57	0.68
1:D:383:GLN:HG3	7:D:1283:HOH:O	1.94	0.68
1:D:602:ASP:OD2	2:D:1006:GOL:H11	1.93	0.68
1:B:301:ARG:HD2	1:D:189:TRP:CZ3	2.28	0.67
1:A:545:HIS:NE2	2:A:807:GOL:H31	2.08	0.67
1:B:602:ASP:OD2	2:B:1006:GOL:H12	1.94	0.66
1:B:46:SER:HA	2:B:1009:GOL:H11	1.77	0.66
5:D:1003:ACT:H3	7:D:1386:HOH:O	1.95	0.66
1:A:68:TRP:CD1	2:A:807:GOL:H12	2.30	0.66
1:B:99:GLU:OE1	7:B:1101:HOH:O	2.13	0.65
1:A:653:THR:CG2	1:A:654:SER:O	2.47	0.62
1:D:68:TRP:CD1	2:D:1006:GOL:H12	2.34	0.62
1:C:653:THR:HG21	1:C:656:ASN:HB2	1.80	0.62
1:A:156:ASP:HB3	1:A:189:TRP:CZ2	2.35	0.62
1:B:546:GLU:OE2	2:B:1006:GOL:H2	2.00	0.62
1:C:653:THR:CG2	1:C:654:SER:O	2.47	0.62
5:C:1004:ACT:H1	7:C:1272:HOH:O	1.99	0.62
1:B:653:THR:HG21	1:B:656:ASN:HB2	1.83	0.61
1:B:653:THR:CG2	1:B:654:SER:O	2.48	0.61
1:D:653:THR:CG2	1:D:654:SER:O	2.48	0.61
1:A:68:TRP:NE1	2:A:807:GOL:H12	2.16	0.61
1:B:545:HIS:NE2	2:B:1006:GOL:C3	2.61	0.61
1:C:384:PHE:C	1:C:388:MET:HE2	2.21	0.60
1:D:653:THR:HG21	1:D:656:ASN:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:TRP:HA	5:C:1003:ACT:H3	1.83	0.60
1:B:54:ARG:NH2	7:B:1104:HOH:O	2.35	0.60
1:A:286[B]:GLU:OE2	7:A:902:HOH:O	2.17	0.59
1:A:653:THR:HG21	1:A:656:ASN:HB2	1.83	0.59
1:D:442:THR:HG21	7:D:1447:HOH:O	1.99	0.59
1:D:154:LEU:HD12	1:D:158:GLN:HG2	1.85	0.57
1:D:88:SER:HA	1:D:199:LYS:HE2	1.87	0.57
1:C:54:ARG:NH2	7:C:1104:HOH:O	2.37	0.56
1:B:653:THR:CG2	1:B:656:ASN:HB2	2.36	0.56
1:A:420:HIS:HE1	7:A:1169:HOH:O	1.88	0.56
1:A:14:ASN:HD22	5:A:805:ACT:H1	1.71	0.55
1:C:653:THR:CG2	1:C:656:ASN:HB2	2.35	0.55
1:C:546:GLU:OE2	2:C:1005:GOL:H2	2.07	0.55
1:C:384:PHE:O	1:C:388:MET:HE2	2.07	0.55
1:B:302:PRO:HB2	1:D:187:THR:O	2.07	0.54
1:A:14:ASN:HD22	5:A:805:ACT:CH3	2.21	0.54
1:A:653:THR:CG2	1:A:656:ASN:HB2	2.38	0.54
1:A:405:GLY:HA2	7:A:1138:HOH:O	2.08	0.53
1:A:702:THR:HG22	7:A:1264:HOH:O	2.08	0.53
1:A:359:MET:HG3	2:A:808:GOL:H11	1.91	0.52
1:D:653:THR:CG2	1:D:656:ASN:HB2	2.38	0.52
5:B:1004:ACT:H1	7:B:1487:HOH:O	2.09	0.52
1:A:312:TRP:CZ3	2:A:808:GOL:H32	2.44	0.52
1:C:602:ASP:OD2	2:C:1005:GOL:H11	2.09	0.52
1:A:54:ARG:NH2	7:A:907:HOH:O	2.42	0.52
1:D:312:TRP:CZ3	2:D:1007:GOL:H32	2.45	0.51
2:C:1005:GOL:O1	2:C:1006:GOL:H2	2.10	0.51
1:B:301:ARG:CD	1:D:189:TRP:CZ3	2.93	0.50
1:C:602:ASP:OD2	2:C:1005:GOL:C1	2.61	0.49
1:C:49:PHE:O	5:C:1003:ACT:H1	2.12	0.49
1:C:153:GLN:HE21	1:C:156:ASP:HA	1.77	0.49
1:C:383:GLN:HG3	7:C:1332:HOH:O	2.12	0.49
1:B:68:TRP:CE2	2:B:1006:GOL:H32	2.47	0.48
1:B:692:GLN:OE1	7:B:1102:HOH:O	2.19	0.48
1:C:292:HIS:CD2	1:C:305:LEU:HD22	2.48	0.48
1:D:156:ASP:HB3	1:D:189:TRP:CZ2	2.49	0.48
1:D:114:ARG:NE	5:D:1005:ACT:H3	2.18	0.48
1:D:60:ARG:NH2	2:D:1009:GOL:H32	2.26	0.48
1:C:385:LEU:HA	1:C:388:MET:HE3	1.96	0.48
1:D:292:HIS:CD2	1:D:305:LEU:HD22	2.50	0.47
1:D:68:TRP:CD1	2:D:1006:GOL:C1	2.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:GLN:NE2	7:C:1105:HOH:O	2.40	0.47
1:D:4:GLN:HG2	7:D:1208:HOH:O	2.15	0.47
1:B:292:HIS:CD2	1:B:305:LEU:HD22	2.49	0.47
1:C:60:ARG:HH12	2:C:1007:GOL:C3	2.23	0.47
1:D:545:HIS:NE2	2:D:1006:GOL:H32	2.30	0.47
1:D:545:HIS:NE2	2:D:1006:GOL:C3	2.78	0.47
1:B:17:SER:CB	6:B:1011:PO4:O3	2.53	0.46
1:D:400:ASN:HB2	7:D:1344:HOH:O	2.15	0.46
1:D:389:LYS:NZ	7:D:1106:HOH:O	2.40	0.46
1:C:519:LEU:HD23	1:C:519:LEU:O	2.16	0.45
1:A:292:HIS:CD2	1:A:305:LEU:HD22	2.51	0.45
1:A:4:GLN:HG2	7:A:965:HOH:O	2.17	0.45
1:B:152:LYS:NZ	1:B:221:GLU:OE2	2.49	0.45
2:B:1006:GOL:O1	2:B:1007:GOL:H2	2.17	0.45
1:C:4:GLN:HG2	7:C:1227:HOH:O	2.16	0.45
1:B:602:ASP:OD2	2:B:1006:GOL:H11	2.15	0.44
1:A:347:LEU:HB3	1:A:364:ILE:HG21	2.00	0.44
1:D:69:MET:SD	1:D:358:LEU:HD12	2.58	0.44
1:A:14:ASN:ND2	5:A:805:ACT:H1	2.32	0.44
1:B:347:LEU:HB3	1:B:364:ILE:HG21	1.99	0.44
1:B:420:HIS:HE1	7:B:1420:HOH:O	2.01	0.43
1:A:709:LEU:HD23	1:A:709:LEU:HA	1.86	0.43
1:A:359:MET:CG	2:A:808:GOL:H11	2.48	0.43
1:B:586:LYS:NZ	1:B:656:ASN:OD1	2.48	0.43
1:B:69:MET:SD	1:B:358:LEU:HD12	2.59	0.43
1:C:586:LYS:NZ	1:C:656:ASN:OD1	2.49	0.43
1:C:68:TRP:NE1	2:C:1005:GOL:H12	2.33	0.43
1:B:72:PHE:HA	1:B:166:TYR:HA	2.00	0.43
1:B:710:SER:CB	7:B:1140:HOH:O	2.58	0.43
1:D:586:LYS:NZ	1:D:656:ASN:OD1	2.50	0.43
1:C:385:LEU:HA	1:C:388:MET:CE	2.47	0.43
1:D:60:ARG:HH22	2:D:1009:GOL:C3	2.29	0.43
1:A:69:MET:SD	1:A:358:LEU:HD12	2.59	0.43
1:C:388:MET:HB3	1:C:436:ILE:HG12	2.02	0.42
1:C:60:ARG:NH1	2:C:1007:GOL:H31	2.27	0.42
1:A:586:LYS:NZ	1:A:656:ASN:OD1	2.51	0.42
1:B:685:ASN:HA	1:B:685:ASN:HD22	1.67	0.42
1:A:226:LEU:HD22	1:A:286[A]:GLU:HG3	2.02	0.42
1:C:563:GLN:N	1:C:564:PRO:CD	2.83	0.42
1:D:563:GLN:N	1:D:564:PRO:CD	2.83	0.42
1:A:563:GLN:N	1:A:564:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:TRP:CD1	1:A:496:SER:HB3	2.56	0.41
1:B:4:GLN:HG2	7:B:1319:HOH:O	2.19	0.41
1:C:46:SER:HA	2:C:1007:GOL:H11	2.03	0.41
1:D:134:TYR:CE1	1:D:139:ASN:HB3	2.55	0.41
1:B:133:ASP:OD2	5:B:1003:ACT:H2	2.21	0.41
1:B:563:GLN:N	1:B:564:PRO:CD	2.84	0.41
1:A:60:ARG:HH12	2:A:809:GOL:H31	1.85	0.41
1:B:546:GLU:OE2	2:B:1006:GOL:H31	2.21	0.41
1:B:488:TRP:CD1	1:B:496:SER:HB3	2.56	0.41
1:A:2:ASN:ND2	1:A:248:HIS:HE1	2.19	0.41
1:C:69:MET:SD	1:C:358:LEU:HD12	2.61	0.41
1:A:72:PHE:HA	1:A:166:TYR:HA	2.02	0.40
1:A:494:GLU:OE1	2:A:807:GOL:H2	2.20	0.40
1:C:162:LYS:HD2	1:C:177:TYR:CE2	2.56	0.40
1:B:709:LEU:HD23	1:B:709:LEU:HA	1.91	0.40
2:C:1005:GOL:O1	2:C:1006:GOL:C2	2.70	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)
7:A:1270:HOH:O	7:B:1445:HOH:O[7_555]	2.08	0.12

## 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	713/721 (99%)	687 (96%)	26 (4%)	0	100	100
1	B	710/721 (98%)	687 (97%)	23 (3%)	0	100	100
1	C	710/721 (98%)	684 (96%)	26 (4%)	0	100	100
1	D	710/721 (98%)	688 (97%)	21 (3%)	1 (0%)	51	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2843/2884 (99%)	2746 (97%)	96 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	490	LYS

### 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	631/637 (99%)	620 (98%)	11 (2%)	60	65
1	B	628/637 (99%)	616 (98%)	12 (2%)	57	61
1	C	628/637 (99%)	615 (98%)	13 (2%)	53	57
1	D	628/637 (99%)	613 (98%)	15 (2%)	49	51
All	All	2515/2548 (99%)	2464 (98%)	51 (2%)	55	59

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	SER
1	A	85	SER
1	A	272	TYR
1	A	309	ASN
1	A	330	TYR
1	A	350	TRP
1	A	476	GLU
1	A	482	ASP
1	A	513	LYS
1	A	640	GLU
1	A	653	THR
1	B	66	SER
1	B	85	SER
1	B	199	LYS

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Mol	Chain	Res	Type
1	B	272	TYR
1	B	309	ASN
1	B	330	TYR
1	B	350	TRP
1	B	399	GLU
1	B	513	LYS
1	B	640	GLU
1	B	653	THR
1	B	700	GLN
1	C	66	SER
1	C	85	SER
1	C	152	LYS
1	C	188	LYS
1	C	222	LYS
1	C	272	TYR
1	C	309	ASN
1	C	315	TYR
1	C	330	TYR
1	C	350	TRP
1	C	513	LYS
1	C	640	GLU
1	C	653	THR
1	D	66	SER
1	D	109	ASN
1	D	255	LYS
1	D	272	TYR
1	D	309	ASN
1	D	330	TYR
1	D	350	TRP
1	D	399	GLU
1	D	442	THR
1	D	447	GLU
1	D	513	LYS
1	D	640	GLU
1	D	653	THR
1	D	667	GLN
1	D	681	GLN

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	150	GLN

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Mol	Chain	Res	Type
1	B	249	ASN
1	B	298	GLN
1	B	394	GLN
1	B	420	HIS
1	B	454	GLN
1	B	648	GLN
1	B	685	ASN
1	B	700	GLN
1	C	15	GLN
1	C	150	GLN
1	C	241	GLN
1	C	242	GLN
1	C	288	GLN
1	C	400	ASN
1	C	460	GLN
1	C	461	GLN
1	C	648	GLN
1	C	700	GLN
1	D	420	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 8 are monoatomic - leaving 29 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	$\# Z  > 2$
5	ACT	D	1004	-	1,3,3	4.38	1 (100%)	0,3,3	0.00	-
5	ACT	A	804	-	1,3,3	6.52	1 (100%)	0,3,3	0.00	-
2	GOL	D	1007	3	5,5,5	0.40	0	5,5,5	0.56	0
2	GOL	B	1007	3	5,5,5	0.27	0	5,5,5	1.02	0
2	GOL	B	1009	-	5,5,5	1.24	1 (20%)	5,5,5	2.05	4 (80%)
6	PO4	B	1011	-	4,4,4	0.91	0	6,6,6	0.77	0
5	ACT	C	1003	-	1,3,3	4.41	1 (100%)	0,3,3	0.00	-
2	GOL	A	807	-	5,5,5	1.00	0	5,5,5	1.85	1 (20%)
5	ACT	D	1005	-	1,3,3	1.24	0	0,3,3	0.00	-
5	ACT	B	1004	-	1,3,3	7.47	1 (100%)	0,3,3	0.00	-
5	ACT	C	1004	-	1,3,3	6.76	1 (100%)	0,3,3	0.00	-
5	ACT	D	1003	-	1,3,3	2.69	1 (100%)	0,3,3	0.00	-
5	ACT	B	1003	-	1,3,3	1.69	0	0,3,3	0.00	-
2	GOL	A	808	3	5,5,5	0.18	0	5,5,5	0.55	0
2	GOL	C	1005	-	5,5,5	0.82	0	5,5,5	1.74	1 (20%)
2	GOL	A	801	-	5,5,5	0.91	0	5,5,5	1.02	0
5	ACT	A	806	-	1,3,3	6.99	1 (100%)	0,3,3	0.00	-
2	GOL	C	1007	-	5,5,5	0.75	0	5,5,5	1.55	1 (20%)
6	PO4	B	1010	-	4,4,4	0.54	0	6,6,6	0.79	0
2	GOL	D	1006	3	5,5,5	0.79	0	5,5,5	1.34	1 (20%)
2	GOL	C	1006	3	5,5,5	0.38	0	5,5,5	0.96	0
2	GOL	B	1006	-	5,5,5	1.21	0	5,5,5	2.10	1 (20%)
2	GOL	D	1008	-	5,5,5	0.88	0	5,5,5	1.05	0
2	GOL	C	1008	-	5,5,5	0.49	0	5,5,5	1.11	0
5	ACT	A	805	-	1,3,3	2.81	1 (100%)	0,3,3	0.00	-
2	GOL	D	1009	-	5,5,5	0.99	0	5,5,5	1.45	1 (20%)
2	GOL	A	809	-	5,5,5	0.83	0	5,5,5	0.87	0
5	ACT	B	1005	-	1,3,3	6.43	1 (100%)	0,3,3	0.00	-
2	GOL	B	1008	-	5,5,5	0.71	0	5,5,5	0.77	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	C	1008	-	-	4/4/4/4	-
2	GOL	D	1007	3	-	3/4/4/4	-
2	GOL	B	1007	3	-	0/4/4/4	-
2	GOL	B	1006	-	-	2/4/4/4	-
2	GOL	A	808	3	-	1/4/4/4	-
2	GOL	C	1005	-	-	0/4/4/4	-
2	GOL	B	1009	-	-	2/4/4/4	-
2	GOL	A	801	-	-	3/4/4/4	-
2	GOL	A	807	-	-	2/4/4/4	-
2	GOL	D	1006	3	-	4/4/4/4	-
2	GOL	D	1009	-	-	4/4/4/4	-
2	GOL	A	809	-	-	0/4/4/4	-
2	GOL	B	1008	-	-	1/4/4/4	-
2	GOL	C	1007	-	-	2/4/4/4	-
2	GOL	C	1006	3	-	0/4/4/4	-
2	GOL	D	1008	-	-	0/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1004	ACT	CH3-C	7.47	1.58	1.48
5	A	806	ACT	CH3-C	6.99	1.57	1.48
5	C	1004	ACT	CH3-C	6.76	1.57	1.48
5	A	804	ACT	CH3-C	6.52	1.57	1.48
5	B	1005	ACT	CH3-C	6.43	1.56	1.48
5	C	1003	ACT	CH3-C	4.41	1.54	1.48
5	D	1004	ACT	CH3-C	4.38	1.54	1.48
5	A	805	ACT	CH3-C	2.81	1.52	1.48
5	D	1003	ACT	CH3-C	2.69	1.52	1.48
2	B	1009	GOL	C3-C2	2.29	1.61	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1006	GOL	O1-C1-C2	4.10	129.88	110.20
2	A	807	GOL	O1-C1-C2	3.51	127.01	110.20
2	C	1005	GOL	O1-C1-C2	3.33	126.18	110.20
2	D	1009	GOL	O3-C3-C2	2.48	122.10	110.20
2	B	1009	GOL	O3-C3-C2	2.47	122.05	110.20
2	C	1007	GOL	O2-C2-C1	-2.44	98.40	109.12
2	B	1009	GOL	O2-C2-C3	2.42	119.78	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1006	GOL	O1-C1-C2	2.36	121.50	110.20
2	B	1009	GOL	O2-C2-C1	-2.13	99.76	109.12
2	B	1009	GOL	C3-C2-C1	2.10	119.88	111.70

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1009	GOL	C1-C2-C3-O3
2	A	807	GOL	C1-C2-C3-O3
2	A	801	GOL	C1-C2-C3-O3
2	C	1007	GOL	C1-C2-C3-O3
2	D	1006	GOL	O1-C1-C2-C3
2	D	1006	GOL	C1-C2-C3-O3
2	C	1008	GOL	O1-C1-C2-C3
2	D	1009	GOL	O1-C1-C2-C3
2	D	1009	GOL	C1-C2-C3-O3
2	C	1007	GOL	O2-C2-C3-O3
2	D	1009	GOL	O1-C1-C2-O2
2	C	1008	GOL	C1-C2-C3-O3
2	A	801	GOL	O2-C2-C3-O3
2	D	1006	GOL	O1-C1-C2-O2
2	D	1006	GOL	O2-C2-C3-O3
2	C	1008	GOL	O1-C1-C2-O2
2	D	1009	GOL	O2-C2-C3-O3
2	B	1009	GOL	O2-C2-C3-O3
2	A	801	GOL	O1-C1-C2-O2
2	B	1006	GOL	O1-C1-C2-O2
2	B	1006	GOL	O2-C2-C3-O3
2	C	1008	GOL	O2-C2-C3-O3
2	B	1008	GOL	O1-C1-C2-C3
2	D	1007	GOL	O2-C2-C3-O3
2	A	807	GOL	O2-C2-C3-O3
2	D	1007	GOL	O1-C1-C2-O2
2	A	808	GOL	O2-C2-C3-O3
2	D	1007	GOL	O1-C1-C2-C3

There are no ring outliers.

20 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1007	GOL	1	0
2	B	1007	GOL	1	0
2	B	1009	GOL	1	0
6	B	1011	PO4	2	0
5	C	1003	ACT	2	0
2	A	807	GOL	4	0
5	D	1005	ACT	3	0
5	B	1004	ACT	1	0
5	C	1004	ACT	1	0
5	D	1003	ACT	1	0
5	B	1003	ACT	1	0
2	A	808	GOL	3	0
2	C	1005	GOL	8	0
2	C	1007	GOL	4	0
2	D	1006	GOL	6	0
2	C	1006	GOL	2	0
2	B	1006	GOL	10	0
5	A	805	ACT	3	0
2	D	1009	GOL	4	0
2	A	809	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	712/721 (98%)	-0.39	13 (1%) 68 75	22, 29, 47, 73	0
1	B	712/721 (98%)	-0.34	12 (1%) 70 76	20, 28, 46, 72	0
1	C	712/721 (98%)	-0.22	20 (2%) 53 62	22, 31, 51, 79	0
1	D	712/721 (98%)	-0.31	13 (1%) 68 75	22, 31, 51, 79	0
All	All	2848/2884 (98%)	-0.31	58 (2%) 65 72	20, 30, 49, 79	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	481	PRO	5.1
1	C	397	GLU	4.3
1	B	397	GLU	3.9
1	C	482	ASP	3.9
1	B	482	ASP	3.8
1	C	191	ALA	3.4
1	B	398	ARG	3.3
1	C	399	GLU	3.0
1	C	398	ARG	2.9
1	C	446	SER	2.9
1	C	670	GLN	2.8
1	B	399	GLU	2.7
1	D	482	ASP	2.7
1	D	670	GLN	2.6
1	B	481	PRO	2.6
1	A	670	GLN	2.6
1	B	671	GLU	2.6
1	B	85	SER	2.5
1	D	566	PHE	2.5
1	B	475	THR	2.5
1	C	447	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	137	LYS	2.4
1	C	478	ASN	2.4
1	C	85	SER	2.4
1	D	481	PRO	2.4
1	C	466	GLU	2.4
1	D	466	GLU	2.4
1	B	446	SER	2.4
1	C	418	THR	2.3
1	A	137	LYS	2.3
1	C	480	ARG	2.3
1	D	447	GLU	2.3
1	A	85	SER	2.3
1	B	312	TRP	2.3
1	A	466	GLU	2.3
1	A	566	PHE	2.3
1	D	671	GLU	2.2
1	D	317	THR	2.2
1	C	315	TYR	2.2
1	C	671	GLU	2.2
1	A	481	PRO	2.2
1	C	312	TRP	2.2
1	A	671	GLU	2.1
1	A	447	GLU	2.1
1	A	314	THR	2.1
1	D	620	TYR	2.1
1	B	137	LYS	2.1
1	D	622	VAL	2.1
1	A	311	PHE	2.1
1	A	399	GLU	2.0
1	A	444	ASN	2.0
1	D	316	LYS	2.0
1	B	505	TYR	2.0
1	A	482	ASP	2.0
1	D	314	THR	2.0
1	C	412	TYR	2.0
1	C	505	TYR	2.0
1	D	318	VAL	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
5	ACT	A	806	4/4	0.56	0.23	42,51,57,63	0
5	ACT	B	1005	4/4	0.57	0.26	37,54,59,62	0
5	ACT	B	1004	4/4	0.60	0.18	30,33,42,51	0
5	ACT	C	1004	4/4	0.62	0.20	29,35,41,50	0
2	GOL	D	1009	6/6	0.66	0.28	49,60,67,76	0
5	ACT	D	1005	4/4	0.68	0.15	40,54,58,60	0
5	ACT	A	805	4/4	0.69	0.31	43,58,60,69	0
5	ACT	A	804	4/4	0.70	0.19	30,38,38,50	0
2	GOL	B	1009	6/6	0.79	0.24	40,49,54,56	0
5	ACT	D	1004	4/4	0.80	0.17	32,34,39,47	0
5	ACT	D	1003	4/4	0.80	0.22	39,47,52,61	0
5	ACT	C	1003	4/4	0.81	0.23	45,46,48,64	0
5	ACT	B	1003	4/4	0.81	0.15	42,53,60,61	0
2	GOL	A	809	6/6	0.82	0.17	44,56,60,64	0
2	GOL	C	1007	6/6	0.82	0.21	45,51,54,59	0
2	GOL	B	1006	6/6	0.85	0.19	28,32,43,58	0
2	GOL	A	807	6/6	0.86	0.21	30,51,60,73	0
2	GOL	A	801	6/6	0.87	0.13	36,52,56,57	0
2	GOL	D	1006	6/6	0.88	0.20	33,43,50,64	0
2	GOL	C	1005	6/6	0.88	0.17	31,44,51,52	0
6	PO4	B	1010	5/5	0.89	0.24	75,84,90,116	0
2	GOL	B	1008	6/6	0.90	0.12	37,45,54,56	0
2	GOL	C	1006	6/6	0.91	0.24	59,73,76,88	0
2	GOL	C	1008	6/6	0.91	0.18	37,52,59,65	0
6	PO4	B	1011	5/5	0.92	0.25	71,84,91,106	0
2	GOL	B	1007	6/6	0.93	0.18	57,61,66,67	0
2	GOL	D	1007	6/6	0.94	0.12	42,53,57,64	0
2	GOL	D	1008	6/6	0.94	0.17	35,44,47,50	0
2	GOL	A	808	6/6	0.94	0.23	54,66,69,81	0
3	CA	A	802	1/1	0.99	0.06	38,38,38,38	0
3	CA	C	1001	1/1	0.99	0.04	41,41,41,41	0
4	K	D	1002	1/1	0.99	0.05	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	K	A	803	1/1	0.99	0.05	29,29,29,29	0
4	K	B	1002	1/1	1.00	0.07	25,25,25,25	0
3	CA	D	1001	1/1	1.00	0.06	39,39,39,39	0
4	K	C	1002	1/1	1.00	0.04	29,29,29,29	0
3	CA	B	1001	1/1	1.00	0.02	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.