wwPDB X-ray Structure Validation Summary Report (i)

Aug 21, 2020 – 03:46 PM BST

PDB ID	:	5NAQ
Title	:	Crystal structure of native 6-phospho-glucosidase LpBgl from Lactobacillus plantarum
Authors	:	Acebron, I.; Mancheno, J.M.
Deposited on	:	2017-02-28
Resolution	:	2.48 Å(reported)

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

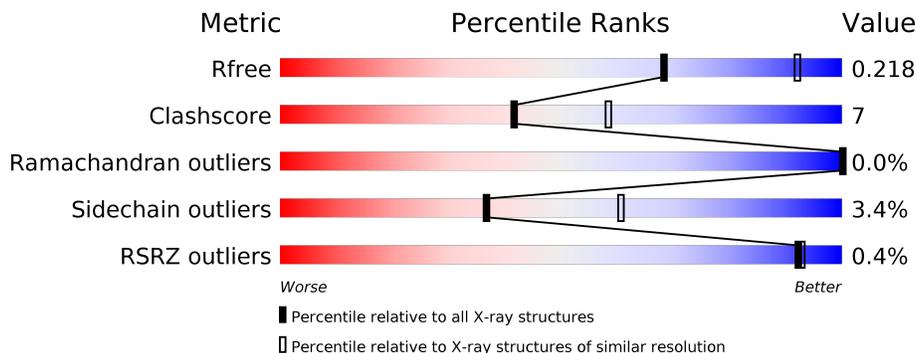|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	Percentile Ranks	Value
Rfree		0.218
Clashscore		7
Ramachandran outliers		0.0%
Sidechain outliers		3.4%
RSRZ outliers		0.4%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 <=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	477	82% · · · 14% · ·
1	B	477	79% · · · 16% · ·
1	C	477	% 78% · · · 16% · ·
1	D	477	82% · · · 14% ·
1	E	477	81% · · · 14% · ·
1	F	477	79% · · · 16% · ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24057 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total 3732	As 1	C 2403	N 628	O 682	S 18	0	0	0
1	B	461	Total 3732	As 1	C 2403	N 628	O 682	S 18	0	0	0
1	C	461	Total 3732	As 1	C 2403	N 628	O 682	S 18	0	0	0
1	D	461	Total 3732	As 1	C 2403	N 628	O 682	S 18	0	0	0
1	E	461	Total 3732	As 1	C 2403	N 628	O 682	S 18	0	0	0
1	F	461	Total 3732	As 1	C 2403	N 628	O 682	S 18	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP F9ULH8
A	-14	GLY	-	expression tag	UNP F9ULH8
A	-13	GLY	-	expression tag	UNP F9ULH8
A	-12	SER	-	expression tag	UNP F9ULH8
A	-11	HIS	-	expression tag	UNP F9ULH8
A	-10	HIS	-	expression tag	UNP F9ULH8
A	-9	HIS	-	expression tag	UNP F9ULH8
A	-8	HIS	-	expression tag	UNP F9ULH8
A	-7	HIS	-	expression tag	UNP F9ULH8
A	-6	HIS	-	expression tag	UNP F9ULH8
A	-5	GLY	-	expression tag	UNP F9ULH8
A	-4	ASP	-	expression tag	UNP F9ULH8
A	-3	ASP	-	expression tag	UNP F9ULH8
A	-2	ASP	-	expression tag	UNP F9ULH8
A	-1	ASP	-	expression tag	UNP F9ULH8
A	0	LYS	-	expression tag	UNP F9ULH8
B	-15	MET	-	initiating methionine	UNP F9ULH8

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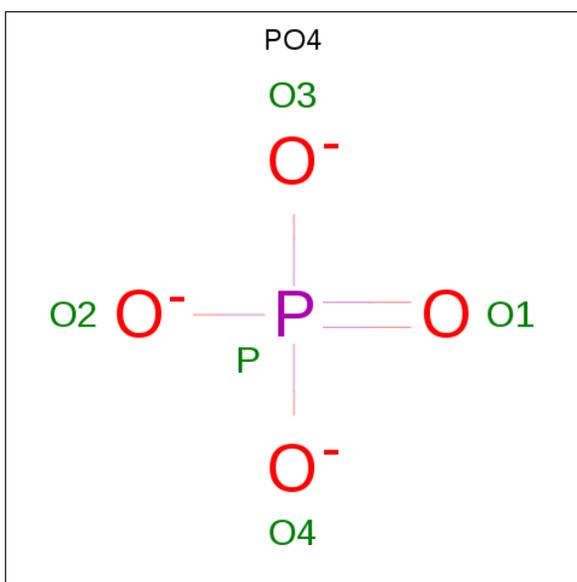
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	GLY	-	expression tag	UNP F9ULH8
B	-13	GLY	-	expression tag	UNP F9ULH8
B	-12	SER	-	expression tag	UNP F9ULH8
B	-11	HIS	-	expression tag	UNP F9ULH8
B	-10	HIS	-	expression tag	UNP F9ULH8
B	-9	HIS	-	expression tag	UNP F9ULH8
B	-8	HIS	-	expression tag	UNP F9ULH8
B	-7	HIS	-	expression tag	UNP F9ULH8
B	-6	HIS	-	expression tag	UNP F9ULH8
B	-5	GLY	-	expression tag	UNP F9ULH8
B	-4	ASP	-	expression tag	UNP F9ULH8
B	-3	ASP	-	expression tag	UNP F9ULH8
B	-2	ASP	-	expression tag	UNP F9ULH8
B	-1	ASP	-	expression tag	UNP F9ULH8
B	0	LYS	-	expression tag	UNP F9ULH8
C	-15	MET	-	initiating methionine	UNP F9ULH8
C	-14	GLY	-	expression tag	UNP F9ULH8
C	-13	GLY	-	expression tag	UNP F9ULH8
C	-12	SER	-	expression tag	UNP F9ULH8
C	-11	HIS	-	expression tag	UNP F9ULH8
C	-10	HIS	-	expression tag	UNP F9ULH8
C	-9	HIS	-	expression tag	UNP F9ULH8
C	-8	HIS	-	expression tag	UNP F9ULH8
C	-7	HIS	-	expression tag	UNP F9ULH8
C	-6	HIS	-	expression tag	UNP F9ULH8
C	-5	GLY	-	expression tag	UNP F9ULH8
C	-4	ASP	-	expression tag	UNP F9ULH8
C	-3	ASP	-	expression tag	UNP F9ULH8
C	-2	ASP	-	expression tag	UNP F9ULH8
C	-1	ASP	-	expression tag	UNP F9ULH8
C	0	LYS	-	expression tag	UNP F9ULH8
D	-15	MET	-	initiating methionine	UNP F9ULH8
D	-14	GLY	-	expression tag	UNP F9ULH8
D	-13	GLY	-	expression tag	UNP F9ULH8
D	-12	SER	-	expression tag	UNP F9ULH8
D	-11	HIS	-	expression tag	UNP F9ULH8
D	-10	HIS	-	expression tag	UNP F9ULH8
D	-9	HIS	-	expression tag	UNP F9ULH8
D	-8	HIS	-	expression tag	UNP F9ULH8
D	-7	HIS	-	expression tag	UNP F9ULH8
D	-6	HIS	-	expression tag	UNP F9ULH8
D	-5	GLY	-	expression tag	UNP F9ULH8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ASP	-	expression tag	UNP F9ULH8
D	-3	ASP	-	expression tag	UNP F9ULH8
D	-2	ASP	-	expression tag	UNP F9ULH8
D	-1	ASP	-	expression tag	UNP F9ULH8
D	0	LYS	-	expression tag	UNP F9ULH8
E	-15	MET	-	initiating methionine	UNP F9ULH8
E	-14	GLY	-	expression tag	UNP F9ULH8
E	-13	GLY	-	expression tag	UNP F9ULH8
E	-12	SER	-	expression tag	UNP F9ULH8
E	-11	HIS	-	expression tag	UNP F9ULH8
E	-10	HIS	-	expression tag	UNP F9ULH8
E	-9	HIS	-	expression tag	UNP F9ULH8
E	-8	HIS	-	expression tag	UNP F9ULH8
E	-7	HIS	-	expression tag	UNP F9ULH8
E	-6	HIS	-	expression tag	UNP F9ULH8
E	-5	GLY	-	expression tag	UNP F9ULH8
E	-4	ASP	-	expression tag	UNP F9ULH8
E	-3	ASP	-	expression tag	UNP F9ULH8
E	-2	ASP	-	expression tag	UNP F9ULH8
E	-1	ASP	-	expression tag	UNP F9ULH8
E	0	LYS	-	expression tag	UNP F9ULH8
F	-15	MET	-	initiating methionine	UNP F9ULH8
F	-14	GLY	-	expression tag	UNP F9ULH8
F	-13	GLY	-	expression tag	UNP F9ULH8
F	-12	SER	-	expression tag	UNP F9ULH8
F	-11	HIS	-	expression tag	UNP F9ULH8
F	-10	HIS	-	expression tag	UNP F9ULH8
F	-9	HIS	-	expression tag	UNP F9ULH8
F	-8	HIS	-	expression tag	UNP F9ULH8
F	-7	HIS	-	expression tag	UNP F9ULH8
F	-6	HIS	-	expression tag	UNP F9ULH8
F	-5	GLY	-	expression tag	UNP F9ULH8
F	-4	ASP	-	expression tag	UNP F9ULH8
F	-3	ASP	-	expression tag	UNP F9ULH8
F	-2	ASP	-	expression tag	UNP F9ULH8
F	-1	ASP	-	expression tag	UNP F9ULH8
F	0	LYS	-	expression tag	UNP F9ULH8

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ — P ═ O O1

P

O⁻

O4

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

- Molecule 3 is water.

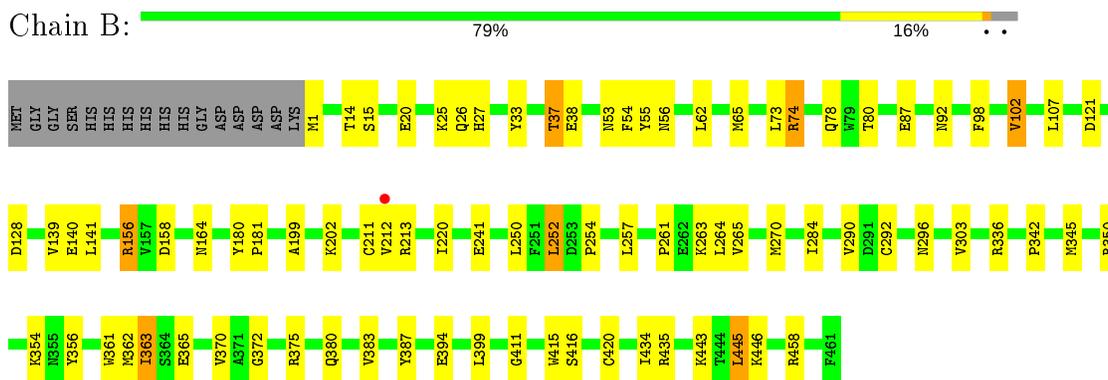| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	333	Total 333	O 333	0	0
3	B	324	Total 324	O 324	0	0
3	C	271	Total 271	O 271	0	0
3	D	271	Total 271	O 271	0	0
3	E	231	Total 231	O 231	0	0
3	F	175	Total 175	O 175	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.
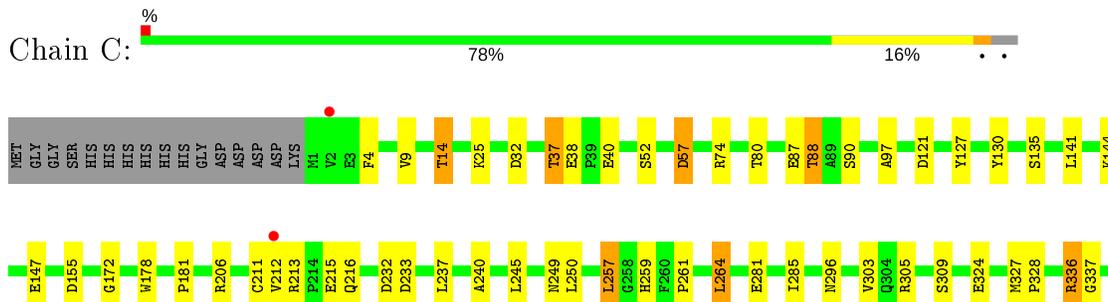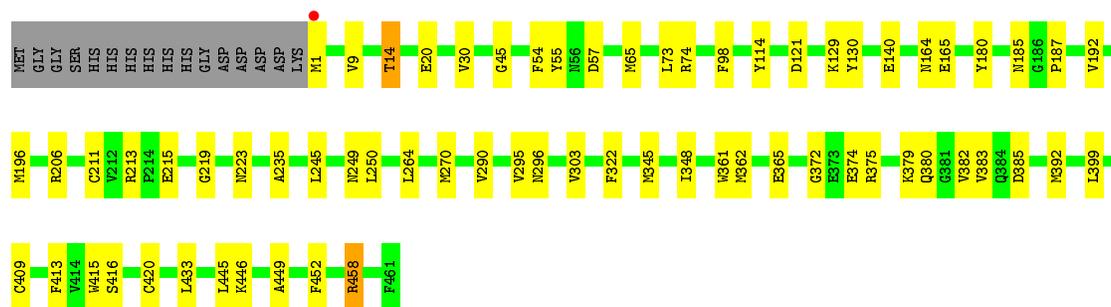
- Molecule 1: Beta-galactosidase

- Molecule 1: Beta-galactosidase
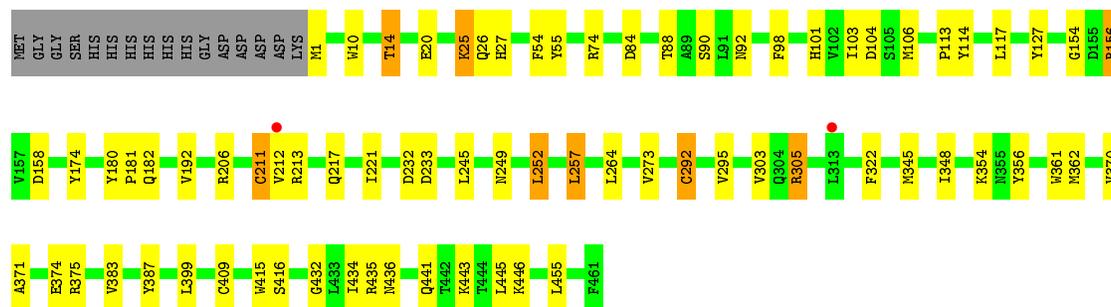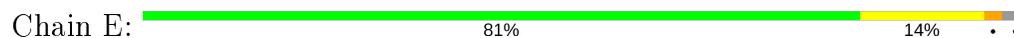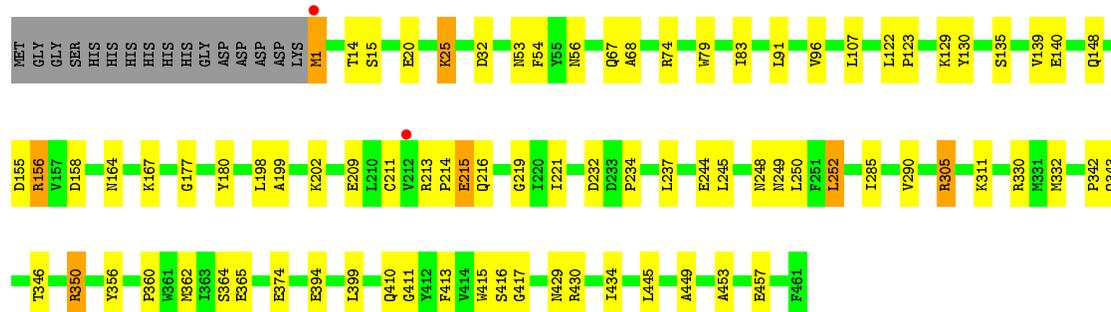

- Molecule 1: Beta-galactosidase

P342 M345 R350 Q353 K354 W361 M362 I363 S364 E365 G372 R375 K379 D385 D386 Y387 L399 G402 S407 N408 C409 Q410 G411 Y412 F413 V414 W415 S416 D419 C420 Y431 I434 R435 N436 Q441 L445 E454 E457 R458 N459 G460 F461

- Molecule 1: Beta-galactosidase

Chain D:

82%   14%

MET GLY GLY SER HIS HIS HIS HIS HIS GLY ASP ASP ASP LYS M1 V9 T14 E20 V30 G45 F54 Y55 N56 D57 M65 L73 R74 F98 Y114 D121 K129 Y130 E140 N164 E165 Y180 N185 G186 P187 V192

M196 R206 C211 V212 R213 P214 E215 G219 N223 A235 L245 N249 L250 L264 N270 V290 V295 V296 V303 F322 M345 I348 W361 M362 E365 G372 E373 E374 R375 K379 Q380 G381 V382 V383 Q384 D385 M392 L399

C409 F413 V414 W415 S416 C420 L433 L445 L446 A449 F452 R458 F461

- Molecule 1: Beta-galactosidase

Chain E:

81%   14%

MET GLY GLY SER HIS HIS HIS HIS HIS GLY ASP ASP ASP LYS M1 W10 T14 E20 K25 Q26 H27 F54 Y55 R74 D84 T88 A89 S90 I91 N92 F98 H101 V102 I103 D104 S105 M106 P113 Y114 L117 Y127 G154 D155 R156

V157 D158 Y174 Y180 P181 Q182 V192 R206 C211 V212 R213 Q217 I221 D232 D233 L245 N249 L252 L257 L264 V273 Q292 V295 V303 Q304 R305 I313 F322 M345 I348 K354 N355 Y356 W361 M362 V370

A371 E374 R375 V383 Y387 L399 C409 W415 S416 G432 L433 I434 R435 N436 Q441 T442 K443 T444 L445 K446 L455 F461

- Molecule 1: Beta-galactosidase

Chain F:

79%   16%

MET GLY GLY SER HIS HIS HIS HIS HIS GLY ASP ASP ASP LYS M1 T14 S15 E20 K25 D32 N53 F54 Y55 N56 Q67 A68 R74 W79 I83 L91 V96 L107 L122 P123 K129 Y130 S135 V139 E140 Q148

D155 R156 V157 D158 N164 K167 G177 Y180 L198 A199 K202 E209 L210 C211 V212 R213 P214 E215 Q216 G219 I220 I221 D232 D233 P234 L237 E244 L245 N248 N249 L250 F251 L252 I285 V290 R305 K311 R330 M331 M332 P342 Q343

T346 R350 Y356 P360 W361 M362 I363 S364 E365 E374 E394 L399 Q410 G411 Y412 F413 V414 W415 S416 G417 N429 R430 I434 L445 A449 A453 E457 F461

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.69Å 191.68Å 105.93Å 90.00° 102.75° 90.00°	Depositor
Resolution (Å)	61.23 – 2.48 61.23 – 2.48	Depositor EDS
% Data completeness (in resolution range)	93.9 (61.23-2.48) 93.9 (61.23-2.48)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.14	Depositor
$<I/\sigma(I)>$ [1]	2.18 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.159 , 0.217 0.161 , 0.218	Depositor DCC
R_{free} test set	6370 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.9	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24057	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: CAS, PO4

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	0.44	0/3843	0.61	0/5236
1	B	0.43	0/3843	0.61	1/5236 (0.0%)
1	C	0.48	3/3843 (0.1%)	0.61	2/5236 (0.0%)
1	D	0.42	0/3843	0.59	2/5236 (0.0%)
1	E	0.50	3/3843 (0.1%)	0.57	0/5236
1	F	0.43	1/3843 (0.0%)	0.56	0/5236
All	All	0.45	7/23058 (0.0%)	0.59	5/31416 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	374	GLU	CD-OE1	-11.86	1.12	1.25
1	E	374	GLU	CD-OE2	-11.16	1.13	1.25
1	C	350	ARG	CZ-NH1	-9.79	1.20	1.33
1	C	350	ARG	NE-CZ	-7.90	1.22	1.33
1	F	215	GLU	CD-OE1	-6.41	1.18	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	350	ARG	NE-CZ-NH1	-10.00	115.30	120.30
1	C	350	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	D	379	LYS	CD-CE-NZ	5.43	124.20	111.70
1	B	445	LEU	CA-CB-CG	5.32	127.53	115.30
1	D	445	LEU	CA-CB-CG	5.12	127.08	115.30

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	3732	0	3509	46	0
1	B	3732	0	3509	52	0
1	C	3732	0	3509	57	0
1	D	3732	0	3509	39	0
1	E	3732	0	3508	50	0
1	F	3732	0	3509	58	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	2	0
2	D	10	0	0	0	0
2	E	10	0	0	1	0
2	F	10	0	0	0	0
3	A	333	0	0	11	0
3	B	324	0	0	5	0
3	C	271	0	0	8	0
3	D	271	0	0	7	0
3	E	231	0	0	10	0
3	F	175	0	0	16	0
All	All	24057	0	21053	304	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 7.

The worst 5 of 304 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:E:104:ASP:OD1	1:E:156:ARG:NH1	1.56	1.37
1:F:53:ASN:HD21	1:F:56:ASN:HD22	1.17	0.89
1:B:241:GLU:OE1	3:B:601:HOH:O	1.88	0.88
1:C:37:THR:HG22	1:C:38:GLU:HG3	1.56	0.88
1:E:158:ASP:OD2	1:E:213:ARG:NH1	2.08	0.87

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	458/477 (96%)	442 (96%)	16 (4%)	0	100	100
1	B	458/477 (96%)	443 (97%)	15 (3%)	0	100	100
1	C	458/477 (96%)	442 (96%)	16 (4%)	0	100	100
1	D	458/477 (96%)	442 (96%)	16 (4%)	0	100	100
1	E	458/477 (96%)	443 (97%)	15 (3%)	0	100	100
1	F	458/477 (96%)	437 (95%)	20 (4%)	1 (0%)	47	66
All	All	2748/2862 (96%)	2649 (96%)	98 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	305	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/399 (97%)	372 (96%)	14 (4%)	35	58
1	B	386/399 (97%)	371 (96%)	15 (4%)	32	55
1	C	386/399 (97%)	369 (96%)	17 (4%)	28	49
1	D	386/399 (97%)	377 (98%)	9 (2%)	50	74
1	E	386/399 (97%)	374 (97%)	12 (3%)	40	64
1	F	386/399 (97%)	375 (97%)	11 (3%)	43	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2316/2394 (97%)	2238 (97%)	78 (3%)	37 61

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	135	SER
1	C	354	LYS
1	F	211	CYS
1	C	250	LEU
1	C	309	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	314	GLN
1	D	164	ASN
1	E	182	GLN
1	C	296	ASN
1	E	436	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	CAS	B	292	1	5,8,9	0.72	0	1,9,11	3.37	1 (100%)
1	CAS	F	292	1	5,8,9	0.93	0	1,9,11	0.20	0
1	CAS	C	292	1	5,8,9	0.90	0	1,9,11	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z|>2$	Counts	RMSZ	$\#|Z|>2$
1	CAS	A	292	1	5,8,9	0.90	0	1,9,11	0.51	0
1	CAS	E	292	1	5,8,9	0.73	0	1,9,11	3.66	1 (100%)
1	CAS	D	292	1	5,8,9	0.97	0	1,9,11	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CAS	B	292	1	-	0/0/7/9	-
1	CAS	F	292	1	-	0/0/7/9	-
1	CAS	C	292	1	-	0/0/7/9	-
1	CAS	A	292	1	-	0/0/7/9	-
1	CAS	E	292	1	-	0/0/7/9	-
1	CAS	D	292	1	-	0/0/7/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	292	CAS	CA-CB-SG	3.66	129.82	114.43
1	B	292	CAS	CA-CB-SG	3.37	128.60	114.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	292	CAS	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	PO4	C	502	-	4,4,4	0.68	0	6,6,6	0.70	0
2	PO4	E	502	-	4,4,4	0.82	0	6,6,6	0.58	0
2	PO4	A	501	-	4,4,4	0.75	0	6,6,6	0.65	0
2	PO4	B	501	-	4,4,4	0.98	0	6,6,6	0.65	0
2	PO4	D	502	-	4,4,4	0.75	0	6,6,6	0.61	0
2	PO4	E	501	-	4,4,4	0.95	0	6,6,6	0.38	0
2	PO4	F	501	-	4,4,4	0.73	0	6,6,6	0.62	0
2	PO4	C	501	-	4,4,4	0.85	0	6,6,6	0.53	0
2	PO4	D	501	-	4,4,4	0.79	0	6,6,6	0.77	0
2	PO4	B	502	-	4,4,4	0.77	0	6,6,6	0.43	0
2	PO4	F	502	-	4,4,4	0.81	0	6,6,6	0.60	0
2	PO4	A	502	-	4,4,4	0.63	0	6,6,6	0.64	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	PO4	1	0
2	E	502	PO4	1	0
2	C	501	PO4	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	460/477 (96%)	-0.41	0	100	100	14, 24, 44, 83	0
1	B	460/477 (96%)	-0.37	1 (0%)	95	95	14, 25, 45, 85	0
1	C	460/477 (96%)	-0.23	5 (1%)	80	82	16, 30, 56, 88	0
1	D	460/477 (96%)	-0.30	1 (0%)	95	95	16, 27, 49, 103	0
1	E	460/477 (96%)	-0.31	2 (0%)	92	93	17, 30, 53, 96	0
1	F	460/477 (96%)	-0.22	2 (0%)	92	93	17, 36, 63, 116	0
All	All	2760/2862 (96%)	-0.31	11 (0%)	92	93	14, 29, 53, 116	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	212	VAL	3.7
1	E	313	LEU	3.5
1	E	212	VAL	3.3
1	C	454	GLU	2.8
1	C	212	VAL	2.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
1	CAS	B	292	9/10	0.88	0.23	29,36,193,196	0
1	CAS	E	292	9/10	0.91	0.21	25,31,183,185	0
1	CAS	F	292	9/10	0.95	0.13	40,43,120,124	0
1	CAS	D	292	9/10	0.96	0.18	25,36,163,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	CAS	C	292	9/10	0.98	0.14	28,32,143,145	0
1	CAS	A	292	9/10	0.98	0.15	19,26,127,129	0

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å²)	Q<0.9
2	PO4	E	502	5/5	0.93	0.18	60,68,71,76	0
2	PO4	C	502	5/5	0.95	0.15	39,61,67,73	0
2	PO4	D	502	5/5	0.95	0.15	41,51,60,69	0
2	PO4	B	502	5/5	0.95	0.12	42,54,61,67	0
2	PO4	F	502	5/5	0.97	0.13	47,53,63,71	0
2	PO4	A	502	5/5	0.97	0.13	31,39,54,57	0
2	PO4	D	501	5/5	0.98	0.14	21,37,44,45	0
2	PO4	E	501	5/5	0.98	0.15	30,32,41,55	0
2	PO4	F	501	5/5	0.98	0.17	31,40,53,54	0
2	PO4	C	501	5/5	0.98	0.13	34,36,44,58	0
2	PO4	A	501	5/5	0.99	0.12	33,42,44,61	0
2	PO4	B	501	5/5	0.99	0.19	34,42,52,61	0

6.5 Other polymers (i)

There are no such residues in this entry.