



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:46 pm BST

PDB ID : 4GZE  
Title : Crystal structure of 6-phospho-beta-glucosidase from *Lactobacillus plantarum* (apo form)  
Authors : Michalska, K.; Hatzos-Skintges, C.; Bearden, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2012-09-06  
Resolution : 2.31 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

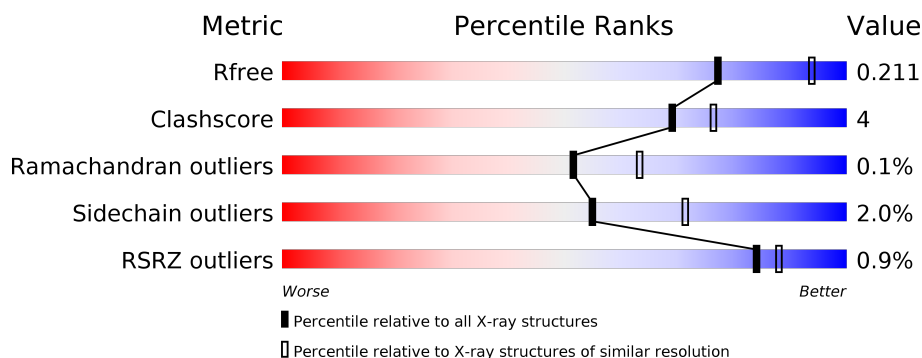
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	481	<div> <div>89%</div> <div>10% .</div> </div>
1	B	481	<div> <div>2%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	C	481	<div> <div>93%</div> <div>5%</div> <div>..</div> </div>
1	D	481	<div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	E	481	<div> <div>2%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	F	481	<div> <div>2%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23591 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 6-phospho-beta-glucosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	Se	0	0	0
			3882	2488	652	722	7	13			
1	B	472	Total	C	N	O	S	Se	0	0	0
			3823	2449	643	712	7	12			
1	C	476	Total	C	N	O	S	Se	0	0	0
			3855	2469	648	719	7	12			
1	D	479	Total	C	N	O	S	Se	0	1	0
			3893	2494	656	723	7	13			
1	E	467	Total	C	N	O	S	Se	0	0	0
			3785	2428	634	703	7	13			
1	F	469	Total	C	N	O	S	Se	0	0	0
			3794	2434	635	705	7	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP F9UU25
A	-1	ASN	-	EXPRESSION TAG	UNP F9UU25
A	0	ALA	-	EXPRESSION TAG	UNP F9UU25
B	-2	SER	-	EXPRESSION TAG	UNP F9UU25
B	-1	ASN	-	EXPRESSION TAG	UNP F9UU25
B	0	ALA	-	EXPRESSION TAG	UNP F9UU25
C	-2	SER	-	EXPRESSION TAG	UNP F9UU25
C	-1	ASN	-	EXPRESSION TAG	UNP F9UU25
C	0	ALA	-	EXPRESSION TAG	UNP F9UU25
D	-2	SER	-	EXPRESSION TAG	UNP F9UU25
D	-1	ASN	-	EXPRESSION TAG	UNP F9UU25
D	0	ALA	-	EXPRESSION TAG	UNP F9UU25
E	-2	SER	-	EXPRESSION TAG	UNP F9UU25
E	-1	ASN	-	EXPRESSION TAG	UNP F9UU25
E	0	ALA	-	EXPRESSION TAG	UNP F9UU25
F	-2	SER	-	EXPRESSION TAG	UNP F9UU25
F	-1	ASN	-	EXPRESSION TAG	UNP F9UU25

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	EXPRESSION TAG	UNP F9UU25

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	A	3	Total Cl 3 3	0	0
2	D	2	Total Cl 2 2	0	0

- Molecule 3 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
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	121	Total O 121 121	0	0
4	B	109	Total O 109 109	0	2

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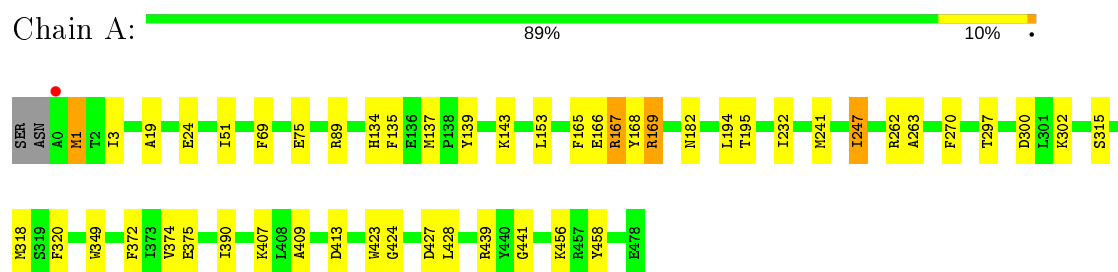
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	115	Total 115	O 115	0	2
4	D	133	Total 133	O 133	0	2
4	E	28	Total 28	O 28	0	0
4	F	41	Total 41	O 41	0	0

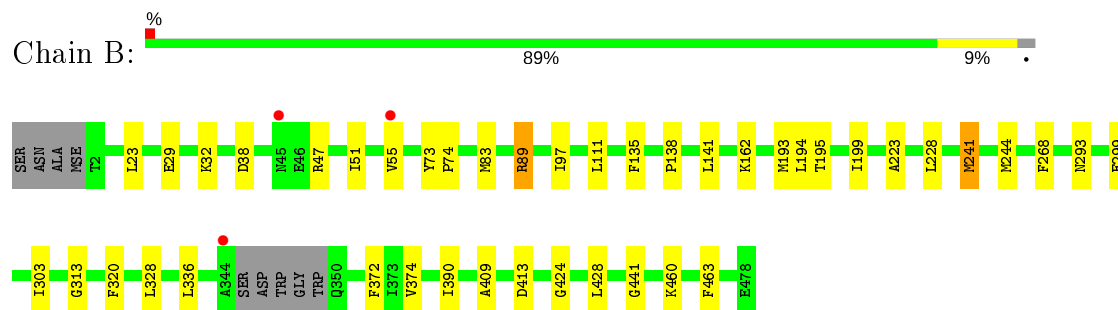
### 3 Residue-property plots

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

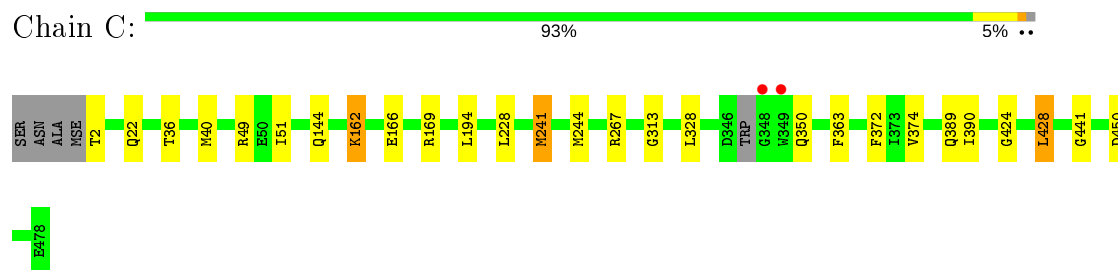
- Molecule 1: 6-phospho-beta-glucosidase



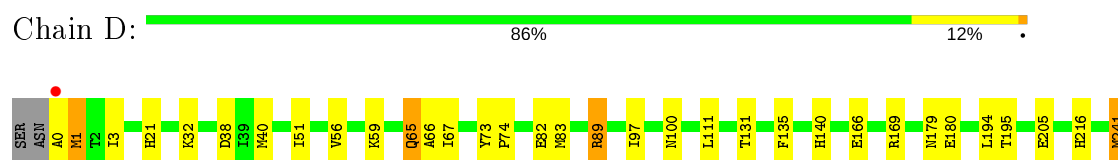
- Molecule 1: 6-phospho-beta-glucosidase

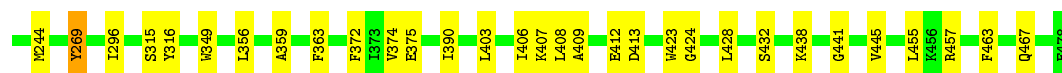


- Molecule 1: 6-phospho-beta-glucosidase

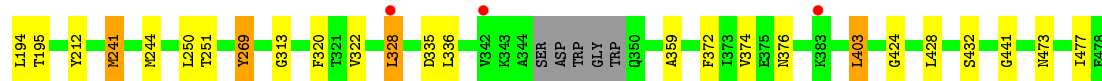
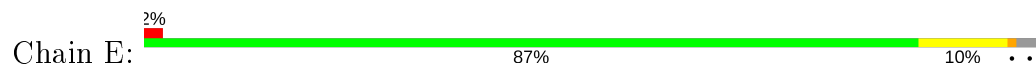


- Molecule 1: 6-phospho-beta-glucosidase

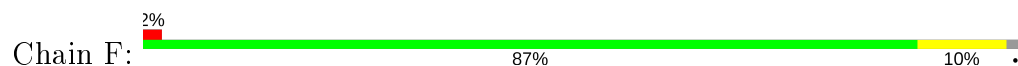




- Molecule 1: 6-phospho-beta-glucosidase



- Molecule 1: 6-phospho-beta-glucosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.09 Å 96.09 Å 289.14 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.31 47.49 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-2.31) 99.5 (47.49-2.31)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.32 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.174 , 0.213 0.173 , 0.211	Depositor DCC
$R_{free}$ test set	1248 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 16.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.328 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
Reported twinning fraction	0.718 for 1.000H, 1.000K, L 0.282 for 1.000K, 1.000H, -L	Depositor
Outliers	0 of 130290 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23591	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.93% 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, CL

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	0.63	0/3980	0.70	2/5377 (0.0%)
1	B	0.64	0/3917	0.70	0/5290
1	C	0.65	0/3951	0.71	0/5337
1	D	0.65	0/3991	0.73	0/5391
1	E	0.54	0/3877	0.64	0/5233
1	F	0.57	0/3887	0.64	0/5247
All	All	0.61	0/23603	0.69	2/31875 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	167	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3882	0	3678	29	0
1	B	3823	0	3628	26	0
1	C	3855	0	3650	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3893	0	3690	41	0
1	E	3785	0	3597	34	0
1	F	3794	0	3604	28	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	D	2	0	0	1	0
3	D	6	0	8	0	0
4	A	121	0	0	2	0
4	B	109	0	0	3	0
4	C	115	0	0	0	0
4	D	133	0	0	0	0
4	E	28	0	0	0	0
4	F	41	0	0	1	0
All	All	23591	0	21855	166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (166) 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:F:424:GLY:O	1:F:441:GLY:HA2	1.89	0.72
1:E:424:GLY:O	1:E:441:GLY:HA2	1.89	0.71
1:F:89:ARG:HD2	1:F:374:VAL:HB	1.74	0.70
1:C:51:ILE:HD13	1:C:194:LEU:HD22	1.75	0.68
1:D:40:MSE:HE3	1:D:194:LEU:HD23	1.76	0.67
1:E:1:MSE:HE1	1:F:328:LEU:HD11	1.77	0.67
1:E:22:GLN:HB3	1:E:428:LEU:HD13	1.77	0.67
1:B:97:ILE:HD12	1:B:111:LEU:HD23	1.77	0.66
1:D:424:GLY:O	1:D:441:GLY:HA2	1.96	0.65
1:B:51:ILE:HD12	1:B:194:LEU:HD22	1.78	0.65
1:D:97:ILE:HD12	1:D:111:LEU:HD23	1.81	0.62
1:D:65:GLN:NE2	1:D:455:LEU:HD21	2.16	0.61
1:D:1:MSE:HE2	1:D:412:GLU:HG3	1.83	0.61
1:D:51:ILE:HD13	1:D:194:LEU:HD22	1.85	0.59
1:D:89:ARG:HD2	1:D:374:VAL:HB	1.83	0.59
1:C:390:ILE:HD12	1:C:390:ILE:N	2.18	0.58
1:A:247:ILE:HD12	1:A:263:ALA:HB1	1.86	0.57
1:A:89:ARG:HD2	1:A:374:VAL:HB	1.87	0.56
1:B:135:PHE:CD1	1:B:195:THR:HB	2.41	0.56
1:F:241:MSE:HE2	1:F:374:VAL:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:THR:O	1:C:2:THR:HG23	2.07	0.55
1:D:135:PHE:CD1	1:D:195:THR:HB	2.41	0.55
1:C:162:LYS:HD3	1:C:228:LEU:HD11	1.88	0.54
1:A:51:ILE:HD13	1:A:194:LEU:HD22	1.89	0.54
1:B:424:GLY:O	1:B:441:GLY:HA2	2.07	0.54
1:F:216:HIS:CE1	1:F:296:ILE:HG23	2.43	0.54
1:D:316:TYR:CG	1:D:356:LEU:HD13	2.43	0.54
1:D:179:ASN:OD1	1:D:241:MSE:HE3	2.08	0.53
1:B:89:ARG:HD2	1:B:374:VAL:HB	1.89	0.53
1:C:241:MSE:HE2	1:C:374:VAL:HG23	1.90	0.53
1:D:67:ILE:HG22	1:D:445:VAL:HG11	1.90	0.53
1:E:92:ILE:CG2	1:E:97:ILE:CD1	2.87	0.53
1:C:328:LEU:HD11	1:D:0:ALA:HB2	1.91	0.53
1:F:373:ILE:HG13	1:F:417:LEU:HD11	1.91	0.53
1:D:244:MSE:HG2	1:D:359:ALA:HB1	1.91	0.53
1:D:67:ILE:CG2	1:D:445:VAL:HG11	2.39	0.52
1:F:87:CYS:HA	1:F:127:GLN:O	2.09	0.52
1:E:403:LEU:HD12	1:E:477:ILE:HG13	1.91	0.52
1:A:318:MSE:HE2	1:A:320:PHE:HE1	1.75	0.51
1:D:73:TYR:CG	1:D:74:PRO:HD3	2.46	0.51
1:E:179:ASN:OD1	1:E:241:MSE:HE3	2.10	0.51
1:E:135:PHE:CD1	1:E:195:THR:HB	2.45	0.51
1:C:328:LEU:HD11	1:D:0:ALA:CB	2.41	0.50
1:E:1:MSE:CE	1:F:328:LEU:HD11	2.41	0.50
1:A:3:ILE:HD12	1:A:407:LYS:HD3	1.92	0.50
1:E:328:LEU:HD11	1:F:1:MSE:HE3	1.93	0.50
1:E:250:LEU:HG	1:E:251:THR:HG23	1.94	0.49
1:C:166:GLU:O	1:C:169:ARG:HG2	2.11	0.49
1:E:32:LYS:HE2	1:E:95:THR:OG1	2.12	0.49
1:E:244:MSE:HG2	1:E:359:ALA:HB1	1.93	0.49
1:F:192:ALA:O	1:F:196:ASP:HB2	2.12	0.49
1:E:424:GLY:O	1:E:441:GLY:CA	2.59	0.49
1:F:44:THR:HA	1:F:435:GLN:NE2	2.28	0.49
1:D:100:ASN:HB3	1:D:140:HIS:CD2	2.47	0.49
1:D:375:GLU:HG3	1:D:423:TRP:HB2	1.94	0.49
1:E:1:MSE:HE1	1:F:328:LEU:CD1	2.43	0.49
1:D:65:GLN:NE2	1:D:66:ALA:O	2.45	0.49
1:E:92:ILE:CG2	1:E:97:ILE:HD11	2.43	0.48
1:D:65:GLN:HE22	1:D:455:LEU:HD21	1.78	0.48
1:F:390:ILE:HG21	1:F:460:LYS:HD3	1.96	0.48
1:B:244:MSE:HE2	1:B:268:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:MSE:HA	1:E:313:GLY:O	2.13	0.48
1:C:389:GLN:C	1:C:390:ILE:HD12	2.34	0.48
1:A:165:PHE:O	1:A:169:ARG:HB3	2.14	0.47
1:B:390:ILE:N	1:B:390:ILE:HD12	2.30	0.47
1:C:244:MSE:HE2	1:C:363:PHE:CZ	2.49	0.47
1:A:139:TYR:CE2	1:A:143:LYS:HD3	2.49	0.47
1:B:193:MSE:CE	1:B:199:ILE:HD12	2.45	0.47
1:A:167:ARG:HG3	1:A:168:TYR:CE1	2.50	0.47
1:A:315:SER:CB	1:A:375:GLU:HB3	2.44	0.47
1:A:409:ALA:O	1:A:413:ASP:HB2	2.14	0.47
1:B:51:ILE:HG22	4:B:698:HOH:O	2.14	0.47
1:E:51:ILE:HD13	1:E:194:LEU:HD22	1.95	0.47
1:B:47:ARG:HD2	1:E:145:TYR:HA	1.96	0.47
1:E:52:THR:OG1	1:E:54:GLY:O	2.31	0.47
1:E:212:TYR:HE1	1:E:269:TYR:CE2	2.34	0.46
1:D:67:ILE:HD12	1:D:457:ARG:NH2	2.31	0.46
1:F:3:ILE:HD12	1:F:407:LYS:HD3	1.97	0.46
1:A:1:MSE:CG	1:B:328:LEU:HD21	2.46	0.46
1:E:328:LEU:HD21	1:F:1:MSE:HB2	1.96	0.46
1:F:320:PHE:HB3	1:F:336:LEU:HD22	1.97	0.46
1:D:32:LYS:NZ	1:D:38:ASP:OD2	2.48	0.46
1:E:320:PHE:HB3	1:E:336:LEU:HD22	1.96	0.46
1:E:130:VAL:HG21	1:E:172:VAL:HG21	1.98	0.46
1:E:56:VAL:HG23	1:E:59:LYS:HG3	1.97	0.46
1:D:241:MSE:HE1	1:D:315:SER:HB3	1.98	0.46
1:D:166:GLU:O	1:D:169:ARG:HG2	2.16	0.45
1:A:390:ILE:N	1:A:390:ILE:HD12	2.31	0.45
1:A:427:ASP:OD2	1:A:439:ARG:HD3	2.15	0.45
1:F:424:GLY:O	1:F:441:GLY:CA	2.63	0.45
1:A:166:GLU:CG	1:A:232:ILE:HD13	2.46	0.45
1:B:162:LYS:HB2	1:B:228:LEU:HD21	1.99	0.45
1:C:40:MSE:HE2	1:C:49:ARG:HD3	1.98	0.45
1:E:89:ARG:HD2	1:E:374:VAL:HB	1.99	0.45
1:F:244:MSE:HG2	1:F:359:ALA:HB1	1.98	0.45
1:B:55:VAL:HG12	4:B:687:HOH:O	2.15	0.45
1:C:424:GLY:O	1:C:441:GLY:HA2	2.17	0.45
1:C:36:THR:CG2	1:C:194:LEU:HD11	2.47	0.45
1:D:432:SER:OG	1:D:438:LYS:NZ	2.48	0.45
1:A:315:SER:HB3	1:A:375:GLU:HB3	1.99	0.44
1:E:32:LYS:HG3	1:E:96:ARG:HG2	1.99	0.44
1:D:409:ALA:O	1:D:413:ASP:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:HG3	1:A:232:ILE:HD13	1.99	0.44
1:D:403:LEU:HA	1:D:406:ILE:HD12	1.98	0.44
1:E:61:TYR:HB2	1:E:64:HIS:CE1	2.53	0.44
1:F:162:LYS:HB2	1:F:228:LEU:HD21	2.00	0.44
1:A:135:PHE:CD1	1:A:195:THR:HB	2.53	0.44
1:A:302:LYS:HG2	4:A:688:HOH:O	2.17	0.44
1:F:366:ARG:HD3	1:F:367:TYR:CZ	2.53	0.44
1:D:56:VAL:CG2	1:D:59:LYS:HG3	2.48	0.43
1:A:19:ALA:HB2	1:A:134:HIS:CE1	2.54	0.43
1:A:75:GLU:HG3	4:A:696:HOH:O	2.18	0.43
1:B:29:GLU:HG2	4:B:616:HOH:O	2.19	0.43
1:B:32:LYS:NZ	1:B:38:ASP:OD2	2.52	0.43
1:B:73:TYR:CG	1:B:74:PRO:HD3	2.52	0.43
1:E:22:GLN:O	1:E:428:LEU:HB2	2.19	0.43
1:B:193:MSE:HE3	1:B:199:ILE:HD12	2.01	0.43
1:E:24:GLU:HA	1:E:69:PHE:HB3	2.01	0.43
1:C:450:ASP:C	1:C:450:ASP:OD1	2.55	0.43
1:D:216:HIS:CE1	1:D:296:ILE:HG12	2.54	0.43
1:E:27:TYR:O	1:E:32:LYS:HD3	2.19	0.43
1:A:456:LYS:HD3	1:A:458:TYR:CZ	2.55	0.42
1:A:137:MSE:HE1	1:A:153:LEU:HD21	2.01	0.42
1:D:1:MSE:HE1	1:D:408:LEU:CD2	2.50	0.42
1:D:82:GLU:O	1:D:467:GLN:NE2	2.42	0.42
1:E:322:VAL:HG12	1:E:335:ASP:O	2.20	0.42
1:F:244:MSE:HE2	1:F:268:PHE:CE1	2.54	0.42
1:B:83:MSE:HE2	1:B:463:PHE:CE1	2.54	0.42
1:D:131:THR:HG21	1:D:179:ASN:HB2	2.00	0.42
1:D:179:ASN:O	1:D:180:GLU:C	2.57	0.42
1:F:399:LEU:O	1:F:403:LEU:HB2	2.19	0.42
1:A:456:LYS:HD3	1:A:458:TYR:OH	2.20	0.42
1:F:136:GLU:HG2	4:F:535:HOH:O	2.19	0.42
1:C:36:THR:HG22	1:C:194:LEU:HD11	2.00	0.42
1:F:81:ALA:HB2	1:F:124:ASN:HB3	2.02	0.42
1:B:135:PHE:CG	1:B:195:THR:HB	2.55	0.42
1:B:320:PHE:HB3	1:B:336:LEU:HD22	2.02	0.42
1:E:328:LEU:HD21	1:F:1:MSE:CB	2.50	0.42
1:F:179:ASN:OD1	1:F:241:MSE:HE3	2.21	0.41
1:D:83:MSE:HE2	1:D:463:PHE:CE1	2.55	0.41
1:D:21:HIS:NE2	2:D:502:CL:CL	2.78	0.41
1:C:22:GLN:O	1:C:428:LEU:HB2	2.20	0.41
1:D:56:VAL:HG22	1:D:59:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:356:LEU:HD12	1:F:356:LEU:O	2.19	0.41
1:A:424:GLY:O	1:A:441:GLY:HA2	2.21	0.41
1:B:390:ILE:HB	1:B:460:LYS:HA	2.01	0.41
1:E:95:THR:CG2	1:E:138:PRO:HA	2.51	0.41
1:F:100:ASN:HB3	1:F:140:HIS:ND1	2.35	0.41
1:C:2:THR:O	1:C:2:THR:CG2	2.67	0.41
1:D:179:ASN:HA	1:D:241:MSE:HB3	2.02	0.41
1:B:223:ALA:HB3	1:B:303:ILE:HG22	2.02	0.41
1:B:241:MSE:HA	1:B:313:GLY:O	2.21	0.41
1:C:241:MSE:HA	1:C:313:GLY:O	2.20	0.41
1:A:1:MSE:HG2	1:B:328:LEU:HD21	2.03	0.41
1:A:297:THR:O	1:A:300:ASP:HB2	2.20	0.41
1:A:182:ASN:HB3	1:A:270:PHE:CD2	2.56	0.40
1:B:138:PRO:HD2	1:B:141:LEU:HD12	2.03	0.40
1:B:409:ALA:O	1:B:413:ASP:HB2	2.21	0.40
1:D:390:ILE:HD12	1:D:390:ILE:N	2.36	0.40
1:C:428:LEU:HD12	1:C:428:LEU:C	2.42	0.40
1:D:244:MSE:HE2	1:D:363:PHE:CZ	2.56	0.40
1:D:3:ILE:HD12	1:D:407:LYS:HD3	2.02	0.40
1:E:92:ILE:HG21	1:E:97:ILE:CD1	2.51	0.40
1:A:375:GLU:HG3	1:A:423:TRP:CE3	2.56	0.40
1:A:24:GLU:HA	1:A:69:PHE:HB3	2.03	0.40
1:D:269:TYR:C	1:D:269:TYR:CD1	2.95	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	477/481 (99%)	464 (97%)	13 (3%)	0	100	100
1	B	468/481 (97%)	452 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	472/481 (98%)	459 (97%)	13 (3%)	0	100	100
1	D	478/481 (99%)	464 (97%)	14 (3%)	0	100	100
1	E	461/481 (96%)	441 (96%)	18 (4%)	2 (0%)	34	41
1	F	463/481 (96%)	449 (97%)	12 (3%)	2 (0%)	34	41
All	All	2819/2886 (98%)	2729 (97%)	86 (3%)	4 (0%)	51	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	376	ASN
1	F	20	ALA
1	E	473	ASN
1	F	477	ILE

### 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	401/390 (103%)	394 (98%)	7 (2%)	60	75
1	B	396/390 (102%)	389 (98%)	7 (2%)	59	74
1	C	399/390 (102%)	392 (98%)	7 (2%)	59	74
1	D	402/390 (103%)	393 (98%)	9 (2%)	52	68
1	E	392/390 (100%)	385 (98%)	7 (2%)	59	74
1	F	393/390 (101%)	383 (98%)	10 (2%)	47	64
All	All	2383/2340 (102%)	2336 (98%)	47 (2%)	55	71

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	169	ARG
1	A	241	MSE

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Mol	Chain	Res	Type
1	A	247	ILE
1	A	349	TRP
1	A	372	PHE
1	A	428	LEU
1	B	23	LEU
1	B	89	ARG
1	B	241	MSE
1	B	293	ASN
1	B	299	GLU
1	B	372	PHE
1	B	428	LEU
1	C	144	GLN
1	C	162	LYS
1	C	241	MSE
1	C	267	ARG
1	C	350	GLN
1	C	372	PHE
1	C	428	LEU
1	D	1	MSE
1	D	65	GLN
1	D	89	ARG
1	D	205	GLU
1	D	241	MSE
1	D	269	TYR
1	D	349	TRP
1	D	372	PHE
1	D	428	LEU
1	E	23	LEU
1	E	241	MSE
1	E	269	TYR
1	E	328	LEU
1	E	372	PHE
1	E	403	LEU
1	E	432	SER
1	F	2	THR
1	F	65	GLN
1	F	83	MSE
1	F	104	SER
1	F	144	GLN
1	F	241	MSE
1	F	318	MSE
1	F	328	LEU

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Mol	Chain	Res	Type
1	F	372	PHE
1	F	428	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	GLN
1	B	293	ASN
1	D	65	GLN
1	D	155	GLN
1	D	159	ASN
1	D	305	GLN
1	E	65	GLN
1	E	274	HIS
1	F	134	HIS
1	F	435	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	D	503	-	5,5,5	0.56	0	5,5,5	0.90	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
3	GOL	D	503	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	503	GOL	C1-C2-C3-O3
3	D	503	GOL	O1-C1-C2-C3
3	D	503	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 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	466/481 (96%)	-0.39	1 (0%) 95 97	25, 35, 49, 75	0
1	B	460/481 (95%)	-0.33	3 (0%) 87 91	26, 36, 52, 90	0
1	C	464/481 (96%)	-0.32	2 (0%) 92 95	24, 35, 50, 86	0
1	D	466/481 (96%)	-0.37	1 (0%) 95 97	25, 33, 48, 68	0
1	E	454/481 (94%)	0.01	8 (1%) 68 75	33, 47, 63, 75	0
1	F	456/481 (94%)	-0.04	10 (2%) 62 69	33, 46, 57, 76	0
All	All	2766/2886 (95%)	-0.24	25 (0%) 84 88	24, 38, 56, 90	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	328	LEU	4.8
1	D	0	ALA	4.1
1	F	328	LEU	3.3
1	F	36	THR	3.2
1	E	55	VAL	2.6
1	C	349	TRP	2.5
1	E	187	PHE	2.5
1	E	60	TYR	2.5
1	E	56	VAL	2.4
1	F	342	VAL	2.4
1	F	200	ILE	2.3
1	F	10	GLU	2.3
1	F	165	PHE	2.3
1	E	342	VAL	2.3
1	F	44	THR	2.2
1	B	55	VAL	2.2
1	F	424	GLY	2.2
1	B	344	ALA	2.2
1	F	51	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	45	ASN	2.2
1	F	63	ASN	2.1
1	A	0	ALA	2.1
1	E	383	LYS	2.1
1	C	348	GLY	2.1
1	E	2	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	CL	D	501	1/1	0.85	0.09	52,52,52,52	0
2	CL	A	502	1/1	0.85	0.12	64,64,64,64	0
2	CL	D	502	1/1	0.91	0.10	50,50,50,50	0
3	GOL	D	503	6/6	0.92	0.15	42,47,49,50	0
2	CL	A	501	1/1	0.92	0.09	50,50,50,50	0
2	CL	B	501	1/1	0.93	0.17	51,51,51,51	0
2	CL	A	503	1/1	0.94	0.12	52,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.