



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:19 PM UTC

PDB ID : 4O8M / pdb_00004o8m
Title : Crystal structure of a trap periplasmic solute binding protein actinobacillus succinogenes 130z, target EFI-510004, with bound L-galactonate
Authors : Vetting, M.W.; Al Obaidi, N.F.; Morisco, L.L.; Wasserman, S.R.; Sojitra, S.; Stead, M.; Attonito, J.D.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hillerich, B.; Love, J.; Seidel, R.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on : 2013-12-28
Resolution : 1.70 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

<https://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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

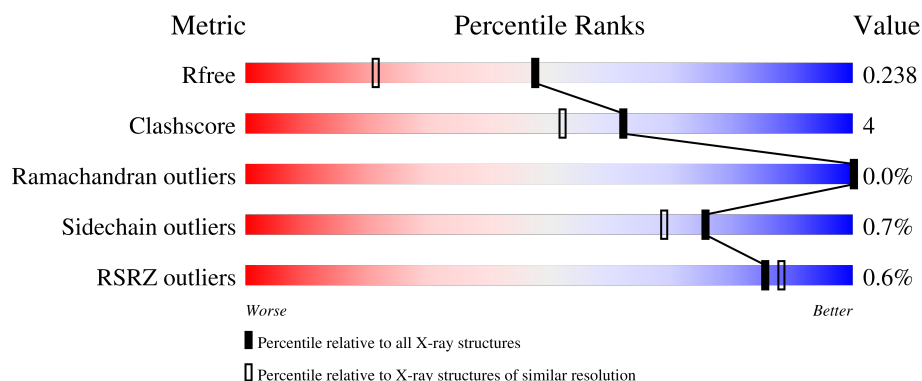
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	346	80% 7% 12%
1	B	346	82% 5% 12%
1	C	346	80% 7% 12%
1	D	346	79% 8% 13%

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	E	346	
1	F	346	
1	G	346	
1	H	346	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	D	401	-	-	X	-
3	SO4	D	403	-	-	X	-
3	SO4	F	401	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41582 atoms, of which 18905 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 TRAP dicarboxylate transporter, DctP subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	303	Total	C	H	N	O	S	0	4	0
			4773	1530	2385	391	459	8			
1	B	303	Total	C	H	N	O	S	0	1	0
			4732	1518	2365	387	454	8			
1	C	303	Total	C	H	N	O	S	0	1	0
			4734	1519	2367	387	453	8			
1	D	301	Total	C	H	N	O	S	0	1	0
			4705	1506	2354	387	450	8			
1	E	303	Total	C	H	N	O	S	0	0	0
			4718	1514	2358	386	452	8			
1	F	303	Total	C	H	N	O	S	0	1	0
			4732	1518	2365	387	454	8			
1	G	302	Total	C	H	N	O	S	0	1	0
			4727	1515	2365	389	450	8			
1	H	302	Total	C	H	N	O	S	0	0	0
			4693	1507	2346	384	448	8			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	329	ALA	-	expression tag	UNP A6VKP1
A	330	GLU	-	expression tag	UNP A6VKP1
A	331	ASN	-	expression tag	UNP A6VKP1
A	332	LEU	-	expression tag	UNP A6VKP1
A	333	TYR	-	expression tag	UNP A6VKP1
A	334	PHE	-	expression tag	UNP A6VKP1
A	335	GLN	-	expression tag	UNP A6VKP1
A	336	GLY	-	expression tag	UNP A6VKP1
A	337	HIS	-	expression tag	UNP A6VKP1
A	338	HIS	-	expression tag	UNP A6VKP1
A	339	HIS	-	expression tag	UNP A6VKP1
A	340	HIS	-	expression tag	UNP A6VKP1
A	341	HIS	-	expression tag	UNP A6VKP1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	342	HIS	-	expression tag	UNP A6VKP1
A	343	HIS	-	expression tag	UNP A6VKP1
A	344	HIS	-	expression tag	UNP A6VKP1
A	345	HIS	-	expression tag	UNP A6VKP1
A	346	HIS	-	expression tag	UNP A6VKP1
B	329	ALA	-	expression tag	UNP A6VKP1
B	330	GLU	-	expression tag	UNP A6VKP1
B	331	ASN	-	expression tag	UNP A6VKP1
B	332	LEU	-	expression tag	UNP A6VKP1
B	333	TYR	-	expression tag	UNP A6VKP1
B	334	PHE	-	expression tag	UNP A6VKP1
B	335	GLN	-	expression tag	UNP A6VKP1
B	336	GLY	-	expression tag	UNP A6VKP1
B	337	HIS	-	expression tag	UNP A6VKP1
B	338	HIS	-	expression tag	UNP A6VKP1
B	339	HIS	-	expression tag	UNP A6VKP1
B	340	HIS	-	expression tag	UNP A6VKP1
B	341	HIS	-	expression tag	UNP A6VKP1
B	342	HIS	-	expression tag	UNP A6VKP1
B	343	HIS	-	expression tag	UNP A6VKP1
B	344	HIS	-	expression tag	UNP A6VKP1
B	345	HIS	-	expression tag	UNP A6VKP1
B	346	HIS	-	expression tag	UNP A6VKP1
C	329	ALA	-	expression tag	UNP A6VKP1
C	330	GLU	-	expression tag	UNP A6VKP1
C	331	ASN	-	expression tag	UNP A6VKP1
C	332	LEU	-	expression tag	UNP A6VKP1
C	333	TYR	-	expression tag	UNP A6VKP1
C	334	PHE	-	expression tag	UNP A6VKP1
C	335	GLN	-	expression tag	UNP A6VKP1
C	336	GLY	-	expression tag	UNP A6VKP1
C	337	HIS	-	expression tag	UNP A6VKP1
C	338	HIS	-	expression tag	UNP A6VKP1
C	339	HIS	-	expression tag	UNP A6VKP1
C	340	HIS	-	expression tag	UNP A6VKP1
C	341	HIS	-	expression tag	UNP A6VKP1
C	342	HIS	-	expression tag	UNP A6VKP1
C	343	HIS	-	expression tag	UNP A6VKP1
C	344	HIS	-	expression tag	UNP A6VKP1
C	345	HIS	-	expression tag	UNP A6VKP1
C	346	HIS	-	expression tag	UNP A6VKP1
D	329	ALA	-	expression tag	UNP A6VKP1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	330	GLU	-	expression tag	UNP A6VKP1
D	331	ASN	-	expression tag	UNP A6VKP1
D	332	LEU	-	expression tag	UNP A6VKP1
D	333	TYR	-	expression tag	UNP A6VKP1
D	334	PHE	-	expression tag	UNP A6VKP1
D	335	GLN	-	expression tag	UNP A6VKP1
D	336	GLY	-	expression tag	UNP A6VKP1
D	337	HIS	-	expression tag	UNP A6VKP1
D	338	HIS	-	expression tag	UNP A6VKP1
D	339	HIS	-	expression tag	UNP A6VKP1
D	340	HIS	-	expression tag	UNP A6VKP1
D	341	HIS	-	expression tag	UNP A6VKP1
D	342	HIS	-	expression tag	UNP A6VKP1
D	343	HIS	-	expression tag	UNP A6VKP1
D	344	HIS	-	expression tag	UNP A6VKP1
D	345	HIS	-	expression tag	UNP A6VKP1
D	346	HIS	-	expression tag	UNP A6VKP1
E	329	ALA	-	expression tag	UNP A6VKP1
E	330	GLU	-	expression tag	UNP A6VKP1
E	331	ASN	-	expression tag	UNP A6VKP1
E	332	LEU	-	expression tag	UNP A6VKP1
E	333	TYR	-	expression tag	UNP A6VKP1
E	334	PHE	-	expression tag	UNP A6VKP1
E	335	GLN	-	expression tag	UNP A6VKP1
E	336	GLY	-	expression tag	UNP A6VKP1
E	337	HIS	-	expression tag	UNP A6VKP1
E	338	HIS	-	expression tag	UNP A6VKP1
E	339	HIS	-	expression tag	UNP A6VKP1
E	340	HIS	-	expression tag	UNP A6VKP1
E	341	HIS	-	expression tag	UNP A6VKP1
E	342	HIS	-	expression tag	UNP A6VKP1
E	343	HIS	-	expression tag	UNP A6VKP1
E	344	HIS	-	expression tag	UNP A6VKP1
E	345	HIS	-	expression tag	UNP A6VKP1
E	346	HIS	-	expression tag	UNP A6VKP1
F	329	ALA	-	expression tag	UNP A6VKP1
F	330	GLU	-	expression tag	UNP A6VKP1
F	331	ASN	-	expression tag	UNP A6VKP1
F	332	LEU	-	expression tag	UNP A6VKP1
F	333	TYR	-	expression tag	UNP A6VKP1
F	334	PHE	-	expression tag	UNP A6VKP1
F	335	GLN	-	expression tag	UNP A6VKP1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	336	GLY	-	expression tag	UNP A6VKP1
F	337	HIS	-	expression tag	UNP A6VKP1
F	338	HIS	-	expression tag	UNP A6VKP1
F	339	HIS	-	expression tag	UNP A6VKP1
F	340	HIS	-	expression tag	UNP A6VKP1
F	341	HIS	-	expression tag	UNP A6VKP1
F	342	HIS	-	expression tag	UNP A6VKP1
F	343	HIS	-	expression tag	UNP A6VKP1
F	344	HIS	-	expression tag	UNP A6VKP1
F	345	HIS	-	expression tag	UNP A6VKP1
F	346	HIS	-	expression tag	UNP A6VKP1
G	329	ALA	-	expression tag	UNP A6VKP1
G	330	GLU	-	expression tag	UNP A6VKP1
G	331	ASN	-	expression tag	UNP A6VKP1
G	332	LEU	-	expression tag	UNP A6VKP1
G	333	TYR	-	expression tag	UNP A6VKP1
G	334	PHE	-	expression tag	UNP A6VKP1
G	335	GLN	-	expression tag	UNP A6VKP1
G	336	GLY	-	expression tag	UNP A6VKP1
G	337	HIS	-	expression tag	UNP A6VKP1
G	338	HIS	-	expression tag	UNP A6VKP1
G	339	HIS	-	expression tag	UNP A6VKP1
G	340	HIS	-	expression tag	UNP A6VKP1
G	341	HIS	-	expression tag	UNP A6VKP1
G	342	HIS	-	expression tag	UNP A6VKP1
G	343	HIS	-	expression tag	UNP A6VKP1
G	344	HIS	-	expression tag	UNP A6VKP1
G	345	HIS	-	expression tag	UNP A6VKP1
G	346	HIS	-	expression tag	UNP A6VKP1
H	329	ALA	-	expression tag	UNP A6VKP1
H	330	GLU	-	expression tag	UNP A6VKP1
H	331	ASN	-	expression tag	UNP A6VKP1
H	332	LEU	-	expression tag	UNP A6VKP1
H	333	TYR	-	expression tag	UNP A6VKP1
H	334	PHE	-	expression tag	UNP A6VKP1
H	335	GLN	-	expression tag	UNP A6VKP1
H	336	GLY	-	expression tag	UNP A6VKP1
H	337	HIS	-	expression tag	UNP A6VKP1
H	338	HIS	-	expression tag	UNP A6VKP1
H	339	HIS	-	expression tag	UNP A6VKP1
H	340	HIS	-	expression tag	UNP A6VKP1
H	341	HIS	-	expression tag	UNP A6VKP1

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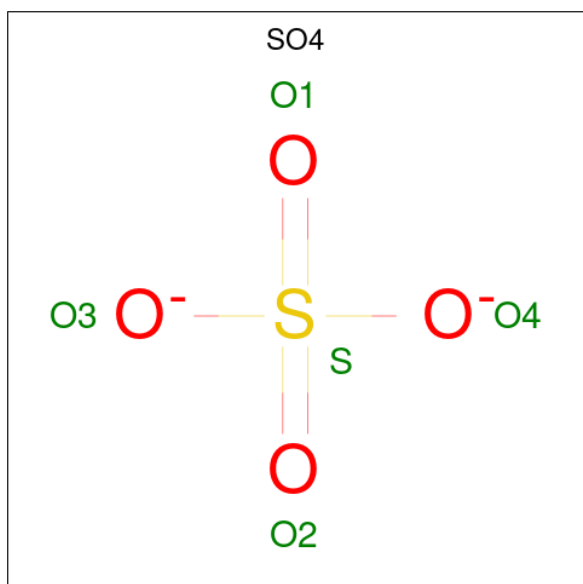
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Chain	Residue	Modelled	Actual	Comment	Reference
H	342	HIS	-	expression tag	UNP A6VKP1
H	343	HIS	-	expression tag	UNP A6VKP1
H	344	HIS	-	expression tag	UNP A6VKP1
H	345	HIS	-	expression tag	UNP A6VKP1
H	346	HIS	-	expression tag	UNP A6VKP1

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



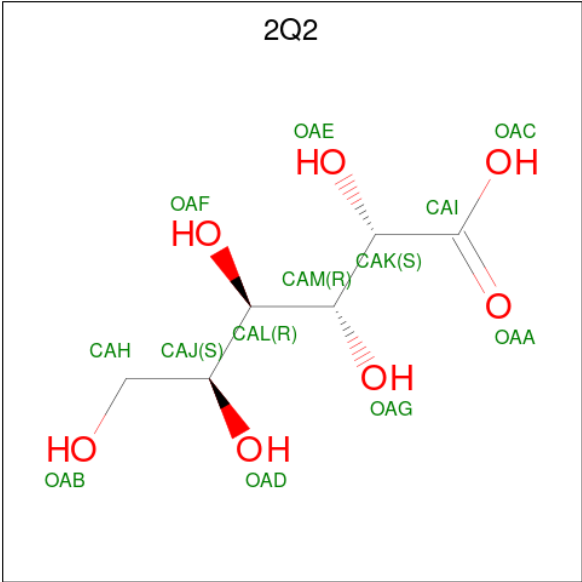
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is L-galactonic acid (CCD ID: 2Q2) (formula: C₆H₁₂O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		
4	E	1	Total	C	O	0	0
			13	6	7		
4	F	1	Total	C	O	0	0
			13	6	7		
4	G	1	Total	C	O	0	0
			13	6	7		
4	H	1	Total	C	O	0	0
			13	6	7		

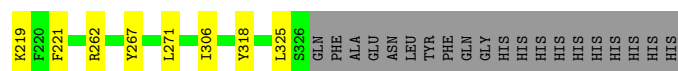
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	413	Total	O	0	0
			413	413		
5	B	455	Total	O	0	1
			456	456		
5	C	496	Total	O	0	1
			497	497		
5	D	442	Total	O	0	0
			442	442		

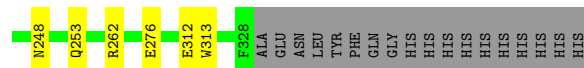
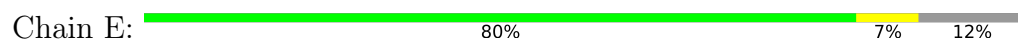
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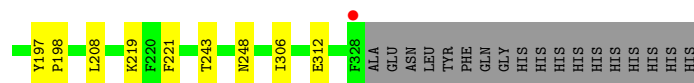
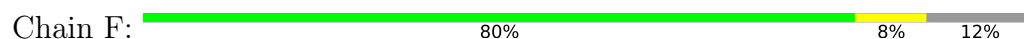
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	470	Total 472	O 472	0	2
5	F	401	Total 401	O 401	0	0
5	G	458	Total 459	O 459	0	1
5	H	440	Total 441	O 441	0	1



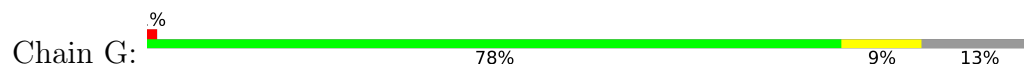
- Molecule 1: TRAP dicarboxylate transporter, DctP subunit



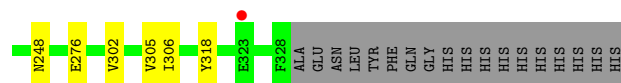
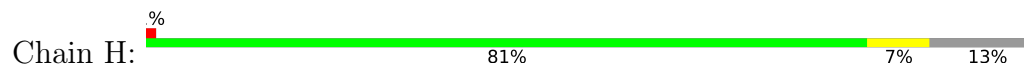
- Molecule 1: TRAP dicarboxylate transporter, DctP subunit



- Molecule 1: TRAP dicarboxylate transporter, DctP subunit



- Molecule 1: TRAP dicarboxylate transporter, DctP subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.23Å 143.59Å 97.46Å 90.00° 99.49° 90.00°	Depositor
Resolution (Å)	31.20 – 1.70 31.20 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (31.20-1.70) 89.4 (31.20-1.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.188 , 0.236 0.190 , 0.238	Depositor DCC
R_{free} test set	14524 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	11.3	Xtriage
Anisotropy	0.912	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	41582	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7829e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2Q2, SO4, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/2442	0.78	0/3314
1	B	0.70	0/2421	0.81	0/3285
1	C	0.69	0/2421	0.82	0/3285
1	D	0.64	1/2404 (0.0%)	0.78	0/3261
1	E	0.69	0/2414	0.81	0/3275
1	F	0.62	0/2421	0.77	0/3285
1	G	0.66	0/2416	0.81	0/3277
1	H	0.62	0/2401	0.79	0/3258
All	All	0.66	1/19340 (0.0%)	0.79	0/26240

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	99	VAL	CA-CB	5.71	1.59	1.54

There are no bond angle outliers.

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	2388	2385	2373	23	0
1	B	2367	2365	2356	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2367	2367	2358	20	0
1	D	2351	2354	2345	23	0
1	E	2360	2358	2350	18	0
1	F	2367	2365	2356	16	0
1	G	2362	2365	2356	21	0
1	H	2347	2346	2338	17	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
2	D	1	0	0	4	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	1	0
3	D	15	0	0	2	0
3	E	5	0	0	0	0
3	F	10	0	0	2	0
3	G	20	0	0	1	0
3	H	10	0	0	1	0
4	A	13	0	11	1	0
4	B	13	0	11	0	0
4	C	13	0	11	0	0
4	D	13	0	11	0	0
4	E	13	0	11	1	0
4	F	13	0	11	1	0
4	G	13	0	11	1	0
4	H	13	0	11	0	0
5	A	413	0	0	12	0
5	B	456	0	0	10	2
5	C	497	0	0	5	1
5	D	442	0	0	6	0
5	E	472	0	0	9	0
5	F	401	0	0	4	0
5	G	459	0	0	8	1
5	H	441	0	0	6	0
All	All	22677	18905	18920	154	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 4.

The worst 5 of 154 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:HIS:ND1	3:F:401:SO4:O4	2.05	0.90
1:G:247:ASN:ND2	5:G:781:HOH:O	2.14	0.80
1:B:247:ASN:OD1	5:B:675:HOH:O	2.01	0.78
1:A:81:LYS:NZ	5:A:840:HOH:O	2.16	0.75
1:C:140:ILE:O	5:C:768:HOH:O	2.05	0.75

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)
5:B:817:HOH:O	5:G:789:HOH:O[2_655]	2.04	0.16
5:B:811:HOH:O	5:C:732:HOH:O[1_554]	2.17	0.03

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	305/346 (88%)	298 (98%)	7 (2%)	0	100	100
1	B	302/346 (87%)	297 (98%)	5 (2%)	0	100	100
1	C	302/346 (87%)	298 (99%)	4 (1%)	0	100	100
1	D	300/346 (87%)	295 (98%)	4 (1%)	1 (0%)	36	22
1	E	301/346 (87%)	297 (99%)	4 (1%)	0	100	100
1	F	302/346 (87%)	298 (99%)	4 (1%)	0	100	100
1	G	301/346 (87%)	297 (99%)	4 (1%)	0	100	100
1	H	300/346 (87%)	295 (98%)	5 (2%)	0	100	100
All	All	2413/2768 (87%)	2375 (98%)	37 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	143	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	266/297 (90%)	264 (99%)	2 (1%)	73	65
1	B	263/297 (89%)	260 (99%)	3 (1%)	65	54
1	C	263/297 (89%)	261 (99%)	2 (1%)	73	65
1	D	261/297 (88%)	260 (100%)	1 (0%)	84	80
1	E	262/297 (88%)	261 (100%)	1 (0%)	84	80
1	F	263/297 (89%)	261 (99%)	2 (1%)	73	65
1	G	262/297 (88%)	259 (99%)	3 (1%)	65	54
1	H	260/297 (88%)	260 (100%)	0	100	100
All	All	2100/2376 (88%)	2086 (99%)	14 (1%)	76	69

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	325	LEU
1	E	165	LYS
1	G	209	GLU
1	G	51	LYS
1	G	208	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	69	GLN
1	G	136	HIS
1	F	172	GLN
1	G	69	GLN
1	G	179	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 ⓘ

Of 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	SO4	G	403	-	4,4,4	0.14	0	6,6,6	0.33	0
4	2Q2	E	402	-	12,12,12	1.14	1 (8%)	15,16,16	1.54	3 (20%)
4	2Q2	A	403	-	12,12,12	0.88	0	15,16,16	1.54	5 (33%)
3	SO4	H	402	-	4,4,4	0.26	0	6,6,6	0.35	0
4	2Q2	D	405	-	12,12,12	0.93	0	15,16,16	1.37	1 (6%)
3	SO4	D	402	-	4,4,4	0.36	0	6,6,6	0.15	0
3	SO4	H	401	-	4,4,4	0.23	0	6,6,6	0.45	0
3	SO4	F	401	-	4,4,4	0.35	0	6,6,6	0.51	0
3	SO4	E	401	-	4,4,4	0.23	0	6,6,6	0.26	0
3	SO4	C	402	-	4,4,4	0.32	0	6,6,6	0.18	0
4	2Q2	G	405	-	12,12,12	1.17	0	15,16,16	1.44	3 (20%)
4	2Q2	H	403	-	12,12,12	0.99	0	15,16,16	1.70	4 (26%)
3	SO4	G	402	-	4,4,4	0.28	0	6,6,6	0.40	0
3	SO4	A	402	-	4,4,4	0.29	0	6,6,6	0.52	0
4	2Q2	C	403	-	12,12,12	0.97	0	15,16,16	1.44	4 (26%)
3	SO4	C	401	-	4,4,4	0.33	0	6,6,6	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	403	-	4,4,4	0.50	0	6,6,6	0.31	0
3	SO4	F	402	-	4,4,4	0.32	0	6,6,6	0.20	0
3	SO4	D	404	-	4,4,4	0.25	0	6,6,6	0.34	0
4	2Q2	B	403	-	12,12,12	1.30	1 (8%)	15,16,16	1.64	4 (26%)
3	SO4	G	404	-	4,4,4	0.27	0	6,6,6	0.15	0
3	SO4	B	402	-	4,4,4	0.48	0	6,6,6	0.38	0
4	2Q2	F	403	-	12,12,12	1.29	1 (8%)	15,16,16	0.92	0
3	SO4	G	401	-	4,4,4	0.26	0	6,6,6	0.22	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
4	2Q2	G	405	-	-	0/18/18/18	-
4	2Q2	E	402	-	-	0/18/18/18	-
4	2Q2	H	403	-	-	0/18/18/18	-
4	2Q2	A	403	-	-	0/18/18/18	-
4	2Q2	F	403	-	-	0/18/18/18	-
4	2Q2	D	405	-	-	0/18/18/18	-
4	2Q2	B	403	-	-	0/18/18/18	-
4	2Q2	C	403	-	-	0/18/18/18	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	2Q2	CAH-CAJ	2.91	1.59	1.52
4	F	403	2Q2	CAH-CAJ	2.19	1.57	1.52
4	E	402	2Q2	CAL-CAM	2.12	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	402	2Q2	CAJ-CAL-CAM	-3.45	107.17	112.48
4	H	403	2Q2	CAJ-CAL-CAM	-3.06	107.77	112.48
4	H	403	2Q2	CAL-CAM-CAK	-2.95	108.40	113.62
4	G	405	2Q2	OAB-CAH-CAJ	-2.81	105.25	111.16
4	B	403	2Q2	CAJ-CAL-CAM	-2.80	108.17	112.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	402	2Q2	1	0
4	A	403	2Q2	1	0
3	H	401	SO4	1	0
3	F	401	SO4	2	0
4	G	405	2Q2	1	0
3	G	402	SO4	1	0
3	C	401	SO4	1	0
3	D	403	SO4	2	0
4	F	403	2Q2	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	303/346 (87%)	-0.34	3 (0%) 79 82	8, 16, 32, 50	4 (1%)
1	B	303/346 (87%)	-0.50	1 (0%) 90 91	5, 13, 30, 46	1 (0%)
1	C	303/346 (87%)	-0.49	2 (0%) 84 86	6, 13, 28, 43	1 (0%)
1	D	301/346 (86%)	-0.38	1 (0%) 90 91	8, 15, 33, 45	1 (0%)
1	E	303/346 (87%)	-0.48	1 (0%) 90 91	6, 14, 31, 52	0
1	F	303/346 (87%)	-0.26	1 (0%) 90 91	9, 18, 37, 53	1 (0%)
1	G	302/346 (87%)	-0.43	2 (0%) 84 86	7, 14, 31, 43	1 (0%)
1	H	302/346 (87%)	-0.31	3 (0%) 79 82	9, 17, 34, 46	0
All	All	2420/2768 (87%)	-0.40	14 (0%) 85 88	5, 15, 33, 53	9 (0%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	82	PHE	3.2
1	C	82	PHE	3.1
1	H	82	PHE	3.0
1	A	82	PHE	2.6
1	D	82	PHE	2.5

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 oligosaccharides 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
3	SO4	D	402	5/5	0.79	0.14	51,52,54,57	0
3	SO4	G	401	5/5	0.84	0.10	49,50,53,59	0
3	SO4	F	401	5/5	0.85	0.13	38,43,48,49	0
3	SO4	G	404	5/5	0.85	0.11	45,50,55,55	0
2	CL	A	401	1/1	0.88	0.15	36,36,36,36	0
3	SO4	A	402	5/5	0.88	0.12	24,30,36,39	0
3	SO4	D	403	5/5	0.89	0.14	18,20,35,40	0
3	SO4	C	401	5/5	0.89	0.14	23,31,35,36	0
3	SO4	H	401	5/5	0.89	0.13	28,39,40,42	0
2	CL	B	401	1/1	0.90	0.15	35,35,35,35	0
3	SO4	F	402	5/5	0.91	0.10	28,41,46,51	0
3	SO4	B	402	5/5	0.92	0.10	25,28,33,33	0
3	SO4	G	402	5/5	0.92	0.14	23,27,42,43	0
3	SO4	H	402	5/5	0.92	0.10	30,32,37,37	0
3	SO4	E	401	5/5	0.93	0.08	18,32,34,37	0
3	SO4	D	404	5/5	0.93	0.10	26,29,37,38	0
3	SO4	C	402	5/5	0.94	0.09	23,28,39,40	0
3	SO4	G	403	5/5	0.96	0.07	26,28,30,39	0
4	2Q2	F	403	13/13	0.96	0.05	8,10,11,16	0
4	2Q2	C	403	13/13	0.97	0.05	5,7,11,14	0
4	2Q2	E	402	13/13	0.97	0.05	4,7,9,10	0
2	CL	D	401	1/1	0.97	0.17	26,26,26,26	0
4	2Q2	G	405	13/13	0.97	0.04	6,7,11,14	0
4	2Q2	H	403	13/13	0.97	0.04	6,8,12,12	0
4	2Q2	A	403	13/13	0.98	0.05	8,9,12,12	0
4	2Q2	D	405	13/13	0.98	0.04	7,8,13,13	0
4	2Q2	B	403	13/13	0.98	0.04	3,6,12,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.