



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 02:32 AM EDT

PDB ID : 6ET2
Title : Crystal structure of PqsBC (C129A) mutant from *Pseudomonas aeruginosa*
(crystal form 3)
Authors : Witzgall, F.; Blankenfeldt, W.
Deposited on : 2017-10-25
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

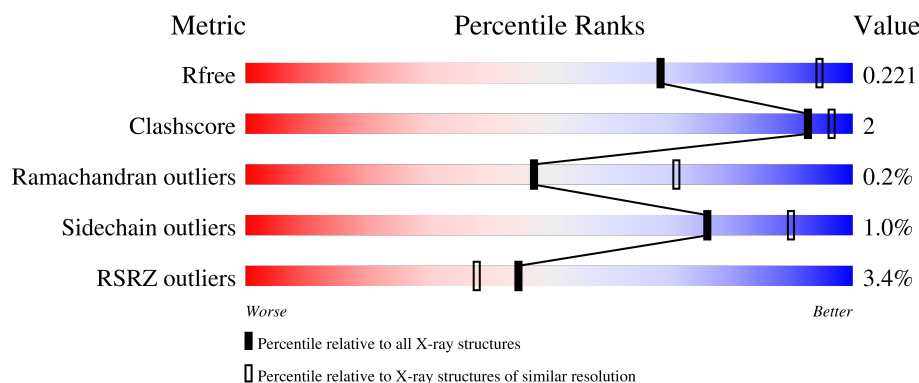
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 $\leq 5\%$. 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	365	<div> <div>2%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	C	365	<div> <div>%</div> <div>90%</div> <div>6%</div> <div>..</div> </div>
1	E	365	<div> <div>7%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	G	365	<div> <div>12%</div> <div>92%</div> <div>.</div> <div>.</div> </div>
1	I	365	<div> <div>%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	365	 93% . .
1	M	365	 10% 90% 7% . .
1	O	365	 3% 92% 5% . .
2	B	283	 2% 97% . .
2	D	283	 95% . .
2	F	283	 2% 96% . .
2	H	283	 4% 97% . .
2	J	283	 94% 5% .
2	L	283	 % 98% . .
2	N	283	 % 96% . .
2	P	283	 3% 97% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 77939 atoms, of which 38341 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 PqsC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	354	Total	C	H	N	O	S	0	0	0
			5383	1725	2668	466	506	18			
1	C	355	Total	C	H	N	O	S	0	1	0
			5411	1735	2682	469	507	18			
1	E	354	Total	C	H	N	O	S	0	1	0
			5358	1725	2645	464	506	18			
1	G	354	Total	C	H	N	O	S	0	1	0
			5357	1724	2643	464	508	18			
1	I	355	Total	C	H	N	O	S	0	0	0
			5410	1732	2680	470	510	18			
1	K	354	Total	C	H	N	O	S	0	0	0
			5382	1726	2666	464	508	18			
1	M	355	Total	C	H	N	O	S	0	0	0
			5362	1722	2648	465	509	18			
1	O	354	Total	C	H	N	O	S	0	0	0
			5353	1719	2644	465	507	18			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP Q9I4X1
A	-15	GLY	-	expression tag	UNP Q9I4X1
A	-14	HIS	-	expression tag	UNP Q9I4X1
A	-13	HIS	-	expression tag	UNP Q9I4X1
A	-12	HIS	-	expression tag	UNP Q9I4X1
A	-11	HIS	-	expression tag	UNP Q9I4X1
A	-10	HIS	-	expression tag	UNP Q9I4X1
A	-9	HIS	-	expression tag	UNP Q9I4X1
A	-8	ALA	-	expression tag	UNP Q9I4X1
A	-7	GLU	-	expression tag	UNP Q9I4X1
A	-6	ASN	-	expression tag	UNP Q9I4X1
A	-5	LEU	-	expression tag	UNP Q9I4X1
A	-4	TYR	-	expression tag	UNP Q9I4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PHE	-	expression tag	UNP Q9I4X1
A	-2	GLN	-	expression tag	UNP Q9I4X1
A	-1	GLY	-	expression tag	UNP Q9I4X1
A	0	HIS	-	expression tag	UNP Q9I4X1
A	129	ALA	CYS	engineered mutation	UNP Q9I4X1
C	-16	MET	-	initiating methionine	UNP Q9I4X1
C	-15	GLY	-	expression tag	UNP Q9I4X1
C	-14	HIS	-	expression tag	UNP Q9I4X1
C	-13	HIS	-	expression tag	UNP Q9I4X1
C	-12	HIS	-	expression tag	UNP Q9I4X1
C	-11	HIS	-	expression tag	UNP Q9I4X1
C	-10	HIS	-	expression tag	UNP Q9I4X1
C	-9	HIS	-	expression tag	UNP Q9I4X1
C	-8	ALA	-	expression tag	UNP Q9I4X1
C	-7	GLU	-	expression tag	UNP Q9I4X1
C	-6	ASN	-	expression tag	UNP Q9I4X1
C	-5	LEU	-	expression tag	UNP Q9I4X1
C	-4	TYR	-	expression tag	UNP Q9I4X1
C	-3	PHE	-	expression tag	UNP Q9I4X1
C	-2	GLN	-	expression tag	UNP Q9I4X1
C	-1	GLY	-	expression tag	UNP Q9I4X1
C	0	HIS	-	expression tag	UNP Q9I4X1
C	129	ALA	CYS	engineered mutation	UNP Q9I4X1
E	-16	MET	-	initiating methionine	UNP Q9I4X1
E	-15	GLY	-	expression tag	UNP Q9I4X1
E	-14	HIS	-	expression tag	UNP Q9I4X1
E	-13	HIS	-	expression tag	UNP Q9I4X1
E	-12	HIS	-	expression tag	UNP Q9I4X1
E	-11	HIS	-	expression tag	UNP Q9I4X1
E	-10	HIS	-	expression tag	UNP Q9I4X1
E	-9	HIS	-	expression tag	UNP Q9I4X1
E	-8	ALA	-	expression tag	UNP Q9I4X1
E	-7	GLU	-	expression tag	UNP Q9I4X1
E	-6	ASN	-	expression tag	UNP Q9I4X1
E	-5	LEU	-	expression tag	UNP Q9I4X1
E	-4	TYR	-	expression tag	UNP Q9I4X1
E	-3	PHE	-	expression tag	UNP Q9I4X1
E	-2	GLN	-	expression tag	UNP Q9I4X1
E	-1	GLY	-	expression tag	UNP Q9I4X1
E	0	HIS	-	expression tag	UNP Q9I4X1
E	129	ALA	CYS	engineered mutation	UNP Q9I4X1
G	-16	MET	-	initiating methionine	UNP Q9I4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-15	GLY	-	expression tag	UNP Q9I4X1
G	-14	HIS	-	expression tag	UNP Q9I4X1
G	-13	HIS	-	expression tag	UNP Q9I4X1
G	-12	HIS	-	expression tag	UNP Q9I4X1
G	-11	HIS	-	expression tag	UNP Q9I4X1
G	-10	HIS	-	expression tag	UNP Q9I4X1
G	-9	HIS	-	expression tag	UNP Q9I4X1
G	-8	ALA	-	expression tag	UNP Q9I4X1
G	-7	GLU	-	expression tag	UNP Q9I4X1
G	-6	ASN	-	expression tag	UNP Q9I4X1
G	-5	LEU	-	expression tag	UNP Q9I4X1
G	-4	TYR	-	expression tag	UNP Q9I4X1
G	-3	PHE	-	expression tag	UNP Q9I4X1
G	-2	GLN	-	expression tag	UNP Q9I4X1
G	-1	GLY	-	expression tag	UNP Q9I4X1
G	0	HIS	-	expression tag	UNP Q9I4X1
G	129	ALA	CYS	engineered mutation	UNP Q9I4X1
I	-16	MET	-	initiating methionine	UNP Q9I4X1
I	-15	GLY	-	expression tag	UNP Q9I4X1
I	-14	HIS	-	expression tag	UNP Q9I4X1
I	-13	HIS	-	expression tag	UNP Q9I4X1
I	-12	HIS	-	expression tag	UNP Q9I4X1
I	-11	HIS	-	expression tag	UNP Q9I4X1
I	-10	HIS	-	expression tag	UNP Q9I4X1
I	-9	HIS	-	expression tag	UNP Q9I4X1
I	-8	ALA	-	expression tag	UNP Q9I4X1
I	-7	GLU	-	expression tag	UNP Q9I4X1
I	-6	ASN	-	expression tag	UNP Q9I4X1
I	-5	LEU	-	expression tag	UNP Q9I4X1
I	-4	TYR	-	expression tag	UNP Q9I4X1
I	-3	PHE	-	expression tag	UNP Q9I4X1
I	-2	GLN	-	expression tag	UNP Q9I4X1
I	-1	GLY	-	expression tag	UNP Q9I4X1
I	0	HIS	-	expression tag	UNP Q9I4X1
I	129	ALA	CYS	engineered mutation	UNP Q9I4X1
K	-16	MET	-	initiating methionine	UNP Q9I4X1
K	-15	GLY	-	expression tag	UNP Q9I4X1
K	-14	HIS	-	expression tag	UNP Q9I4X1
K	-13	HIS	-	expression tag	UNP Q9I4X1
K	-12	HIS	-	expression tag	UNP Q9I4X1
K	-11	HIS	-	expression tag	UNP Q9I4X1
K	-10	HIS	-	expression tag	UNP Q9I4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	HIS	-	expression tag	UNP Q9I4X1
K	-8	ALA	-	expression tag	UNP Q9I4X1
K	-7	GLU	-	expression tag	UNP Q9I4X1
K	-6	ASN	-	expression tag	UNP Q9I4X1
K	-5	LEU	-	expression tag	UNP Q9I4X1
K	-4	TYR	-	expression tag	UNP Q9I4X1
K	-3	PHE	-	expression tag	UNP Q9I4X1
K	-2	GLN	-	expression tag	UNP Q9I4X1
K	-1	GLY	-	expression tag	UNP Q9I4X1
K	0	HIS	-	expression tag	UNP Q9I4X1
K	129	ALA	CYS	engineered mutation	UNP Q9I4X1
M	-16	MET	-	initiating methionine	UNP Q9I4X1
M	-15	GLY	-	expression tag	UNP Q9I4X1
M	-14	HIS	-	expression tag	UNP Q9I4X1
M	-13	HIS	-	expression tag	UNP Q9I4X1
M	-12	HIS	-	expression tag	UNP Q9I4X1
M	-11	HIS	-	expression tag	UNP Q9I4X1
M	-10	HIS	-	expression tag	UNP Q9I4X1
M	-9	HIS	-	expression tag	UNP Q9I4X1
M	-8	ALA	-	expression tag	UNP Q9I4X1
M	-7	GLU	-	expression tag	UNP Q9I4X1
M	-6	ASN	-	expression tag	UNP Q9I4X1
M	-5	LEU	-	expression tag	UNP Q9I4X1
M	-4	TYR	-	expression tag	UNP Q9I4X1
M	-3	PHE	-	expression tag	UNP Q9I4X1
M	-2	GLN	-	expression tag	UNP Q9I4X1
M	-1	GLY	-	expression tag	UNP Q9I4X1
M	0	HIS	-	expression tag	UNP Q9I4X1
M	129	ALA	CYS	engineered mutation	UNP Q9I4X1
O	-16	MET	-	initiating methionine	UNP Q9I4X1
O	-15	GLY	-	expression tag	UNP Q9I4X1
O	-14	HIS	-	expression tag	UNP Q9I4X1
O	-13	HIS	-	expression tag	UNP Q9I4X1
O	-12	HIS	-	expression tag	UNP Q9I4X1
O	-11	HIS	-	expression tag	UNP Q9I4X1
O	-10	HIS	-	expression tag	UNP Q9I4X1
O	-9	HIS	-	expression tag	UNP Q9I4X1
O	-8	ALA	-	expression tag	UNP Q9I4X1
O	-7	GLU	-	expression tag	UNP Q9I4X1
O	-6	ASN	-	expression tag	UNP Q9I4X1
O	-5	LEU	-	expression tag	UNP Q9I4X1
O	-4	TYR	-	expression tag	UNP Q9I4X1

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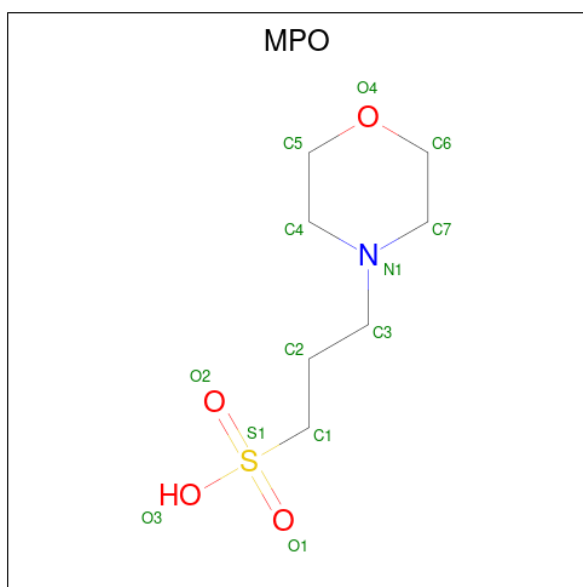
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Chain	Residue	Modelled	Actual	Comment	Reference
O	-3	PHE	-	expression tag	UNP Q9I4X1
O	-2	GLN	-	expression tag	UNP Q9I4X1
O	-1	GLY	-	expression tag	UNP Q9I4X1
O	0	HIS	-	expression tag	UNP Q9I4X1
O	129	ALA	CYS	engineered mutation	UNP Q9I4X1

- Molecule 2 is a protein called PqsB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	280	Total	C	H	N	O	S	0	0	0
			4234	1336	2119	376	395	8			
2	D	279	Total	C	H	N	O	S	0	1	0
			4224	1334	2114	375	393	8			
2	F	280	Total	C	H	N	O	S	0	1	0
			4255	1341	2129	379	398	8			
2	H	280	Total	C	H	N	O	S	0	0	0
			4237	1335	2122	379	393	8			
2	J	280	Total	C	H	N	O	S	0	0	0
			4233	1335	2117	378	395	8			
2	L	280	Total	C	H	N	O	S	0	1	0
			4254	1340	2130	379	397	8			
2	N	280	Total	C	H	N	O	S	0	0	0
			4239	1337	2121	376	397	8			
2	P	279	Total	C	H	N	O	S	0	0	0
			4206	1330	2101	371	396	8			

- Molecule 3 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C₇H₁₅NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 27	C 7	H 14	N 1	O 4	S 1	0	0
3	C	1	Total 27	C 7	H 14	N 1	O 4	S 1	0	0
3	E	1	Total 27	C 7	H 14	N 1	O 4	S 1	0	0
3	G	1	Total 27	C 7	H 14	N 1	O 4	S 1	0	0
3	I	1	Total 27	C 7	H 14	N 1	O 4	S 1	0	0
3	K	1	Total 27	C 7	H 14	N 1	O 4	S 1	0	0
3	M	1	Total 27	C 7	H 14	N 1	O 4	S 1	0	0
3	O	1	Total 27	C 7	H 14	N 1	O 4	S 1	0	0

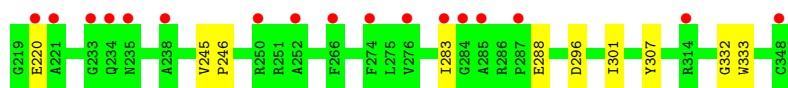
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	81	Total	O	0	0
			81	81		
4	C	83	Total	O	0	0
			83	83		
4	D	59	Total	O	0	0
			59	59		

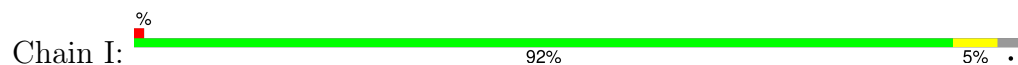
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	22	Total 22	O 22	0	0
4	F	56	Total 56	O 56	0	0
4	G	6	Total 6	O 6	0	0
4	H	18	Total 18	O 18	0	0
4	I	94	Total 94	O 94	0	0
4	J	94	Total 94	O 94	0	0
4	K	82	Total 82	O 82	0	0
4	L	59	Total 59	O 59	0	0
4	M	25	Total 25	O 25	0	0
4	N	44	Total 44	O 44	0	0
4	O	23	Total 23	O 23	0	0
4	P	18	Total 18	O 18	0	0



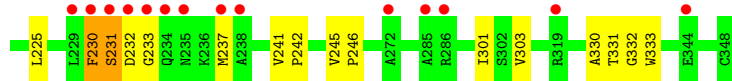
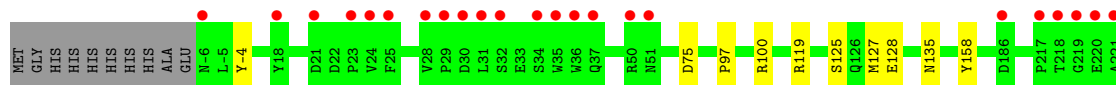
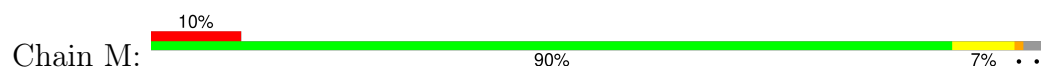
• Molecule 1: PqsC



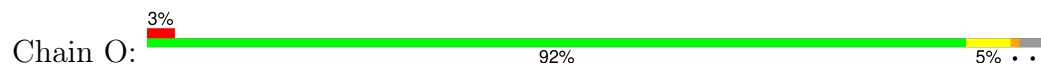
• Molecule 1: PqsC



• Molecule 1: PqsC



• Molecule 1: PqsC



• Molecule 2: PqsB



• Molecule 2: PqsB

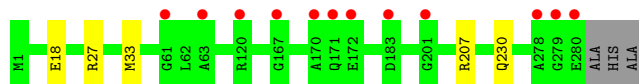




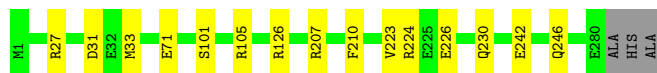
● Molecule 2: PqsB



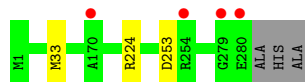
● Molecule 2: PqsB



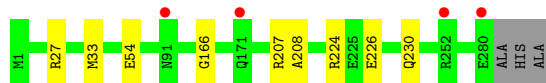
● Molecule 2: PqsB



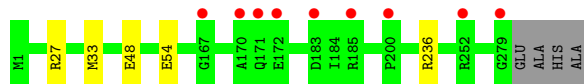
● Molecule 2: PqsB



● Molecule 2: PqsB



● Molecule 2: PqsB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.43Å 170.18Å 148.38Å 90.00° 100.97° 90.00°	Depositor
Resolution (Å)	48.98 – 2.60 48.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.98-2.60) 99.9 (48.98-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.61Å)	Xtriage
Refinement program	PHENIX dev_2875	Depositor
R, R_{free}	0.184 , 0.220 0.185 , 0.221	Depositor DCC
R_{free} test set	8943 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	77939	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.70% 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: MPO

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	0.27	0/2777	0.47	0/3771
1	C	0.27	0/2794	0.49	0/3793
1	E	0.28	0/2779	0.47	0/3777
1	G	0.28	0/2780	0.46	0/3779
1	I	0.28	0/2792	0.47	0/3791
1	K	0.27	0/2778	0.48	0/3772
1	M	0.26	0/2776	0.45	0/3773
1	O	0.27	0/2771	0.47	0/3766
2	B	0.28	0/2156	0.48	0/2930
2	D	0.27	0/2154	0.47	0/2928
2	F	0.27	0/2170	0.47	0/2949
2	H	0.26	0/2156	0.46	0/2930
2	J	0.27	0/2157	0.49	0/2932
2	L	0.27	0/2168	0.47	0/2946
2	N	0.27	0/2159	0.47	0/2934
2	P	0.27	0/2146	0.46	0/2918
All	All	0.27	0/39513	0.47	0/53689

There are no bond length outliers.

There are no bond angle outliers.

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	2715	2668	2670	10	0
1	C	2729	2682	2684	14	0
1	E	2713	2645	2647	15	0
1	G	2714	2643	2645	10	0
1	I	2730	2680	2682	11	0
1	K	2716	2666	2668	7	0
1	M	2714	2648	2650	15	1
1	O	2709	2644	2646	11	0
2	B	2115	2119	2119	4	0
2	D	2110	2114	2114	5	0
2	F	2126	2129	2129	3	0
2	H	2115	2122	2122	1	1
2	J	2116	2117	2117	9	0
2	L	2124	2130	2130	0	1
2	N	2118	2121	2121	4	0
2	P	2105	2101	2101	2	1
3	A	13	14	15	0	0
3	C	13	14	15	1	0
3	E	13	14	15	0	0
3	G	13	14	15	0	0
3	I	13	14	15	0	0
3	K	13	14	15	0	0
3	M	13	14	15	1	0
3	O	13	14	15	0	0
4	A	61	0	0	0	0
4	B	81	0	0	2	0
4	C	83	0	0	2	0
4	D	59	0	0	1	0
4	E	22	0	0	0	0
4	F	56	0	0	2	0
4	G	6	0	0	0	0
4	H	18	0	0	0	0
4	I	94	0	0	3	0
4	J	94	0	0	3	0
4	K	82	0	0	1	0
4	L	59	0	0	0	0
4	M	25	0	0	1	0
4	N	44	0	0	1	0
4	O	23	0	0	1	0
4	P	18	0	0	1	0
All	All	39598	38341	38365	119	2

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 2.

The worst 5 of 119 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:64:GLU:HB3	1:E:68:ARG:HH12	1.22	1.03
1:E:19:GLU:OE2	1:E:43:ARG:NE	1.98	0.96
1:E:64:GLU:HB3	1:E:68:ARG:NH1	1.81	0.94
2:B:226:GLU:OE2	4:B:301:HOH:O	1.85	0.92
1:C:288:GLU:OE2	4:C:1001:HOH:O	1.93	0.85

All (2) 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)
2:L:253:ASP:OD2	1:M:-4:TYR:OH[2_445]	2.12	0.08
2:H:18:GLU:OE2	2:P:236:ARG:HH12[1_545]	1.59	0.01

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	352/365 (96%)	341 (97%)	10 (3%)	1 (0%)	41	64
1	C	354/365 (97%)	344 (97%)	9 (2%)	1 (0%)	41	64
1	E	353/365 (97%)	344 (98%)	8 (2%)	1 (0%)	41	64
1	G	353/365 (97%)	343 (97%)	9 (2%)	1 (0%)	41	64
1	I	353/365 (97%)	343 (97%)	9 (2%)	1 (0%)	41	64
1	K	352/365 (96%)	340 (97%)	11 (3%)	1 (0%)	41	64
1	M	353/365 (97%)	345 (98%)	6 (2%)	2 (1%)	25	47
1	O	352/365 (96%)	340 (97%)	11 (3%)	1 (0%)	41	64
2	B	278/283 (98%)	274 (99%)	4 (1%)	0	100	100
2	D	278/283 (98%)	273 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	279/283 (99%)	274 (98%)	5 (2%)	0	100	100
2	H	278/283 (98%)	274 (99%)	4 (1%)	0	100	100
2	J	278/283 (98%)	273 (98%)	5 (2%)	0	100	100
2	L	279/283 (99%)	273 (98%)	6 (2%)	0	100	100
2	N	278/283 (98%)	273 (98%)	5 (2%)	0	100	100
2	P	277/283 (98%)	272 (98%)	5 (2%)	0	100	100
All	All	5047/5184 (97%)	4926 (98%)	112 (2%)	9 (0%)	47	71

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	231	SER
1	A	301	ILE
1	C	301	ILE
1	E	301	ILE
1	G	301	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	284/299 (95%)	282 (99%)	2 (1%)	84	94
1	C	284/299 (95%)	281 (99%)	3 (1%)	73	88
1	E	281/299 (94%)	277 (99%)	4 (1%)	67	85
1	G	282/299 (94%)	280 (99%)	2 (1%)	84	94
1	I	286/299 (96%)	284 (99%)	2 (1%)	84	94
1	K	284/299 (95%)	281 (99%)	3 (1%)	73	88
1	M	283/299 (95%)	280 (99%)	3 (1%)	73	88
1	O	282/299 (94%)	278 (99%)	4 (1%)	67	85
2	B	219/223 (98%)	217 (99%)	2 (1%)	78	91
2	D	218/223 (98%)	216 (99%)	2 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	221/223 (99%)	218 (99%)	3 (1%)	67	85
2	H	219/223 (98%)	217 (99%)	2 (1%)	78	91
2	J	219/223 (98%)	217 (99%)	2 (1%)	78	91
2	L	221/223 (99%)	219 (99%)	2 (1%)	78	91
2	N	220/223 (99%)	217 (99%)	3 (1%)	67	85
2	P	218/223 (98%)	216 (99%)	2 (1%)	78	91
All	All	4021/4176 (96%)	3980 (99%)	41 (1%)	76	90

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	224	ARG
1	O	44	ARG
1	M	158	TYR
2	N	27	ARG
1	O	158	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	291	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 monosaccharides 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	MPO	C	900	-	13,13,13	1.38	3 (23%)	17,17,17	1.73	4 (23%)
3	MPO	I	900	-	13,13,13	1.46	3 (23%)	17,17,17	1.93	5 (29%)
3	MPO	E	900	-	13,13,13	1.43	3 (23%)	17,17,17	2.00	6 (35%)
3	MPO	A	900	-	13,13,13	1.39	3 (23%)	17,17,17	2.00	6 (35%)
3	MPO	G	900	-	13,13,13	1.44	3 (23%)	17,17,17	1.85	5 (29%)
3	MPO	O	900	-	13,13,13	1.46	3 (23%)	17,17,17	2.02	5 (29%)
3	MPO	K	900	-	13,13,13	1.42	3 (23%)	17,17,17	1.78	4 (23%)
3	MPO	M	900	-	13,13,13	1.45	3 (23%)	17,17,17	1.82	6 (35%)

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	MPO	C	900	-	-	0/7/15/15	0/1/1/1
3	MPO	I	900	-	-	1/7/15/15	0/1/1/1
3	MPO	E	900	-	-	4/7/15/15	0/1/1/1
3	MPO	A	900	-	-	4/7/15/15	0/1/1/1
3	MPO	G	900	-	-	3/7/15/15	0/1/1/1
3	MPO	O	900	-	-	2/7/15/15	0/1/1/1
3	MPO	K	900	-	-	3/7/15/15	0/1/1/1
3	MPO	M	900	-	-	2/7/15/15	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	900	MPO	C1-S1	3.30	1.82	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	900	MPO	C1-S1	3.25	1.82	1.77
3	G	900	MPO	C1-S1	3.14	1.82	1.77
3	E	900	MPO	C1-S1	3.13	1.82	1.77
3	M	900	MPO	C1-S1	3.09	1.81	1.77

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	900	MPO	O3-S1-O2	-4.58	99.95	111.40
3	A	900	MPO	O3-S1-O1	-4.23	100.82	111.40
3	C	900	MPO	O2-S1-O1	-4.19	100.18	113.82
3	I	900	MPO	O2-S1-O1	-4.13	100.40	113.82
3	G	900	MPO	O3-S1-O2	-4.08	101.19	111.40

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	900	MPO	S1-C1-C2-C3
3	O	900	MPO	S1-C1-C2-C3
3	O	900	MPO	C1-C2-C3-N1
3	G	900	MPO	C2-C3-N1-C4
3	A	900	MPO	C2-C3-N1-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	900	MPO	1	0
3	M	900	MPO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	354/365 (96%)	0.05	7 (1%) 65 60	25, 42, 75, 108	0
1	C	355/365 (97%)	0.00	3 (0%) 86 84	24, 38, 66, 122	0
1	E	354/365 (96%)	0.38	27 (7%) 13 10	36, 62, 98, 131	0
1	G	354/365 (96%)	0.71	42 (11%) 4 3	44, 71, 109, 139	0
1	I	355/365 (97%)	-0.13	3 (0%) 86 84	22, 40, 72, 107	0
1	K	354/365 (96%)	-0.05	1 (0%) 94 93	23, 40, 68, 101	0
1	M	355/365 (97%)	0.55	37 (10%) 6 4	42, 70, 109, 159	0
1	O	354/365 (96%)	0.23	11 (3%) 49 42	33, 61, 91, 147	0
2	B	280/283 (98%)	0.05	5 (1%) 68 64	23, 33, 58, 95	0
2	D	279/283 (98%)	-0.14	1 (0%) 92 91	25, 40, 68, 107	0
2	F	280/283 (98%)	0.08	6 (2%) 63 58	29, 45, 76, 111	0
2	H	280/283 (98%)	0.29	12 (4%) 35 28	42, 58, 88, 141	0
2	J	280/283 (98%)	-0.15	0 100 100	21, 33, 57, 85	0
2	L	280/283 (98%)	0.03	4 (1%) 75 71	24, 37, 61, 99	0
2	N	280/283 (98%)	-0.10	4 (1%) 75 71	26, 45, 70, 94	0
2	P	279/283 (98%)	0.20	9 (3%) 47 40	37, 58, 86, 106	0
All	All	5073/5184 (97%)	0.14	172 (3%) 45 38	21, 49, 90, 159	0

The worst 5 of 172 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	279	GLY	9.2
1	G	233	GLY	6.1
1	G	218	THR	5.7
1	E	233	GLY	5.6
2	H	279	GLY	5.5

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 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(\AA^2)	Q<0.9
3	MPO	M	900	13/13	0.88	0.27	38,47,59,62	27
3	MPO	O	900	13/13	0.89	0.24	78,86,100,101	0
3	MPO	E	900	13/13	0.92	0.19	65,67,80,80	27
3	MPO	G	900	13/13	0.92	0.19	86,92,110,110	0
3	MPO	A	900	13/13	0.93	0.22	62,72,85,86	0
3	MPO	I	900	13/13	0.93	0.23	57,67,79,80	0
3	MPO	C	900	13/13	0.94	0.24	51,60,72,72	0
3	MPO	K	900	13/13	0.94	0.23	51,67,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.