



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 09:03 am BST

PDB ID : 4ZNG
Title : X-ray crystallography of recombinant *Lactococcus lactis* prolidase
Authors : Kgosisejo, O.; Grochulski, P.; Tanaka, T.
Deposited on : 2015-05-04
Resolution : 2.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

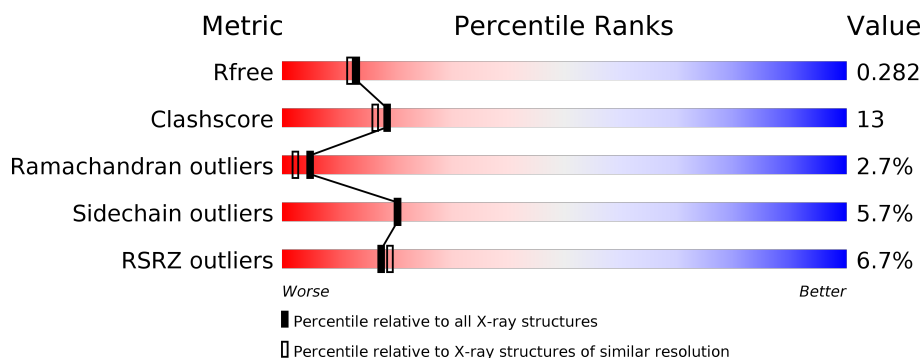
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	362	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>.</div> </div> </div>
1	B	362	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>...</div> </div> </div>
1	C	362	<div> <div>15%</div> <div> <div></div> <div>61%</div> <div>27%</div> <div>7%</div> <div>...</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8636 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 Prolidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	352	Total	C	N	O	S	0	0	0
			2708	1717	443	533	15			
1	B	360	Total	C	N	O	S	0	0	0
			2787	1763	464	544	16			
1	A	362	Total	C	N	O	S	0	0	0
			2806	1777	466	546	17			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	As	C	O	0	0
			5	1	2	2		
3	A	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

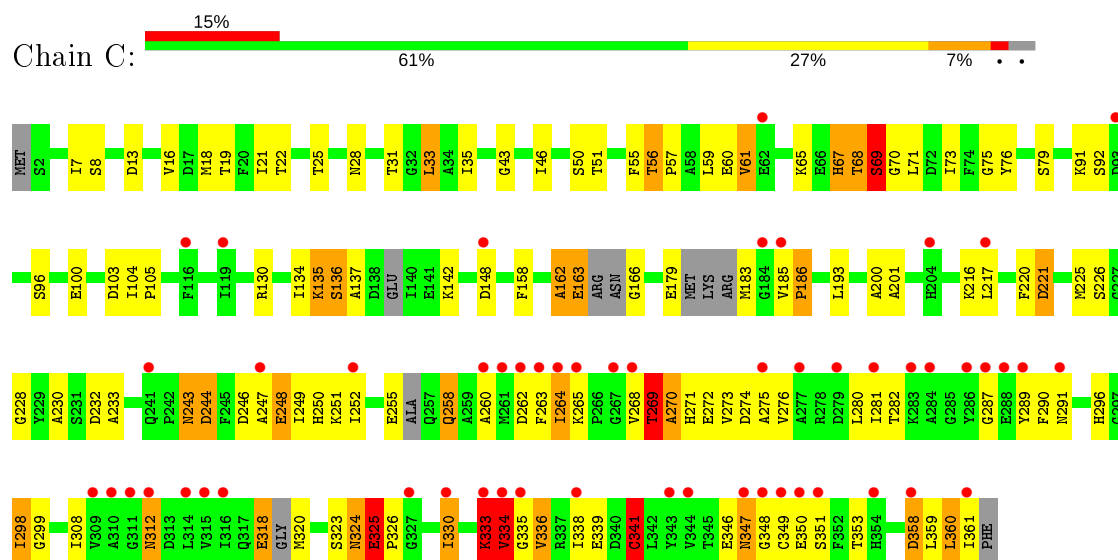
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	52	Total 52	O 52	0	0
5	B	118	Total 118	O 118	0	0
5	A	144	Total 144	O 144	0	0

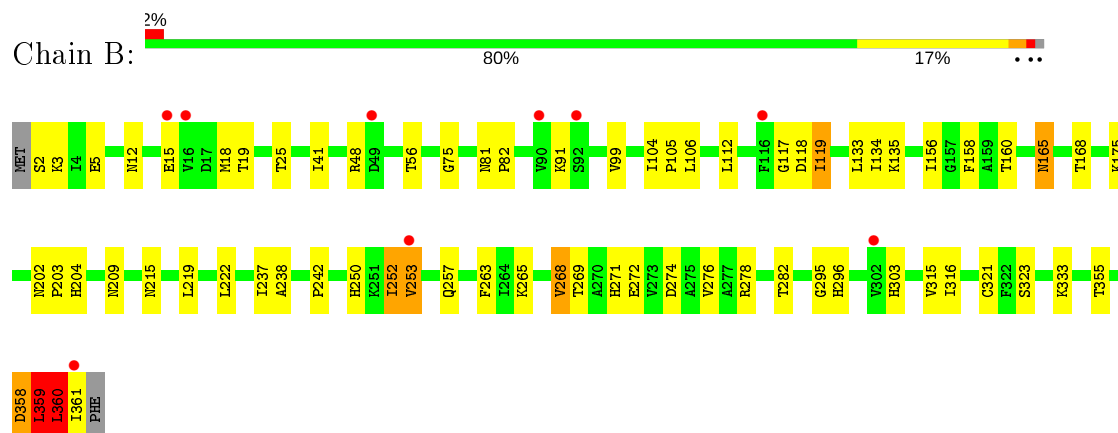
3 Residue-property plots [i](#)

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.

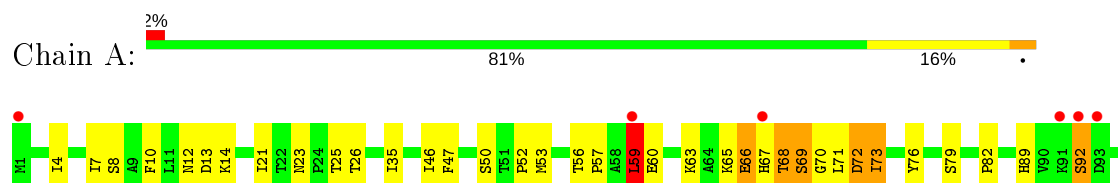
• Molecule 1: Prolidase

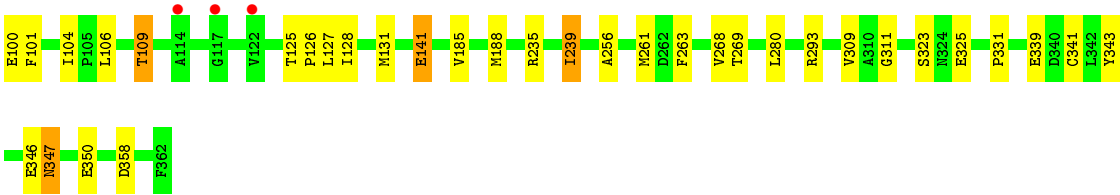


• Molecule 1: Prolidase



• Molecule 1: Prolidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.13Å 76.99Å 88.92Å 90.00° 112.39° 90.00°	Depositor
Resolution (Å)	49.83 – 2.25 49.45 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.83-2.25) 99.9 (49.45-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.220 , 0.280 0.227 , 0.282	Depositor DCC
R_{free} test set	3153 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8636	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CAC, GOL, MN

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	0.73	0/2861	0.87	4/3870 (0.1%)
1	B	0.69	1/2841 (0.0%)	0.85	3/3844 (0.1%)
1	C	0.53	0/2757	0.75	1/3730 (0.0%)
All	All	0.66	1/8459 (0.0%)	0.83	8/11444 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	7
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	360	LEU	N-CA	5.66	1.57	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	LEU	N-CA-C	7.69	131.76	111.00
1	B	253	VAL	N-CA-C	-6.28	94.05	111.00
1	B	359	LEU	CA-CB-CG	6.25	129.68	115.30
1	C	325	GLU	O-C-N	-6.18	109.35	121.10
1	A	235	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	239	ILE	CG1-CB-CG2	-5.46	99.38	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	59	LEU	CB-CG-CD1	5.11	119.69	111.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	GLY	Peptide
1	A	67	HIS	Peptide
1	B	15	GLU	Peptide
1	B	165	ASN	Peptide
1	B	252	ILE	Peptide
1	B	359	LEU	Peptide
1	C	248	GLU	Peptide
1	C	263	PHE	Peptide
1	C	270	ALA	Peptide
1	C	312	ASN	Peptide
1	C	325	GLU	Mainchain
1	C	333	LYS	Peptide
1	C	67	HIS	Peptide

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	2806	0	2756	50	0
1	B	2787	0	2734	50	0
1	C	2708	0	2629	121	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	6	0	8	2	0
5	A	144	0	0	6	1
5	B	118	0	0	10	1
5	C	52	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8636	0	8127	217	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 13.

All (217) 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:C:296:HIS:HD2	1:C:325:GLU:OE2	1.34	1.06
1:C:296:HIS:CD2	1:C:325:GLU:OE2	2.14	1.01
1:C:324:ASN:O	1:C:339:GLU:HA	1.66	0.93
1:A:127:LEU:HG	1:A:131:MET:HE2	1.52	0.92
1:A:12:ASN:ND2	5:A:501:HOH:O	2.01	0.91
1:A:263:PHE:CE2	1:A:268:VAL:HG11	2.07	0.89
1:C:193:LEU:O	1:C:220:PHE:O	1.98	0.82
1:C:221:ASP:HA	1:C:233:ALA:O	1.79	0.82
1:B:238:ALA:HB3	1:B:360:LEU:HD23	1.63	0.78
1:B:112:LEU:C	5:B:514:HOH:O	2.23	0.77
1:C:330:ILE:O	1:C:333:LYS:HB2	1.86	0.76
1:A:65:LYS:O	1:A:68:THR:HA	1.85	0.75
1:A:35:ILE:HD11	1:A:60:GLU:OE2	1.85	0.75
1:B:282:THR:OG1	5:B:501:HOH:O	2.03	0.75
1:C:333:LYS:O	1:C:334:VAL:HG23	1.87	0.74
1:C:162:ALA:O	5:C:501:HOH:O	2.05	0.74
1:B:215:ASN:ND2	5:B:502:HOH:O	2.08	0.74
1:B:156:ILE:O	1:B:160:THR:HG23	1.88	0.73
1:B:250:HIS:O	1:B:253:VAL:O	2.06	0.73
1:C:325:GLU:HB3	1:C:339:GLU:HG3	1.71	0.73
1:B:165:ASN:O	1:B:165:ASN:CG	2.29	0.72
1:A:343:TYR:OH	5:A:502:HOH:O	2.08	0.71
1:C:318:GLU:C	1:C:320:MET:N	2.44	0.71
1:C:28:ASN:N	5:C:504:HOH:O	2.14	0.70
1:C:33:LEU:HD21	1:C:35:ILE:HB	1.73	0.70
1:C:25:THR:C	5:C:504:HOH:O	2.31	0.69
1:B:268:VAL:O	5:B:503:HOH:O	2.10	0.69
1:C:334:VAL:O	1:C:334:VAL:HG12	1.93	0.69
1:A:68:THR:O	1:A:69:SER:OG	2.11	0.69
1:C:341:CYS:N	5:C:506:HOH:O	2.25	0.68
1:C:91:LYS:O	1:C:92:SER:OG	2.09	0.68
1:C:359:LEU:O	5:C:503:HOH:O	2.13	0.67
1:C:268:VAL:HG23	1:C:272:GLU:OE1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:LYS:O	1:C:68:THR:OG1	2.12	0.67
1:C:61:VAL:HG23	1:C:73:ILE:HG22	1.75	0.67
1:C:249:ILE:HG22	1:C:336:VAL:HG11	1.76	0.67
1:C:360:LEU:O	1:C:360:LEU:HD23	1.94	0.67
1:B:3:LYS:N	1:B:5:GLU:OE1	2.28	0.66
1:C:216:LYS:NZ	5:C:507:HOH:O	2.28	0.66
1:C:201:ALA:HB2	1:C:333:LYS:HE2	1.77	0.66
1:C:185:VAL:HG22	1:C:186:PRO:HD2	1.78	0.66
1:C:325:GLU:HB3	1:C:339:GLU:CG	2.26	0.65
1:B:316:ILE:N	5:B:503:HOH:O	2.26	0.65
1:A:358:ASP:OD2	5:A:503:HOH:O	2.15	0.65
1:C:333:LYS:HG2	1:C:334:VAL:HB	1.79	0.65
1:A:69:SER:HB2	1:A:70:GLY:HA2	1.79	0.65
1:A:56:THR:HG22	1:A:57:PRO:O	1.98	0.63
1:C:282:THR:HG22	1:C:287:GLY:HA3	1.80	0.63
1:C:264:ILE:HG12	1:C:349:CYS:SG	2.37	0.63
1:A:347:ASN:C	1:A:347:ASN:OD1	2.38	0.63
1:B:274:ASP:OD1	1:B:278:ARG:NH1	2.32	0.62
1:C:158:PHE:HB3	1:C:361:ILE:HD12	1.81	0.62
1:C:280:LEU:HD23	1:C:280:LEU:O	1.99	0.62
1:C:56:THR:HG23	1:C:60:GLU:HB2	1.81	0.62
1:C:272:GLU:HG3	1:C:273:VAL:N	2.15	0.62
1:A:256:ALA:HB2	1:A:280:LEU:HD22	1.83	0.61
1:B:133:LEU:HG	1:B:134:ILE:HD12	1.83	0.60
1:C:264:ILE:CG1	1:C:349:CYS:SG	2.90	0.59
1:C:246:ASP:OD2	1:C:334:VAL:HG22	2.03	0.59
1:C:308:ILE:O	1:C:308:ILE:HG22	2.02	0.59
1:A:26:THR:HG21	1:A:100:GLU:OE2	2.03	0.59
1:C:200:ALA:HB3	1:C:335:GLY:HA3	1.85	0.59
1:C:142:LYS:NZ	1:C:226:SER:O	2.35	0.59
1:C:264:ILE:HG23	1:C:265:LYS:N	2.18	0.59
1:B:282:THR:O	5:B:504:HOH:O	2.17	0.58
1:C:258:GLN:HE21	1:C:258:GLN:HA	1.68	0.58
1:C:225:MET:SD	1:C:230:ALA:HB2	2.44	0.57
1:C:346:GLU:OE1	1:C:346:GLU:N	2.37	0.57
1:A:10:PHE:O	1:A:13:ASP:O	2.22	0.57
1:A:263:PHE:CZ	1:A:268:VAL:HG11	2.40	0.57
1:B:117:GLY:O	1:B:119:ILE:HG23	2.05	0.57
1:B:41:ILE:HD12	1:B:41:ILE:N	2.20	0.57
1:B:360:LEU:O	1:B:361:ILE:HB	2.05	0.56
1:A:293:ARG:HB3	1:A:309:VAL:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ASP:HA	5:C:538:HOH:O	2.06	0.56
1:C:268:VAL:O	1:C:269:THR:O	2.22	0.56
1:C:25:THR:O	5:C:504:HOH:O	2.17	0.56
1:C:264:ILE:HG12	1:C:349:CYS:HB2	1.88	0.56
1:C:248:GLU:OE2	1:C:251:LYS:N	2.40	0.55
1:C:246:ASP:OD1	1:C:334:VAL:CG2	2.54	0.55
1:C:272:GLU:CG	1:C:273:VAL:N	2.70	0.55
1:C:320:MET:N	5:C:510:HOH:O	2.38	0.55
1:C:246:ASP:CG	1:C:334:VAL:HG13	2.27	0.55
1:A:268:VAL:HG12	1:A:269:THR:N	2.22	0.55
1:B:2:SER:OG	1:B:5:GLU:OE1	2.25	0.55
1:C:334:VAL:O	1:C:334:VAL:CG1	2.55	0.55
1:C:323:SER:HA	1:C:341:CYS:HA	1.90	0.54
1:A:346:GLU:OE1	5:A:504:HOH:O	2.18	0.54
1:B:269:THR:OG1	1:B:272:GLU:HG2	2.08	0.54
1:A:141:GLU:OE2	5:A:505:HOH:O	2.18	0.53
1:C:336:VAL:HG13	1:C:336:VAL:O	2.08	0.53
1:C:326:PRO:HD2	1:C:338:ILE:O	2.09	0.53
1:C:67:HIS:HA	1:C:68:THR:HB	1.90	0.53
1:C:318:GLU:O	1:C:320:MET:N	2.42	0.53
1:B:160:THR:HG21	1:B:175:LYS:HG2	1.90	0.53
1:A:268:VAL:HG12	1:A:269:THR:H	1.74	0.53
1:B:2:SER:OG	1:B:5:GLU:CD	2.47	0.53
1:C:323:SER:OG	1:C:341:CYS:HB3	2.10	0.52
1:A:72:ASP:O	1:A:73:ILE:HB	2.09	0.52
1:C:135:LYS:C	1:C:137:ALA:H	2.13	0.52
1:C:134:ILE:HG22	1:C:318:GLU:O	2.10	0.52
1:C:56:THR:HG22	1:C:57:PRO:O	2.09	0.51
1:C:31:THR:HG22	1:C:33:LEU:HB3	1.92	0.51
1:C:243:ASN:O	1:C:247:ALA:HB2	2.10	0.51
1:C:258:GLN:HE21	1:C:258:GLN:CA	2.20	0.51
1:A:76:TYR:CE1	1:A:82:PRO:HG3	2.46	0.51
1:C:330:ILE:HG13	1:C:333:LYS:HG3	1.92	0.51
1:C:273:VAL:C	1:C:275:ALA:H	2.13	0.51
1:A:293:ARG:CB	1:A:309:VAL:HG12	2.40	0.51
1:B:219:LEU:HD23	1:B:219:LEU:C	2.31	0.51
1:A:13:ASP:O	1:A:14:LYS:HB2	2.11	0.51
1:A:185:VAL:O	4:A:404:GOL:O3	2.30	0.50
1:C:347:ASN:HB2	1:C:348:GLY:C	2.32	0.50
1:C:21:ILE:O	1:C:43:GLY:HA2	2.12	0.50
1:C:272:GLU:HG3	1:C:273:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:VAL:HG21	5:C:513:HOH:O	2.12	0.50
1:C:269:THR:O	1:C:272:GLU:CD	2.51	0.49
1:C:333:LYS:HG2	1:C:334:VAL:CB	2.42	0.49
1:A:127:LEU:HG	1:A:131:MET:CE	2.34	0.49
1:C:232:ASP:OD2	1:C:339:GLU:OE2	2.30	0.49
1:A:323:SER:HA	1:A:341:CYS:HA	1.95	0.49
1:C:244:ASP:HA	1:C:247:ALA:HB2	1.94	0.49
1:B:5:GLU:CD	1:B:5:GLU:H	2.16	0.49
1:C:246:ASP:OD1	1:C:334:VAL:HG21	2.13	0.49
1:C:255:GLU:OE1	1:C:280:LEU:HD21	2.13	0.49
1:B:242:PRO:HD3	1:B:360:LEU:HD21	1.94	0.48
1:C:258:GLN:NE2	1:C:258:GLN:HA	2.28	0.48
1:C:13:ASP:O	1:A:14:LYS:NZ	2.46	0.48
1:A:8:SER:OG	1:A:47:PHE:O	2.24	0.48
1:C:330:ILE:HG13	1:C:333:LYS:CB	2.44	0.48
1:C:246:ASP:OD1	1:C:334:VAL:CG1	2.62	0.47
1:C:252:ILE:HG22	1:C:281:ILE:HD12	1.95	0.47
1:B:263:PHE:CD2	1:B:276:VAL:HG21	2.49	0.47
1:C:348:GLY:O	1:C:349:CYS:SG	2.70	0.47
1:C:163:GLU:OE2	1:C:166:GLY:N	2.47	0.47
1:A:128:ILE:HA	1:A:131:MET:HE3	1.97	0.47
1:C:250:HIS:CE1	5:C:538:HOH:O	2.68	0.47
1:A:325:GLU:HB3	1:A:339:GLU:HG3	1.97	0.47
1:C:69:SER:N	1:C:70:GLY:HA2	2.30	0.47
1:B:106:LEU:HD23	1:A:101:PHE:CE1	2.50	0.46
1:C:264:ILE:HG13	1:C:349:CYS:SG	2.56	0.46
1:C:347:ASN:HB2	1:C:348:GLY:CA	2.46	0.46
1:B:18:MET:HG2	1:B:19:THR:O	2.16	0.46
1:A:343:TYR:CE1	1:A:350:GLU:HB3	2.51	0.46
1:B:257:GLN:HB3	5:B:517:HOH:O	2.16	0.46
1:C:243:ASN:ND2	5:C:507:HOH:O	2.49	0.46
1:C:325:GLU:HB3	1:C:339:GLU:HB2	1.97	0.45
1:A:7:ILE:O	1:A:10:PHE:HB3	2.16	0.45
1:B:222:LEU:C	1:B:222:LEU:HD12	2.37	0.45
1:C:185:VAL:CG2	1:C:186:PRO:HD2	2.44	0.45
1:C:264:ILE:HG12	1:C:349:CYS:CB	2.47	0.45
1:C:50:SER:CB	5:C:536:HOH:O	2.65	0.45
1:A:52:PRO:O	1:A:72:ASP:HB2	2.17	0.45
1:B:271:HIS:C	1:B:271:HIS:CD2	2.90	0.45
1:C:7:ILE:HG21	1:C:46:ILE:HD12	1.99	0.45
1:C:100:GLU:O	1:C:104:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ASP:O	1:C:105:PRO:HD3	2.17	0.44
1:C:268:VAL:CG2	1:C:272:GLU:OE1	2.64	0.44
1:B:296:HIS:CG	1:B:303:HIS:HD2	2.34	0.44
1:C:248:GLU:HB3	1:C:251:LYS:CB	2.46	0.44
1:A:188:MET:HG2	4:A:404:GOL:H11	1.98	0.44
1:C:33:LEU:C	1:C:33:LEU:HD23	2.37	0.44
1:A:4:ILE:HG23	1:A:46:ILE:HG13	2.00	0.44
1:C:347:ASN:CB	1:C:348:GLY:CA	2.96	0.44
1:C:179:GLU:OE2	5:C:505:HOH:O	2.21	0.44
1:A:63:LYS:HA	1:A:66:GLU:HB2	1.99	0.44
1:B:56:THR:O	1:B:75:GLY:HA2	2.18	0.44
1:B:158:PHE:CD1	1:B:237:ILE:HD13	2.53	0.43
1:C:217:LEU:HD11	1:C:246:ASP:HB3	2.00	0.43
1:B:250:HIS:C	1:B:253:VAL:O	2.56	0.43
1:A:23:ASN:OD1	1:A:25:THR:HB	2.19	0.43
1:A:331:PRO:HB3	5:A:608:HOH:O	2.18	0.43
1:B:168:THR:HG21	1:B:209:ASN:OD1	2.19	0.43
1:C:270:ALA:HB3	1:C:312:ASN:O	2.18	0.43
1:C:270:ALA:C	1:C:272:GLU:N	2.71	0.43
1:C:298:ILE:HG13	1:C:299:GLY:N	2.34	0.43
1:A:263:PHE:HE2	1:A:268:VAL:HG11	1.71	0.43
1:C:282:THR:HG22	1:C:287:GLY:CA	2.47	0.43
1:B:135:LYS:HG2	1:B:321:CYS:SG	2.59	0.43
1:C:16:VAL:HG13	1:C:96:SER:HB3	2.01	0.43
1:A:128:ILE:HD13	1:A:131:MET:HE3	2.00	0.42
1:C:272:GLU:CG	1:C:273:VAL:H	2.32	0.42
1:B:358:ASP:O	1:B:359:LEU:HD22	2.18	0.42
1:B:2:SER:C	1:B:5:GLU:OE1	2.57	0.42
1:B:99:VAL:HB	1:B:104:ILE:HD12	2.01	0.42
1:B:12:ASN:HA	1:B:48:ARG:NE	2.34	0.42
1:B:278:ARG:NH1	5:B:508:HOH:O	2.30	0.42
1:B:3:LYS:NZ	5:B:512:HOH:O	2.38	0.42
1:A:53:MET:HA	1:A:72:ASP:HB3	2.02	0.42
1:B:315:VAL:HG13	5:B:503:HOH:O	2.19	0.42
1:C:333:LYS:NZ	1:C:335:GLY:HA2	2.35	0.42
1:B:105:PRO:HA	1:A:104:ILE:O	2.19	0.42
1:B:202:ASN:OD1	1:B:203:PRO:HD2	2.20	0.42
1:C:166:GLY:HA2	5:C:523:HOH:O	2.20	0.42
1:C:269:THR:C	1:C:272:GLU:HB3	2.40	0.42
1:C:16:VAL:HG13	1:C:96:SER:CB	2.50	0.42
1:C:233:ALA:HB2	1:C:353:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ASP:O	1:C:247:ALA:C	2.58	0.42
1:C:244:ASP:HA	1:C:247:ALA:CB	2.50	0.41
1:C:55:PHE:CZ	1:C:76:TYR:CD1	3.08	0.41
1:A:125:THR:HB	1:A:126:PRO:HD3	2.02	0.41
1:C:18:MET:HG2	1:C:19:THR:N	2.34	0.41
1:C:35:ILE:HD11	1:C:60:GLU:CB	2.50	0.41
1:A:106:LEU:O	1:A:109:THR:HG22	2.20	0.41
1:B:295:GLY:HA3	1:B:323:SER:O	2.21	0.41
1:B:250:HIS:CE1	1:B:358:ASP:O	2.74	0.41
1:C:61:VAL:HG23	1:C:73:ILE:CG2	2.48	0.41
1:C:56:THR:O	1:C:75:GLY:HA2	2.19	0.41
1:B:204:HIS:ND1	1:A:63:LYS:HG3	2.36	0.41
1:B:250:HIS:CE1	1:B:359:LEU:HD22	2.56	0.41
1:B:81:ASN:HA	1:B:82:PRO:HD2	1.95	0.41
1:B:272:GLU:O	1:B:276:VAL:HG23	2.21	0.41
1:C:246:ASP:CG	1:C:334:VAL:CG1	2.90	0.41
1:A:70:GLY:O	1:A:71:LEU:HD12	2.21	0.40
1:A:59:LEU:H	1:A:59:LEU:CD1	2.34	0.40
1:C:325:GLU:HB3	1:C:339:GLU:CB	2.51	0.40
1:A:21:ILE:HG23	1:A:100:GLU:OE1	2.21	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)
5:B:540:HOH:O	5:A:503:HOH:O[4_445]	2.00	0.20

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	360/362 (99%)	333 (92%)	22 (6%)	5 (1%)	11 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	358/362 (99%)	332 (93%)	21 (6%)	5 (1%)	11	7
1	C	340/362 (94%)	281 (83%)	40 (12%)	19 (6%)	2	0
All	All	1058/1086 (97%)	946 (89%)	83 (8%)	29 (3%)	5	2

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	69	SER
1	C	221	ASP
1	C	243	ASN
1	C	260	ALA
1	C	264	ILE
1	C	269	THR
1	C	271	HIS
1	C	334	VAL
1	C	341	CYS
1	B	360	LEU
1	A	72	ASP
1	C	186	PRO
1	C	289	TYR
1	C	347	ASN
1	B	252	ILE
1	B	358	ASP
1	A	69	SER
1	A	73	ILE
1	C	228	GLY
1	C	274	ASP
1	C	333	LYS
1	A	68	THR
1	A	92	SER
1	C	68	THR
1	C	162	ALA
1	C	136	SER
1	B	118	ASP
1	B	355	THR
1	C	336	VAL

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	303/303 (100%)	292 (96%)	11 (4%)	35	42
1	B	301/303 (99%)	293 (97%)	8 (3%)	44	54
1	C	292/303 (96%)	260 (89%)	32 (11%)	6	4
All	All	896/909 (99%)	845 (94%)	51 (6%)	20	20

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

Mol	Chain	Res	Type
1	C	8	SER
1	C	22	THR
1	C	33	LEU
1	C	51	THR
1	C	56	THR
1	C	59	LEU
1	C	61	VAL
1	C	69	SER
1	C	71	LEU
1	C	79	SER
1	C	130	ARG
1	C	135	LYS
1	C	136	SER
1	C	148	ASP
1	C	163	GLU
1	C	183	MET
1	C	244	ASP
1	C	258	GLN
1	C	262	ASP
1	C	269	THR
1	C	290	PHE
1	C	291	ASN
1	C	298	ILE
1	C	318	GLU
1	C	324	ASN
1	C	330	ILE
1	C	334	VAL
1	C	341	CYS
1	C	350	GLU
1	C	351	SER

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Mol	Chain	Res	Type
1	C	358	ASP
1	C	360	LEU
1	B	25	THR
1	B	91	LYS
1	B	119	ILE
1	B	265	LYS
1	B	268	VAL
1	B	333	LYS
1	B	359	LEU
1	B	360	LEU
1	A	50	SER
1	A	59	LEU
1	A	66	GLU
1	A	79	SER
1	A	89	HIS
1	A	92	SER
1	A	109	THR
1	A	141	GLU
1	A	239	ILE
1	A	261	MET
1	A	347	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	258	GLN
1	C	296	HIS
1	C	324	ASN
1	B	303	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 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	$\# Z > 2$
4	GOL	A	404	-	5,5,5	0.39	0	5,5,5	1.18	0
3	CAC	A	403	2	0,4,4	0.00	-	0,6,6	0.00	-
3	CAC	B	401	2	0,4,4	0.00	-	0,6,6	0.00	-

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
4	GOL	A	404	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	GOL	O1-C1-C2-C3
4	A	404	GOL	C1-C2-C3-O3
4	A	404	GOL	O2-C2-C3-O3
4	A	404	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	GOL	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	362/362 (100%)	0.25	9 (2%) 57 60	23, 47, 87, 115	0
1	B	360/362 (99%)	0.23	9 (2%) 57 60	30, 53, 82, 108	0
1	C	352/362 (97%)	0.98	54 (15%) 2 2	52, 82, 120, 183	0
All	All	1074/1086 (98%)	0.48	72 (6%) 17 19	23, 61, 107, 183	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	348	GLY	10.4
1	C	335	GLY	8.4
1	C	286	TYR	6.7
1	C	347	ASN	6.7
1	C	252	ILE	5.6
1	C	310	ALA	5.5
1	C	263	PHE	5.4
1	C	289	TYR	5.0
1	C	334	VAL	4.9
1	C	267	GLY	4.6
1	C	291	ASN	4.6
1	C	343	TYR	4.5
1	B	92	SER	4.3
1	C	344	VAL	4.2
1	C	275	ALA	4.1
1	C	314	LEU	3.9
1	C	312	ASN	3.8
1	C	184	GLY	3.7
1	C	265	LYS	3.5
1	A	92	SER	3.3
1	C	268	VAL	3.3
1	C	279	ASP	3.2
1	C	350	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	311	GLY	3.1
1	C	327	GLY	3.1
1	C	116	PHE	3.1
1	C	185	VAL	3.1
1	C	287	GLY	3.0
1	C	361	ILE	3.0
1	A	59	LEU	3.0
1	C	217	LEU	3.0
1	C	349	CYS	2.9
1	A	1	MET	2.9
1	C	309	VAL	2.8
1	C	283	LYS	2.8
1	C	351	SER	2.8
1	C	262	ASP	2.8
1	C	284	ALA	2.8
1	B	253	VAL	2.7
1	C	316	ILE	2.7
1	C	264	ILE	2.7
1	C	119	ILE	2.7
1	C	277	ALA	2.7
1	C	288	GLU	2.7
1	C	358	ASP	2.6
1	A	91	LYS	2.4
1	C	62	GLU	2.4
1	C	330	ILE	2.4
1	C	354	HIS	2.3
1	B	116	PHE	2.3
1	A	67	HIS	2.3
1	C	241	GLN	2.3
1	A	114	ALA	2.3
1	C	148	ASP	2.2
1	B	15	GLU	2.2
1	A	93	ASP	2.2
1	C	333	LYS	2.2
1	C	261	MET	2.2
1	C	315	VAL	2.1
1	C	260	ALA	2.1
1	B	90	VAL	2.1
1	C	338	ILE	2.1
1	A	117	GLY	2.1
1	B	302	VAL	2.1
1	A	122	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	247	ALA	2.1
1	C	93	ASP	2.0
1	C	204	HIS	2.0
1	C	281	ILE	2.0
1	B	361	ILE	2.0
1	B	16	VAL	2.0
1	B	49	ASP	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	C	401	1/1	0.74	0.21	58,58,58,58	0
3	CAC	A	403	5/5	0.97	0.14	51,54,65,66	0
3	CAC	B	401	5/5	0.98	0.16	44,67,81,85	0
4	GOL	A	404	6/6	0.98	0.16	33,35,36,37	0
2	MN	A	402	1/1	0.98	0.17	27,27,27,27	0
2	MN	B	403	1/1	0.98	0.16	40,40,40,40	0
2	MN	A	401	1/1	0.99	0.17	31,31,31,31	0
2	MN	B	402	1/1	1.00	0.15	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.