



wwPDB X-ray Structure Validation Summary Report i

Sep 12, 2023 – 05:46 PM EDT

PDB ID : 4NF0
Title : CRYSTAL STRUCTURE OF A TRAP PERIPLASMIC SOLUTE BINDING PROTEIN FROM PSEUDOMONAS AERUGINOSA PAO1 (PA4616), TARGET EFI-510182, WITH BOUND L-Malate
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Deposited on : 2013-10-30
Resolution : 1.85 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 i 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](#) 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 : 2.35.1
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)

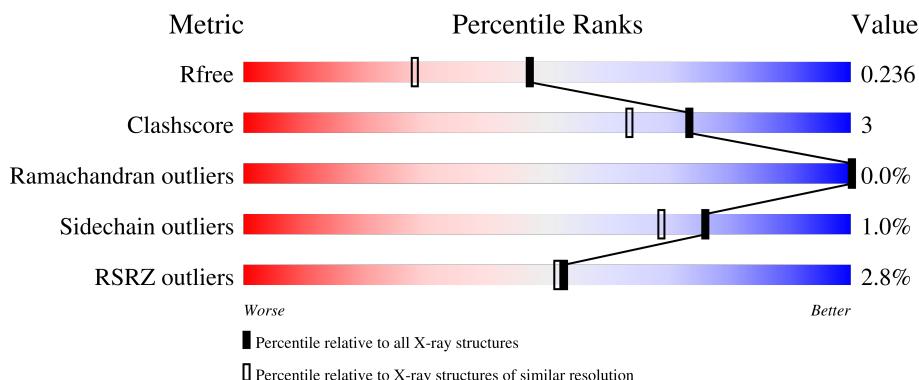
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

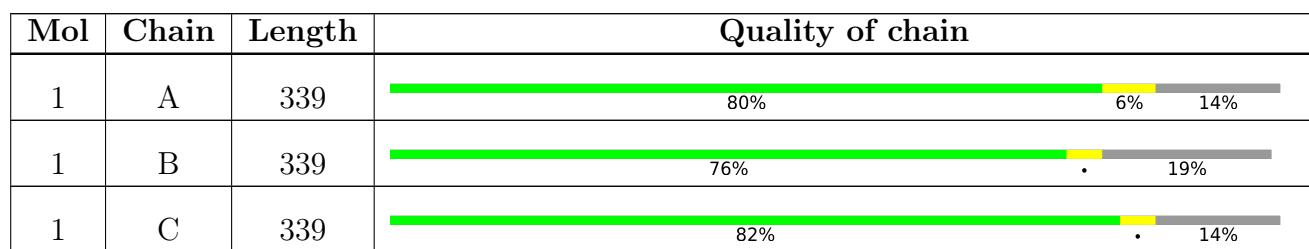
The reported resolution of this entry is 1.85 Å.

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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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.



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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.35.1

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2 Entry composition [\(i\)](#)

There are 4 unique types of molecules in this entry. The entry contains 19172 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 Probable c4-dicarboxylate-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total 2299	C 1462	N 395	O 435	S 7	0	0	0
1	B	273	Total 2156	C 1369	N 370	O 410	S 7	0	0	0
1	C	291	Total 2297	C 1464	N 393	O 433	S 7	0	1	0
1	D	289	Total 2280	C 1448	N 391	O 434	S 7	0	1	0
1	E	233	Total 1780	C 1127	N 301	O 346	S 6	0	0	0
1	F	288	Total 2281	C 1451	N 392	O 431	S 7	0	0	0
1	G	287	Total 2276	C 1449	N 392	O 428	S 7	0	0	0
1	H	261	Total 2056	C 1308	N 348	O 393	S 7	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	ALA	-	expression tag	UNP Q9HVH5
A	335	GLU	-	expression tag	UNP Q9HVH5
A	336	ASN	-	expression tag	UNP Q9HVH5
A	337	LEU	-	expression tag	UNP Q9HVH5
A	338	TYR	-	expression tag	UNP Q9HVH5
A	339	PHE	-	expression tag	UNP Q9HVH5
A	340	GLN	-	expression tag	UNP Q9HVH5
B	334	ALA	-	expression tag	UNP Q9HVH5
B	335	GLU	-	expression tag	UNP Q9HVH5
B	336	ASN	-	expression tag	UNP Q9HVH5
B	337	LEU	-	expression tag	UNP Q9HVH5
B	338	TYR	-	expression tag	UNP Q9HVH5
B	339	PHE	-	expression tag	UNP Q9HVH5

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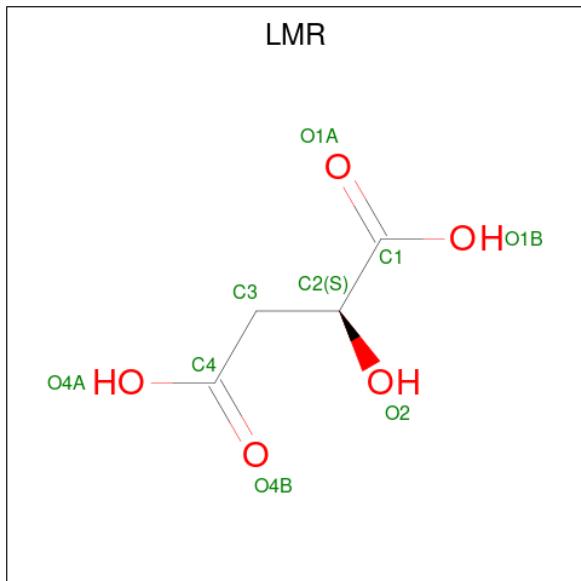
Chain	Residue	Modelled	Actual	Comment	Reference
B	340	GLN	-	expression tag	UNP Q9HVF5
C	334	ALA	-	expression tag	UNP Q9HVF5
C	335	GLU	-	expression tag	UNP Q9HVF5
C	336	ASN	-	expression tag	UNP Q9HVF5
C	337	LEU	-	expression tag	UNP Q9HVF5
C	338	TYR	-	expression tag	UNP Q9HVF5
C	339	PHE	-	expression tag	UNP Q9HVF5
C	340	GLN	-	expression tag	UNP Q9HVF5
D	334	ALA	-	expression tag	UNP Q9HVF5
D	335	GLU	-	expression tag	UNP Q9HVF5
D	336	ASN	-	expression tag	UNP Q9HVF5
D	337	LEU	-	expression tag	UNP Q9HVF5
D	338	TYR	-	expression tag	UNP Q9HVF5
D	339	PHE	-	expression tag	UNP Q9HVF5
D	340	GLN	-	expression tag	UNP Q9HVF5
E	334	ALA	-	expression tag	UNP Q9HVF5
E	335	GLU	-	expression tag	UNP Q9HVF5
E	336	ASN	-	expression tag	UNP Q9HVF5
E	337	LEU	-	expression tag	UNP Q9HVF5
E	338	TYR	-	expression tag	UNP Q9HVF5
E	339	PHE	-	expression tag	UNP Q9HVF5
E	340	GLN	-	expression tag	UNP Q9HVF5
F	334	ALA	-	expression tag	UNP Q9HVF5
F	335	GLU	-	expression tag	UNP Q9HVF5
F	336	ASN	-	expression tag	UNP Q9HVF5
F	337	LEU	-	expression tag	UNP Q9HVF5
F	338	TYR	-	expression tag	UNP Q9HVF5
F	339	PHE	-	expression tag	UNP Q9HVF5
F	340	GLN	-	expression tag	UNP Q9HVF5
G	334	ALA	-	expression tag	UNP Q9HVF5
G	335	GLU	-	expression tag	UNP Q9HVF5
G	336	ASN	-	expression tag	UNP Q9HVF5
G	337	LEU	-	expression tag	UNP Q9HVF5
G	338	TYR	-	expression tag	UNP Q9HVF5
G	339	PHE	-	expression tag	UNP Q9HVF5
G	340	GLN	-	expression tag	UNP Q9HVF5
H	334	ALA	-	expression tag	UNP Q9HVF5
H	335	GLU	-	expression tag	UNP Q9HVF5
H	336	ASN	-	expression tag	UNP Q9HVF5
H	337	LEU	-	expression tag	UNP Q9HVF5
H	338	TYR	-	expression tag	UNP Q9HVF5
H	339	PHE	-	expression tag	UNP Q9HVF5

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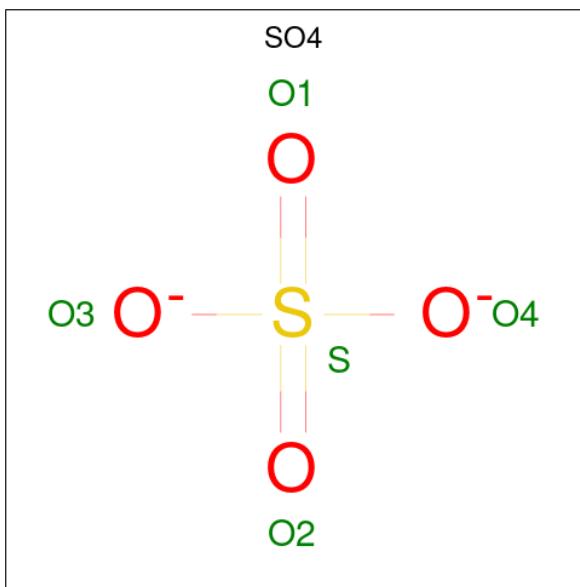
Chain	Residue	Modelled	Actual	Comment	Reference
H	340	GLN	-	expression tag	UNP Q9HVH5

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: C₄H₆O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 4 5	0	0
2	B	1	Total C O 9 4 5	0	0
2	C	1	Total C O 9 4 5	0	0
2	D	1	Total C O 9 4 5	0	0
2	F	1	Total C O 9 4 5	0	0
2	G	1	Total C O 9 4 5	0	0
2	H	1	Total C O 9 4 5	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	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
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	221	Total O 221 221	0	0
4	B	221	Total O 221 221	0	0
4	C	270	Total O 270 270	0	0
4	D	263	Total O 263 263	0	0
4	E	100	Total O 100 100	0	0
4	F	201	Total O 201 201	0	0

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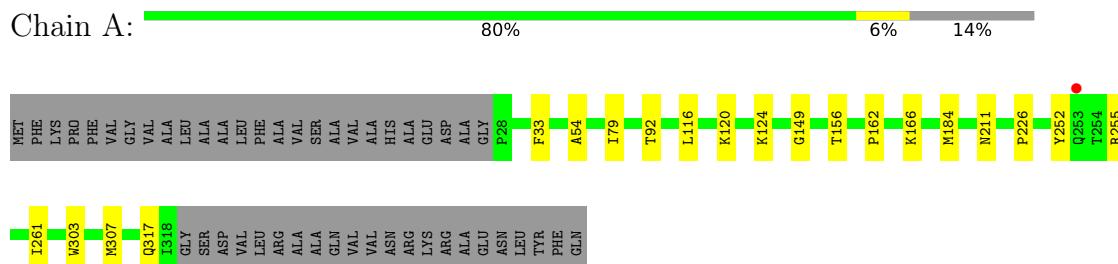
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	261	Total O 261 261	0	0
4	H	117	Total O 117 117	0	0

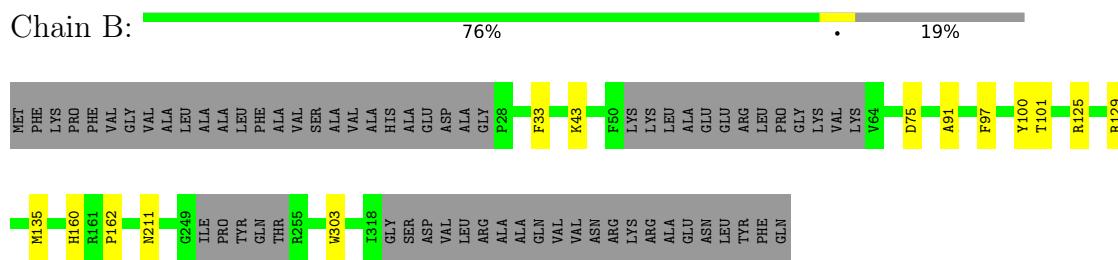
3 Residue-property plots

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.

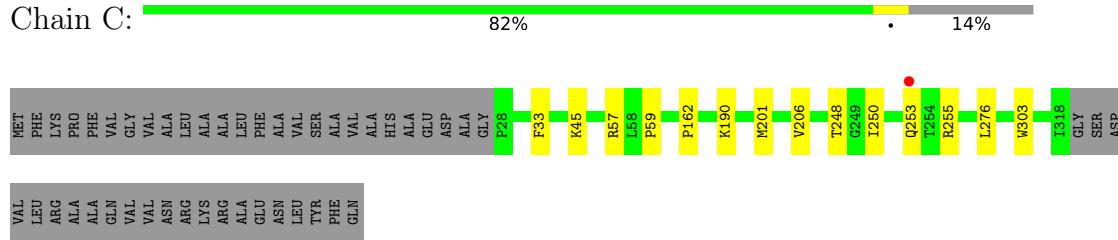
- Molecule 1: Probable c4-dicarboxylate-binding protein



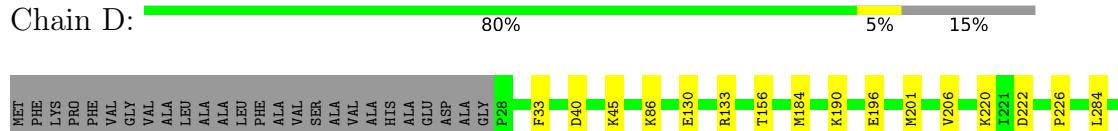
- Molecule 1: Probable c4-dicarboxylate-binding protein

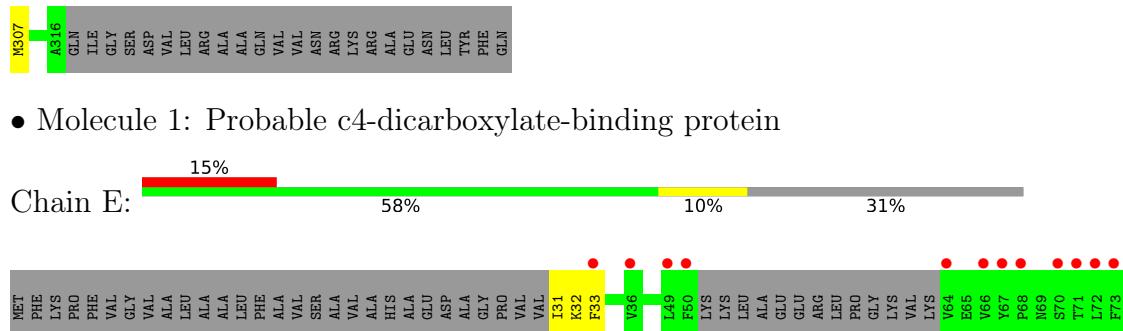


- Molecule 1: Probable c4-dicarboxylate-binding protein



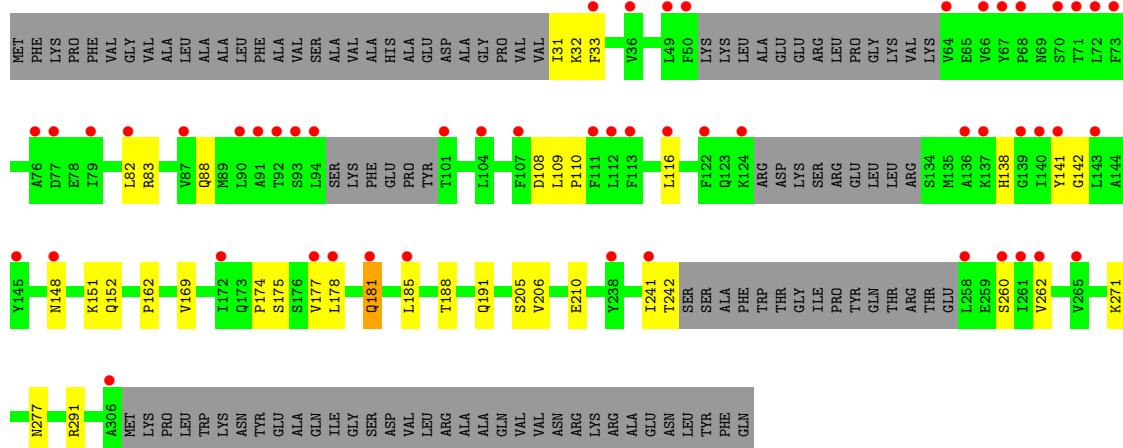
- Molecule 1: Probable c4-dicarboxylate-binding protein



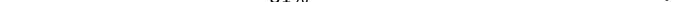


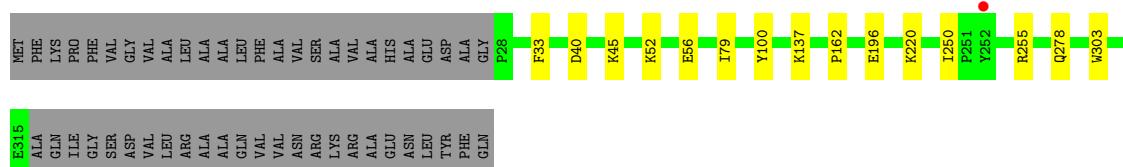
- Molecule 1: Probable c4-dicarboxylate-binding protein

Chain E: 15% 58% 10% 31%

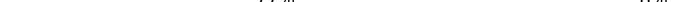


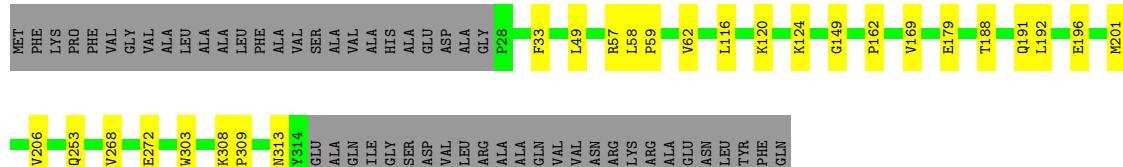
- Molecule 1: Probable c4-dicarboxylate-binding protein

Chain F:  81% • 15%



- Molecule 1: Probable c4-dicarboxylate-binding protein

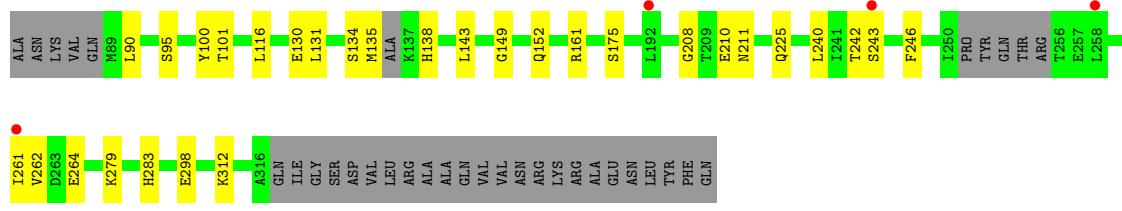
Chain G:  77% 8% 15%



- Molecule 1: Probable c4-dicarboxylate-binding protein

Chain H: 2% 65% 12% 23%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.96 Å 73.91 Å 122.14 Å 99.01° 91.59° 95.09°	Depositor
Resolution (Å)	33.56 – 1.85 120.52 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.1 (33.56-1.85) 96.6 (120.52-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ ¹	3.67 (at 1.84 Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R , R_{free}	0.195 , 0.239 0.195 , 0.236	Depositor DCC
R_{free} test set	10265 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.3	EDS
L-test for twinning ²	$< L > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19172	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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 35.14 % 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 6.1104e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

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

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	0.35	0/2345	0.47	0/3170
1	B	0.38	0/2197	0.51	0/2967
1	C	0.40	0/2343	0.51	0/3168
1	D	0.39	0/2326	0.51	0/3147
1	E	0.41	0/1808	0.54	0/2446
1	F	0.37	0/2327	0.51	0/3144
1	G	0.40	0/2322	0.51	0/3136
1	H	0.35	0/2094	0.50	0/2826
All	All	0.38	0/17762	0.51	0/24004

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 [\(i\)](#)

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	2299	0	2302	10	0
1	B	2156	0	2146	12	0
1	C	2297	0	2302	8	0
1	D	2280	0	2265	11	0
1	E	1780	0	1732	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2281	0	2289	9	0
1	G	2276	0	2294	18	0
1	H	2056	0	2023	23	1
2	A	9	0	4	0	0
2	B	9	0	4	0	0
2	C	9	0	4	0	0
2	D	9	0	4	0	0
2	F	9	0	4	0	0
2	G	9	0	4	0	0
2	H	9	0	4	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	F	5	0	0	0	0
4	A	221	0	0	2	0
4	B	221	0	0	2	0
4	C	270	0	0	0	0
4	D	263	0	0	3	1
4	E	100	0	0	2	0
4	F	201	0	0	1	0
4	G	261	0	0	7	0
4	H	117	0	0	1	0
All	All	19172	0	17381	114	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 3.

The worst 5 of 114 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:B:97:PHE:HB3	1:B:135:MET:HE3	1.61	0.82
1:B:135:MET:SD	4:B:608:HOH:O	2.41	0.78
1:C:250:ILE:O	1:C:255:ARG:NH2	2.20	0.73
1:F:40:ASP:OD1	1:F:45:LYS:NZ	2.21	0.73
1:G:179:GLU:OE1	1:G:191:GLN:NE2	2.21	0.72

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:GLU:OE2	4:D:678:HOH:O[1_544]	2.02	0.18

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	289/339 (85%)	283 (98%)	6 (2%)	0	100 100
1	B	267/339 (79%)	262 (98%)	5 (2%)	0	100 100
1	C	290/339 (86%)	284 (98%)	6 (2%)	0	100 100
1	D	288/339 (85%)	284 (99%)	4 (1%)	0	100 100
1	E	223/339 (66%)	216 (97%)	7 (3%)	0	100 100
1	F	286/339 (84%)	281 (98%)	5 (2%)	0	100 100
1	G	285/339 (84%)	277 (97%)	8 (3%)	0	100 100
1	H	251/339 (74%)	241 (96%)	9 (4%)	1 (0%)	34 19
All	All	2179/2712 (80%)	2128 (98%)	50 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	77	ASP

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	245/281 (87%)	243 (99%)	2 (1%)	81 76
1	B	230/281 (82%)	227 (99%)	3 (1%)	69 58
1	C	244/281 (87%)	242 (99%)	2 (1%)	81 76
1	D	242/281 (86%)	241 (100%)	1 (0%)	91 89
1	E	185/281 (66%)	178 (96%)	7 (4%)	33 16
1	F	244/281 (87%)	243 (100%)	1 (0%)	91 89
1	G	244/281 (87%)	243 (100%)	1 (0%)	91 89
1	H	217/281 (77%)	215 (99%)	2 (1%)	78 72
All	All	1851/2248 (82%)	1832 (99%)	19 (1%)	76 69

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	262	VAL
1	H	33	PHE
1	H	211	ASN
1	G	33	PHE
1	E	31	ILE

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	105	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 (i)

13 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	SO4	B	403	-	4,4,4	0.13	0	6,6,6	0.25	0
2	LMR	C	401	-	8,8,8	1.12	0	10,10,10	1.33	2 (20%)
3	SO4	D	402	-	4,4,4	0.18	0	6,6,6	0.24	0
2	LMR	A	401	-	8,8,8	1.09	0	10,10,10	1.35	1 (10%)
2	LMR	F	401	-	8,8,8	1.12	0	10,10,10	1.56	3 (30%)
2	LMR	B	401	-	8,8,8	1.27	1 (12%)	10,10,10	1.52	3 (30%)
3	SO4	C	402	-	4,4,4	0.15	0	6,6,6	0.23	0
3	SO4	D	403	-	4,4,4	0.12	0	6,6,6	0.17	0
3	SO4	F	402	-	4,4,4	0.13	0	6,6,6	0.12	0
2	LMR	H	401	-	8,8,8	1.16	0	10,10,10	1.41	2 (20%)
3	SO4	B	402	-	4,4,4	0.15	0	6,6,6	0.08	0
2	LMR	D	401	-	8,8,8	1.22	0	10,10,10	1.50	1 (10%)
2	LMR	G	401	-	8,8,8	1.14	0	10,10,10	1.31	1 (10%)

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
2	LMR	C	401	-	-	2/8/8/8	-
2	LMR	A	401	-	-	2/8/8/8	-
2	LMR	F	401	-	-	2/8/8/8	-
2	LMR	B	401	-	-	2/8/8/8	-
2	LMR	H	401	-	-	3/8/8/8	-
2	LMR	D	401	-	-	2/8/8/8	-
2	LMR	G	401	-	-	3/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	LMR	C2-C1	2.40	1.55	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	LMR	O1A-C1-C2	-2.98	116.71	122.54
2	D	401	LMR	O1A-C1-C2	-2.92	116.82	122.54
2	A	401	LMR	O1A-C1-C2	-2.83	117.02	122.54
2	B	401	LMR	O1A-C1-C2	-2.82	117.03	122.54
2	F	401	LMR	O1A-C1-C2	-2.78	117.10	122.54

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	LMR	O1B-C1-C2-C3
2	F	401	LMR	O1B-C1-C2-C3
2	G	401	LMR	O1B-C1-C2-C3
2	B	401	LMR	O1B-C1-C2-C3
2	C	401	LMR	O1A-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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	291/339 (85%)	-0.30	1 (0%) 94 93	16, 28, 48, 61	0
1	B	273/339 (80%)	-0.27	0 100 100	13, 26, 48, 60	0
1	C	291/339 (85%)	-0.36	1 (0%) 94 93	12, 24, 43, 71	0
1	D	289/339 (85%)	-0.39	0 100 100	12, 22, 41, 53	0
1	E	233/339 (68%)	1.02	52 (22%) 0 0	23, 52, 75, 90	0
1	F	288/339 (84%)	-0.27	1 (0%) 94 93	15, 28, 48, 61	0
1	G	287/339 (84%)	-0.34	0 100 100	12, 24, 40, 52	0
1	H	261/339 (76%)	0.05	6 (2%) 60 59	18, 38, 60, 79	0
All	All	2213/2712 (81%)	-0.14	61 (2%) 53 52	12, 28, 58, 90	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	258	LEU	8.2
1	E	104	LEU	4.6
1	E	124	LYS	4.5
1	H	64	VAL	4.2
1	E	90	LEU	4.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.3 Carbohydrates [\(i\)](#)

There are no 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(Å ²)	Q<0.9
2	LMR	H	401	9/9	0.78	0.15	25,26,30,31	0
3	SO4	C	402	5/5	0.89	0.16	45,50,57,64	0
3	SO4	B	403	5/5	0.95	0.08	42,51,55,55	0
3	SO4	D	403	5/5	0.95	0.10	50,52,53,54	0
3	SO4	B	402	5/5	0.96	0.11	37,40,48,57	0
3	SO4	F	402	5/5	0.96	0.07	59,60,66,69	0
2	LMR	C	401	9/9	0.97	0.07	13,16,19,20	0
2	LMR	F	401	9/9	0.97	0.08	14,18,19,21	0
3	SO4	D	402	5/5	0.97	0.10	35,36,40,41	0
2	LMR	A	401	9/9	0.97	0.09	19,21,25,26	0
2	LMR	B	401	9/9	0.97	0.09	13,17,18,19	0
2	LMR	G	401	9/9	0.98	0.07	14,16,17,19	0
2	LMR	D	401	9/9	0.98	0.07	10,12,15,15	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.