WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 28, 2024 – 05:29 pm GMT

PDB ID	:	5CW7
Title	:	Crystal structure of the PaaA2-ParE2 antitoxin-toxin complex
Authors	:	Sterckx, Y.G.-J.; Loris, R.
Deposited on	:	2015-07-27
Resolution	:	2.83 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.83 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.
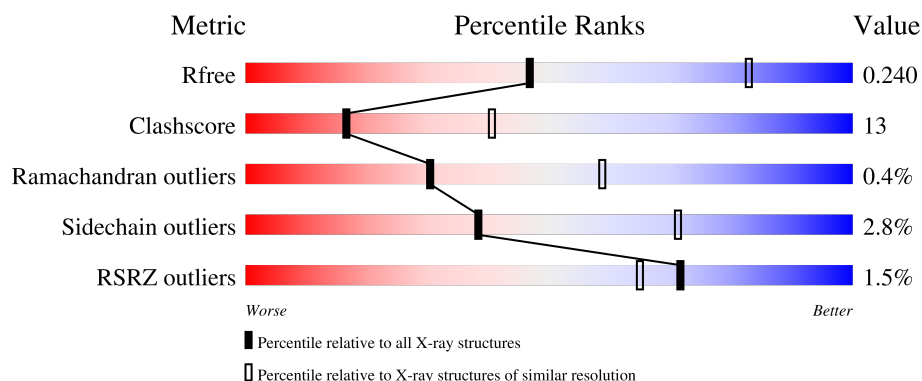
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4293 (2.84-2.80)
Clashscore	180529	4801 (2.84-2.80)
Ramachandran outliers	177936	4739 (2.84-2.80)
Sidechain outliers	177891	4741 (2.84-2.80)
RSRZ outliers	164620	4295 (2.84-2.80)

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 of 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	71	75% 7% · 15%
1	C	71	49% 30% · 20%
1	E	71	55% 25% · 17%
1	G	71	66% 18% · 14%
1	I	71	55% 28% 17%

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Mol	Chain	Length	Quality of chain
1	K	71	4% 61% 23% 14%
1	M	71	4% 59% 20% 20%
1	O	71	% 61% 24% 15%
2	B	100	% 72% 19% 5%
2	D	100	73% 16% 6% 5%
2	F	100	75% 19%
2	H	100	% 69% 23% 5%
2	J	100	2% 76% 18% 5%
2	L	100	% 71% 20% 5%
2	N	100	% 75% 20% 5%
2	P	100	% 76% 18% 5%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 10547 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 PAAA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	60	Total 478	C 295	N 89	O 91	Se 3	0	0	0
1	C	57	Total 455	C 286	N 83	O 83	Se 3	0	0	0
1	E	59	Total 478	C 297	N 90	O 88	Se 3	0	1	0
1	G	61	Total 471	C 292	N 87	O 89	Se 3	0	0	0
1	I	59	Total 476	C 294	N 89	O 90	Se 3	0	0	0
1	K	61	Total 466	C 291	N 86	O 86	Se 3	0	0	0
1	M	57	Total 459	C 285	N 83	O 88	Se 3	0	0	0
1	O	60	Total 478	C 297	N 89	O 89	Se 3	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
A	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
A	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
A	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
A	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
A	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
A	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
A	0	ASP	-	expression tag	UNP A0A0F6F6Q9
A	1	LYS	-	expression tag	UNP A0A0F6F6Q9
C	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
C	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
C	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
C	-4	LYS	-	expression tag	UNP A0A0F6F6Q9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
C	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
C	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
C	0	ASP	-	expression tag	UNP A0A0F6F6Q9
C	1	LYS	-	expression tag	UNP A0A0F6F6Q9
E	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
E	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
E	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
E	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
E	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
E	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
E	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
E	0	ASP	-	expression tag	UNP A0A0F6F6Q9
E	1	LYS	-	expression tag	UNP A0A0F6F6Q9
G	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
G	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
G	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
G	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
G	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
G	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
G	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
G	0	ASP	-	expression tag	UNP A0A0F6F6Q9
G	1	LYS	-	expression tag	UNP A0A0F6F6Q9
I	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
I	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
I	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
I	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
I	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
I	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
I	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
I	0	ASP	-	expression tag	UNP A0A0F6F6Q9
I	1	LYS	-	expression tag	UNP A0A0F6F6Q9
K	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
K	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
K	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
K	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
K	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
K	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
K	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
K	0	ASP	-	expression tag	UNP A0A0F6F6Q9
K	1	LYS	-	expression tag	UNP A0A0F6F6Q9
M	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
M	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
M	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
M	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
M	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
M	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
M	0	ASP	-	expression tag	UNP A0A0F6F6Q9
M	1	LYS	-	expression tag	UNP A0A0F6F6Q9
O	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
O	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
O	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
O	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
O	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
O	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
O	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
O	0	ASP	-	expression tag	UNP A0A0F6F6Q9
O	1	LYS	-	expression tag	UNP A0A0F6F6Q9

- Molecule 2 is a protein called Plasmid stabilization protein ParE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	95	Total 780	C 502	N 136	O 140	S 1	Se 1	0	0	0
2	D	95	Total 776	C 500	N 136	O 138	S 1	Se 1	0	0	0
2	F	96	Total 790	C 508	N 139	O 141	S 1	Se 1	0	0	0
2	H	95	Total 771	C 498	N 133	O 138	S 1	Se 1	0	0	0
2	J	95	Total 776	C 500	N 136	O 138	S 1	Se 1	0	0	0
2	L	95	Total 776	C 500	N 136	O 138	S 1	Se 1	0	0	0
2	N	95	Total 776	C 500	N 136	O 138	S 1	Se 1	0	0	0
2	P	95	Total 786	C 506	N 138	O 140	S 1	Se 1	0	1	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	-	initiating methionine	UNP A0A0D7C2L1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	93	LEU	-	expression tag	UNP A0A0D7C2L1
B	94	GLU	-	expression tag	UNP A0A0D7C2L1
B	95	HIS	-	expression tag	UNP A0A0D7C2L1
B	96	HIS	-	expression tag	UNP A0A0D7C2L1
B	97	HIS	-	expression tag	UNP A0A0D7C2L1
B	98	HIS	-	expression tag	UNP A0A0D7C2L1
B	99	HIS	-	expression tag	UNP A0A0D7C2L1
B	100	HIS	-	expression tag	UNP A0A0D7C2L1
D	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
D	93	LEU	-	expression tag	UNP A0A0D7C2L1
D	94	GLU	-	expression tag	UNP A0A0D7C2L1
D	95	HIS	-	expression tag	UNP A0A0D7C2L1
D	96	HIS	-	expression tag	UNP A0A0D7C2L1
D	97	HIS	-	expression tag	UNP A0A0D7C2L1
D	98	HIS	-	expression tag	UNP A0A0D7C2L1
D	99	HIS	-	expression tag	UNP A0A0D7C2L1
D	100	HIS	-	expression tag	UNP A0A0D7C2L1
F	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
F	93	LEU	-	expression tag	UNP A0A0D7C2L1
F	94	GLU	-	expression tag	UNP A0A0D7C2L1
F	95	HIS	-	expression tag	UNP A0A0D7C2L1
F	96	HIS	-	expression tag	UNP A0A0D7C2L1
F	97	HIS	-	expression tag	UNP A0A0D7C2L1
F	98	HIS	-	expression tag	UNP A0A0D7C2L1
F	99	HIS	-	expression tag	UNP A0A0D7C2L1
F	100	HIS	-	expression tag	UNP A0A0D7C2L1
H	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
H	93	LEU	-	expression tag	UNP A0A0D7C2L1
H	94	GLU	-	expression tag	UNP A0A0D7C2L1
H	95	HIS	-	expression tag	UNP A0A0D7C2L1
H	96	HIS	-	expression tag	UNP A0A0D7C2L1
H	97	HIS	-	expression tag	UNP A0A0D7C2L1
H	98	HIS	-	expression tag	UNP A0A0D7C2L1
H	99	HIS	-	expression tag	UNP A0A0D7C2L1
H	100	HIS	-	expression tag	UNP A0A0D7C2L1
J	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
J	93	LEU	-	expression tag	UNP A0A0D7C2L1
J	94	GLU	-	expression tag	UNP A0A0D7C2L1
J	95	HIS	-	expression tag	UNP A0A0D7C2L1
J	96	HIS	-	expression tag	UNP A0A0D7C2L1
J	97	HIS	-	expression tag	UNP A0A0D7C2L1
J	98	HIS	-	expression tag	UNP A0A0D7C2L1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	99	HIS	-	expression tag	UNP A0A0D7C2L1
J	100	HIS	-	expression tag	UNP A0A0D7C2L1
L	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
L	93	LEU	-	expression tag	UNP A0A0D7C2L1
L	94	GLU	-	expression tag	UNP A0A0D7C2L1
L	95	HIS	-	expression tag	UNP A0A0D7C2L1
L	96	HIS	-	expression tag	UNP A0A0D7C2L1
L	97	HIS	-	expression tag	UNP A0A0D7C2L1
L	98	HIS	-	expression tag	UNP A0A0D7C2L1
L	99	HIS	-	expression tag	UNP A0A0D7C2L1
L	100	HIS	-	expression tag	UNP A0A0D7C2L1
N	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
N	93	LEU	-	expression tag	UNP A0A0D7C2L1
N	94	GLU	-	expression tag	UNP A0A0D7C2L1
N	95	HIS	-	expression tag	UNP A0A0D7C2L1
N	96	HIS	-	expression tag	UNP A0A0D7C2L1
N	97	HIS	-	expression tag	UNP A0A0D7C2L1
N	98	HIS	-	expression tag	UNP A0A0D7C2L1
N	99	HIS	-	expression tag	UNP A0A0D7C2L1
N	100	HIS	-	expression tag	UNP A0A0D7C2L1
P	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
P	93	LEU	-	expression tag	UNP A0A0D7C2L1
P	98	GLU	-	expression tag	UNP A0A0D7C2L1
P	99	HIS	-	expression tag	UNP A0A0D7C2L1
P	100	HIS	-	expression tag	UNP A0A0D7C2L1
P	101	HIS	-	expression tag	UNP A0A0D7C2L1
P	102	HIS	-	expression tag	UNP A0A0D7C2L1
P	103	HIS	-	expression tag	UNP A0A0D7C2L1
P	104	HIS	-	expression tag	UNP A0A0D7C2L1

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1 C2

HO

O1

OH

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	F	1	Total 6	C 3	O 3	0	0
3	H	1	Total 6	C 3	O 3	0	0
3	L	1	Total 6	C 3	O 3	0	0
3	L	1	Total 6	C 3	O 3	0	0
3	N	1	Total 6	C 3	O 3	0	0
3	P	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total 34	O 34	0	0
4	B	42	Total 42	O 42	0	0
4	C	33	Total 33	O 33	0	0
4	D	49	Total 49	O 49	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	26	Total 26	O 26	0	0
4	F	47	Total 47	O 47	0	0
4	G	15	Total 15	O 15	0	0
4	H	45	Total 45	O 45	0	0
4	I	12	Total 12	O 12	0	0
4	J	30	Total 30	O 30	0	0
4	K	15	Total 15	O 15	0	0
4	L	28	Total 28	O 28	0	0
4	M	22	Total 22	O 22	0	0
4	N	41	Total 41	O 41	0	0
4	O	26	Total 26	O 26	0	0
4	P	42	Total 42	O 42	0	0

3 Residue-property plots ⓘ

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: PAAA2
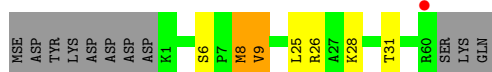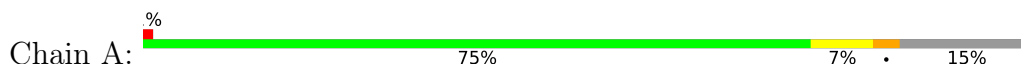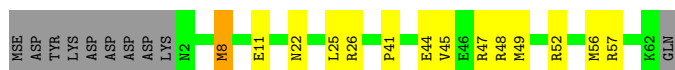
Chain A:

- Molecule 1: PAAA2

Chain C:

- Molecule 1: PAAA2

Chain E:

- Molecule 1: PAAA2

Chain G:

- Molecule 1: PAAA2

Chain I:

- Molecule 1: PAAA2

Chain K:

• Molecule 1: PAAA2

Chain M:

• Molecule 1: PAAA2

Chain O:

• Molecule 2: Plasmid stabilization protein ParE

Chain B:

• Molecule 2: Plasmid stabilization protein ParE

Chain D:

• Molecule 2: Plasmid stabilization protein ParE

Chain F:

• Molecule 2: Plasmid stabilization protein ParE

Chain H:

• Molecule 2: Plasmid stabilization protein ParE

Chain J:

M1 W6 D13 L14 I21 E30 Q34 R37 V40 S44 P47 Y48 L49 D54 R55 V56 L59 R73 N83 R88 R89 L93 E94 H95 HIS HIS HIS HIS

• Molecule 2: Plasmid stabilization protein ParE

Chain L:

M1 L2 L5 W6 S19 Y20 F24 R35 L36 R37 G38 C39 P47 Y48 L49 Y50 R55 I62 V63 A64 H65 P66 N67 S78 H86 A87 R88 R89 L93 E94 H95 HIS HIS HIS HIS

• Molecule 2: Plasmid stabilization protein ParE

Chain N:

M1 L5 W6 D11 L14 I21 Q34 R35 L36 R37 V40 L49 R55 R60 A64 H65 S78 I85 R88 R89 Q90 L93 E94 H95 HIS HIS HIS HIS

• Molecule 2: Plasmid stabilization protein ParE

Chain P:

M1 L5 S19 Y20 I21 E30 Q34 R35 V40 L43 L49 Y50 D54 R55 V56 L59 R60 A64 H65 P66 N67 I85 R88 L93 GLU H99 H100 HIS HIS HIS HIS
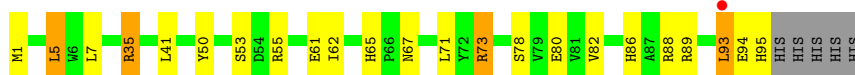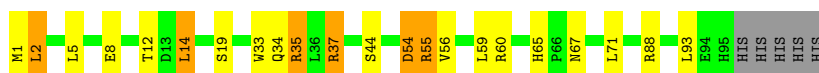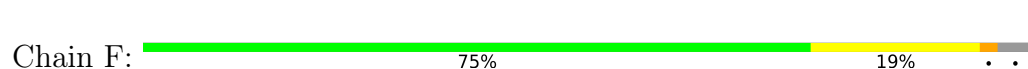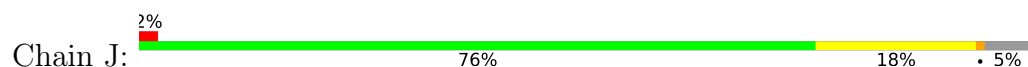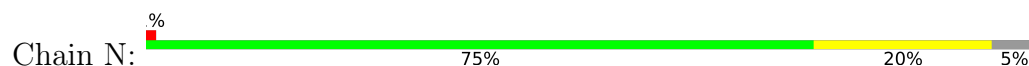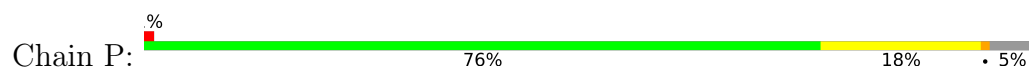
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	90.54Å 90.54Å 412.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.83 49.37 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.37-2.83) 99.8 (49.37-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.185 , 0.240 0.185 , 0.240	Depositor DCC
R_{free} test set	2117 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.9	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.7	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10547	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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:
GOL

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	0.57	0/484	0.68	1/649 (0.2%)
1	C	0.59	0/461	0.65	0/616
1	E	0.63	0/487	0.74	0/651
1	G	0.55	0/477	0.71	1/641 (0.2%)
1	I	0.63	0/482	0.66	0/645
1	K	0.67	0/472	0.71	0/634
1	M	0.69	0/465	0.67	0/623
1	O	0.62	0/484	0.71	0/648
2	B	0.64	0/802	0.69	0/1099
2	D	0.81	2/798 (0.3%)	0.81	2/1094 (0.2%)
2	F	0.64	0/813	0.75	1/1114 (0.1%)
2	H	0.71	0/793	0.73	1/1088 (0.1%)
2	J	0.68	1/798 (0.1%)	0.66	1/1094 (0.1%)
2	L	0.74	2/798 (0.3%)	0.83	2/1094 (0.2%)
2	N	0.70	1/798 (0.1%)	0.71	1/1094 (0.1%)
2	P	0.71	1/811 (0.1%)	0.67	0/1110
All	All	0.67	7/10223 (0.1%)	0.72	10/13894 (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
2	B	0	1
2	D	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	55	ARG	NE-CZ	-7.37	1.23	1.33
2	D	55	ARG	CZ-NH1	-7.21	1.23	1.33
2	L	49	LEU	C-N	-6.86	1.18	1.34
2	P	49	LEU	C-N	-6.09	1.20	1.34
2	L	39	CYS	CB-SG	-5.89	1.72	1.81

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	55	ARG	NE-CZ-NH1	-8.25	116.17	120.30
2	F	49	LEU	CB-CG-CD2	-6.10	100.63	111.00
2	L	5	LEU	CA-CB-CG	6.00	129.11	115.30
1	G	8	MSE	CG-SE-CE	5.85	111.77	98.90
2	N	14	LEU	CB-CG-CD2	-5.78	101.18	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	93	LEU	Peptide
2	D	93	LEU	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	478	0	449	4	0
1	C	455	0	441	26	0
1	E	478	0	465	13	0
1	G	471	0	437	15	0
1	I	476	0	456	24	0
1	K	466	0	433	20	0
1	M	459	0	436	15	0
1	O	478	0	456	17	0
2	B	780	0	776	28	0
2	D	776	0	772	29	0
2	F	790	0	783	19	0
2	H	771	0	763	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	776	0	772	18	0
2	L	776	0	771	34	0
2	N	776	0	772	26	0
2	P	786	0	779	16	0
3	B	12	0	16	3	0
3	F	6	0	8	1	0
3	H	6	0	8	0	0
3	L	12	0	16	1	0
3	N	6	0	8	0	0
3	P	6	0	8	0	0
4	A	34	0	0	1	0
4	B	42	0	0	1	0
4	C	33	0	0	3	0
4	D	49	0	0	3	0
4	E	26	0	0	2	0
4	F	47	0	0	0	1
4	G	15	0	0	0	0
4	H	45	0	0	0	0
4	I	12	0	0	1	0
4	J	30	0	0	1	0
4	K	15	0	0	2	0
4	L	28	0	0	0	0
4	M	22	0	0	0	0
4	N	41	0	0	3	1
4	O	26	0	0	2	0
4	P	42	0	0	0	0
All	All	10547	0	9825	253	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.

The worst 5 of 253 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:I:8:MSE:SE	1:I:8:MSE:CE	2.16	1.43
1:I:8:MSE:SE	2:L:89:ARG:HH22	1.58	1.36
1:I:8:MSE:SE	2:L:89:ARG:HH12	1.65	1.30
1:I:8:MSE:SE	2:L:89:ARG:NH2	2.20	1.25
1:I:8:MSE:SE	2:L:89:ARG:NH1	2.26	1.16

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:318:HOH:O	4:N:308:HOH:O[5_555]	2.10	0.10

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	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
1	C	55/71 (78%)	54 (98%)	0	1 (2%)	7	22
1	E	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
1	G	59/71 (83%)	56 (95%)	3 (5%)	0	100	100
1	I	57/71 (80%)	56 (98%)	1 (2%)	0	100	100
1	K	59/71 (83%)	58 (98%)	0	1 (2%)	7	24
1	M	55/71 (78%)	51 (93%)	3 (6%)	1 (2%)	7	22
1	O	58/71 (82%)	57 (98%)	0	1 (2%)	7	24
2	B	93/100 (93%)	90 (97%)	3 (3%)	0	100	100
2	D	93/100 (93%)	91 (98%)	2 (2%)	0	100	100
2	F	94/100 (94%)	91 (97%)	3 (3%)	0	100	100
2	H	93/100 (93%)	91 (98%)	2 (2%)	0	100	100
2	J	93/100 (93%)	89 (96%)	3 (3%)	1 (1%)	12	35
2	L	93/100 (93%)	89 (96%)	4 (4%)	0	100	100
2	N	93/100 (93%)	91 (98%)	2 (2%)	0	100	100
2	P	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
All	All	1203/1368 (88%)	1167 (97%)	31 (3%)	5 (0%)	30	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	94	GLU
1	M	3	ARG
1	C	59	GLU
1	O	59	GLU
1	K	7	PRO

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	47/60 (78%)	45 (96%)	2 (4%)	25	56
1	C	45/60 (75%)	43 (96%)	2 (4%)	24	55
1	E	49/60 (82%)	44 (90%)	5 (10%)	6	18
1	G	46/60 (77%)	46 (100%)	0	100	100
1	I	49/60 (82%)	49 (100%)	0	100	100
1	K	44/60 (73%)	43 (98%)	1 (2%)	45	77
1	M	47/60 (78%)	47 (100%)	0	100	100
1	O	47/60 (78%)	47 (100%)	0	100	100
2	B	87/91 (96%)	84 (97%)	3 (3%)	32	64
2	D	86/91 (94%)	81 (94%)	5 (6%)	17	43
2	F	88/91 (97%)	86 (98%)	2 (2%)	45	77
2	H	85/91 (93%)	81 (95%)	4 (5%)	22	52
2	J	86/91 (94%)	84 (98%)	2 (2%)	45	77
2	L	86/91 (94%)	84 (98%)	2 (2%)	45	77
2	N	86/91 (94%)	85 (99%)	1 (1%)	67	89
2	P	88/91 (97%)	85 (97%)	3 (3%)	32	64
All	All	1066/1208 (88%)	1034 (97%)	32 (3%)	38	69

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	40	VAL

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Mol	Chain	Res	Type
2	P	43	LEU
1	E	3	ARG
2	D	54	ASP
2	P	54[A]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	34	GLN
2	L	65	HIS
2	P	65	HIS
2	L	86	HIS
1	C	17	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

8 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
3	GOL	L	202	-	5,5,5	0.56	0	5,5,5	0.53	0
3	GOL	B	202	-	5,5,5	0.43	0	5,5,5	0.46	0
3	GOL	L	201	-	5,5,5	0.40	0	5,5,5	0.55	0
3	GOL	N	201	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	P	201	-	5,5,5	0.38	0	5,5,5	0.47	0
3	GOL	B	201	-	5,5,5	0.36	0	5,5,5	0.62	0
3	GOL	F	201	-	5,5,5	0.49	0	5,5,5	0.41	0
3	GOL	H	201	-	5,5,5	0.46	0	5,5,5	0.33	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	L	202	-	-	0/4/4/4	-
3	GOL	B	202	-	-	1/4/4/4	-
3	GOL	L	201	-	-	1/4/4/4	-
3	GOL	N	201	-	-	4/4/4/4	-
3	GOL	P	201	-	-	2/4/4/4	-
3	GOL	B	201	-	-	4/4/4/4	-
3	GOL	F	201	-	-	2/4/4/4	-
3	GOL	H	201	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	GOL	C1-C2-C3-O3
3	H	201	GOL	O1-C1-C2-C3
3	H	201	GOL	C1-C2-C3-O3
3	H	201	GOL	O2-C2-C3-O3
3	N	201	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	202	GOL	2	0
3	L	201	GOL	1	0
3	B	201	GOL	1	0
3	F	201	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	P	1
2	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	49:LEU	C	50:TYR	N	1.20
1	L	49:LEU	C	50:TYR	N	1.18

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	57/71 (80%)	-0.52	1 (1%)	67	60	39, 44, 93, 124	0
1	C	54/71 (76%)	-0.20	2 (3%)	45	37	34, 46, 87, 137	0
1	E	56/71 (78%)	-0.40	1 (1%)	67	60	36, 44, 86, 96	0
1	G	58/71 (81%)	-0.27	0	100	100	41, 55, 99, 149	0
1	I	56/71 (78%)	-0.30	0	100	100	37, 56, 92, 116	0
1	K	58/71 (81%)	-0.10	3 (5%)	34	26	37, 57, 96, 117	0
1	M	54/71 (76%)	-0.15	3 (5%)	31	24	36, 49, 92, 123	0
1	O	57/71 (80%)	-0.48	1 (1%)	67	60	41, 48, 87, 94	0
2	B	94/100 (94%)	-0.60	1 (1%)	77	72	32, 39, 75, 119	0
2	D	94/100 (94%)	-0.69	0	100	100	30, 36, 56, 111	0
2	F	95/100 (95%)	-0.75	0	100	100	30, 36, 59, 79	0
2	H	94/100 (94%)	-0.48	1 (1%)	77	72	33, 43, 81, 107	0
2	J	94/100 (94%)	-0.47	2 (2%)	63	55	34, 47, 70, 144	0
2	L	94/100 (94%)	-0.41	1 (1%)	77	72	35, 47, 77, 123	0
2	N	94/100 (94%)	-0.56	1 (1%)	77	72	34, 41, 59, 92	0
2	P	94/100 (94%)	-0.57	1 (1%)	77	72	34, 42, 68, 99	0
All	All	1203/1368 (87%)	-0.47	18 (1%)	71	65	30, 45, 86, 149	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	93	LEU	5.3
1	C	4	ALA	4.7
2	L	89	ARG	4.2
1	E	60	ARG	3.9
2	J	94	GLU	3.7

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 monosaccharides 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, 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
3	GOL	L	202	6/6	0.85	0.20	63,71,74,75	0
3	GOL	L	201	6/6	0.86	0.13	59,60,61,63	0
3	GOL	N	201	6/6	0.88	0.13	56,66,68,73	0
3	GOL	H	201	6/6	0.90	0.12	59,61,65,69	0
3	GOL	B	201	6/6	0.91	0.13	68,68,70,72	0
3	GOL	B	202	6/6	0.93	0.09	45,55,58,61	0
3	GOL	F	201	6/6	0.94	0.10	51,54,57,57	0
3	GOL	P	201	6/6	0.94	0.10	53,63,68,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.