



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:37 PM UTC

PDB ID : 8EKG / pdb_00008ekg
Title : MHETase variant Thr159Val, Met192Tyr, Tyr252Phe, Tyr503Trp
Authors : Saunders, J.W.; Frkic, R.L.; Jackson, C.J.
Deposited on : 2022-09-20
Resolution : 2.65 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	:	4-5-2 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)
Validation Pipeline (wwPDB-VP)	:	2.49

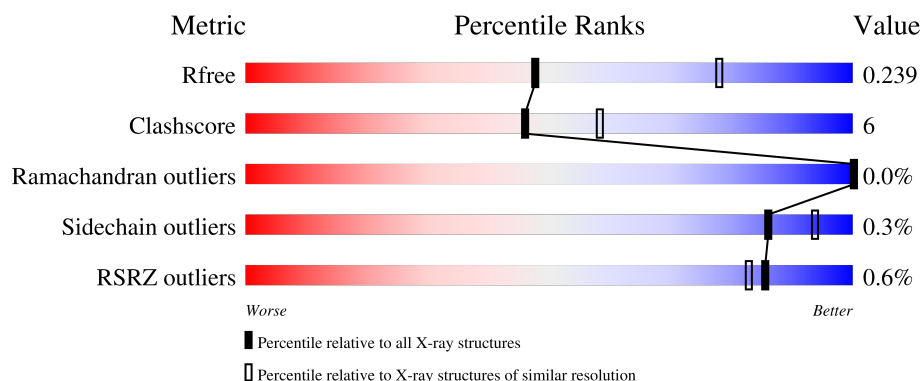
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	592	
1	B	592	
1	C	592	
1	D	592	
1	E	592	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	592	% 80% 15% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25228 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 Mono(2-hydroxyethyl) terephthalate hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	P	S	0	0	0
			4128	2583	726	791	1	27			
1	B	557	Total	C	N	O	P	S	0	0	0
			4123	2580	725	790	1	27			
1	C	557	Total	C	N	O	P	S	0	0	0
			4123	2580	725	790	1	27			
1	D	557	Total	C	N	O	P	S	0	0	0
			4123	2580	725	790	1	27			
1	E	558	Total	C	N	O	P	S	0	0	0
			4128	2583	726	791	1	27			
1	F	557	Total	C	N	O	P	S	0	0	0
			4123	2580	725	790	1	27			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP A0A0K8P8E7
A	13	GLU	-	expression tag	UNP A0A0K8P8E7
A	14	ASN	-	expression tag	UNP A0A0K8P8E7
A	15	LEU	-	expression tag	UNP A0A0K8P8E7
A	16	TYR	-	expression tag	UNP A0A0K8P8E7
A	17	PHE	-	expression tag	UNP A0A0K8P8E7
A	18	GLN	-	expression tag	UNP A0A0K8P8E7
A	19	GLY	-	expression tag	UNP A0A0K8P8E7
A	159	VAL	THR	engineered mutation	UNP A0A0K8P8E7
A	192	TYR	MET	engineered mutation	UNP A0A0K8P8E7
A	252	PHE	TYR	engineered mutation	UNP A0A0K8P8E7
A	503	TRP	TYR	engineered mutation	UNP A0A0K8P8E7
B	12	MET	-	initiating methionine	UNP A0A0K8P8E7
B	13	GLU	-	expression tag	UNP A0A0K8P8E7
B	14	ASN	-	expression tag	UNP A0A0K8P8E7
B	15	LEU	-	expression tag	UNP A0A0K8P8E7
B	16	TYR	-	expression tag	UNP A0A0K8P8E7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	PHE	-	expression tag	UNP A0A0K8P8E7
B	18	GLN	-	expression tag	UNP A0A0K8P8E7
B	19	GLY	-	expression tag	UNP A0A0K8P8E7
B	159	VAL	THR	engineered mutation	UNP A0A0K8P8E7
B	192	TYR	MET	engineered mutation	UNP A0A0K8P8E7
B	252	PHE	TYR	engineered mutation	UNP A0A0K8P8E7
B	503	TRP	TYR	engineered mutation	UNP A0A0K8P8E7
C	12	MET	-	initiating methionine	UNP A0A0K8P8E7
C	13	GLU	-	expression tag	UNP A0A0K8P8E7
C	14	ASN	-	expression tag	UNP A0A0K8P8E7
C	15	LEU	-	expression tag	UNP A0A0K8P8E7
C	16	TYR	-	expression tag	UNP A0A0K8P8E7
C	17	PHE	-	expression tag	UNP A0A0K8P8E7
C	18	GLN	-	expression tag	UNP A0A0K8P8E7
C	19	GLY	-	expression tag	UNP A0A0K8P8E7
C	159	VAL	THR	engineered mutation	UNP A0A0K8P8E7
C	192	TYR	MET	engineered mutation	UNP A0A0K8P8E7
C	252	PHE	TYR	engineered mutation	UNP A0A0K8P8E7
C	503	TRP	TYR	engineered mutation	UNP A0A0K8P8E7
D	12	MET	-	initiating methionine	UNP A0A0K8P8E7
D	13	GLU	-	expression tag	UNP A0A0K8P8E7
D	14	ASN	-	expression tag	UNP A0A0K8P8E7
D	15	LEU	-	expression tag	UNP A0A0K8P8E7
D	16	TYR	-	expression tag	UNP A0A0K8P8E7
D	17	PHE	-	expression tag	UNP A0A0K8P8E7
D	18	GLN	-	expression tag	UNP A0A0K8P8E7
D	19	GLY	-	expression tag	UNP A0A0K8P8E7
D	159	VAL	THR	engineered mutation	UNP A0A0K8P8E7
D	192	TYR	MET	engineered mutation	UNP A0A0K8P8E7
D	252	PHE	TYR	engineered mutation	UNP A0A0K8P8E7
D	503	TRP	TYR	engineered mutation	UNP A0A0K8P8E7
E	12	MET	-	initiating methionine	UNP A0A0K8P8E7
E	13	GLU	-	expression tag	UNP A0A0K8P8E7
E	14	ASN	-	expression tag	UNP A0A0K8P8E7
E	15	LEU	-	expression tag	UNP A0A0K8P8E7
E	16	TYR	-	expression tag	UNP A0A0K8P8E7
E	17	PHE	-	expression tag	UNP A0A0K8P8E7
E	18	GLN	-	expression tag	UNP A0A0K8P8E7
E	19	GLY	-	expression tag	UNP A0A0K8P8E7
E	159	VAL	THR	engineered mutation	UNP A0A0K8P8E7
E	192	TYR	MET	engineered mutation	UNP A0A0K8P8E7
E	252	PHE	TYR	engineered mutation	UNP A0A0K8P8E7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	503	TRP	TYR	engineered mutation	UNP A0A0K8P8E7
F	12	MET	-	initiating methionine	UNP A0A0K8P8E7
F	13	GLU	-	expression tag	UNP A0A0K8P8E7
F	14	ASN	-	expression tag	UNP A0A0K8P8E7
F	15	LEU	-	expression tag	UNP A0A0K8P8E7
F	16	TYR	-	expression tag	UNP A0A0K8P8E7
F	17	PHE	-	expression tag	UNP A0A0K8P8E7
F	18	GLN	-	expression tag	UNP A0A0K8P8E7
F	19	GLY	-	expression tag	UNP A0A0K8P8E7
F	159	VAL	THR	engineered mutation	UNP A0A0K8P8E7
F	192	TYR	MET	engineered mutation	UNP A0A0K8P8E7
F	252	PHE	TYR	engineered mutation	UNP A0A0K8P8E7
F	503	TRP	TYR	engineered mutation	UNP A0A0K8P8E7

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	O	S	0	0
			5	4	1		

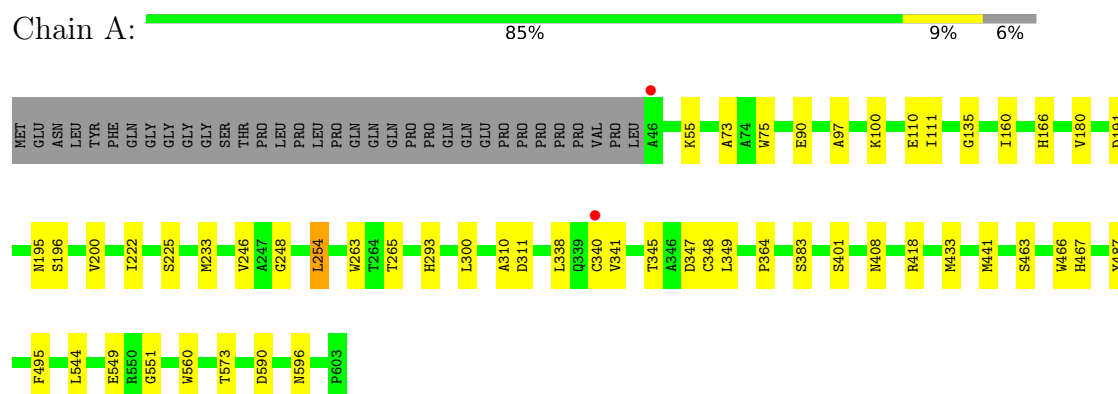
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	70	Total	O	0	0
			70	70		
6	B	91	Total	O	0	0
			91	91		
6	C	71	Total	O	0	0
			71	71		
6	D	64	Total	O	0	0
			64	64		
6	E	52	Total	O	0	0
			52	52		
6	F	55	Total	O	0	0
			55	55		

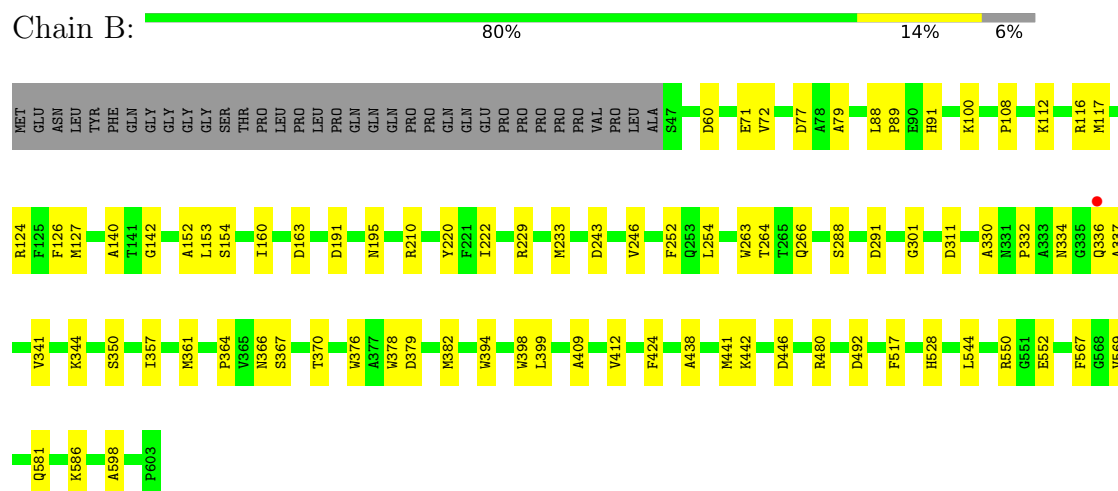
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

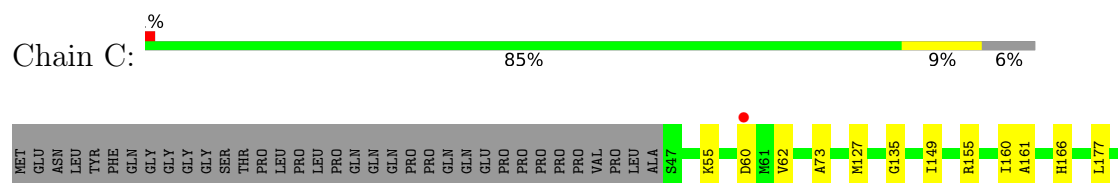
- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

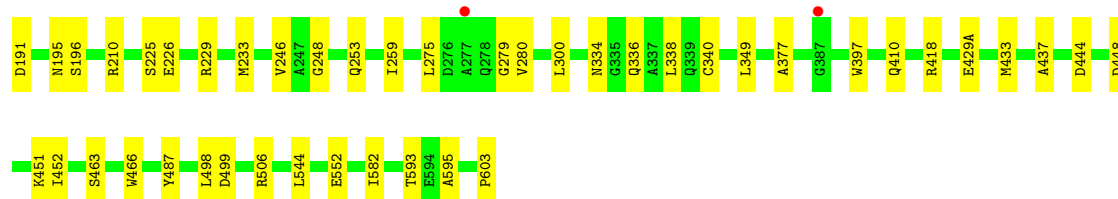


- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase



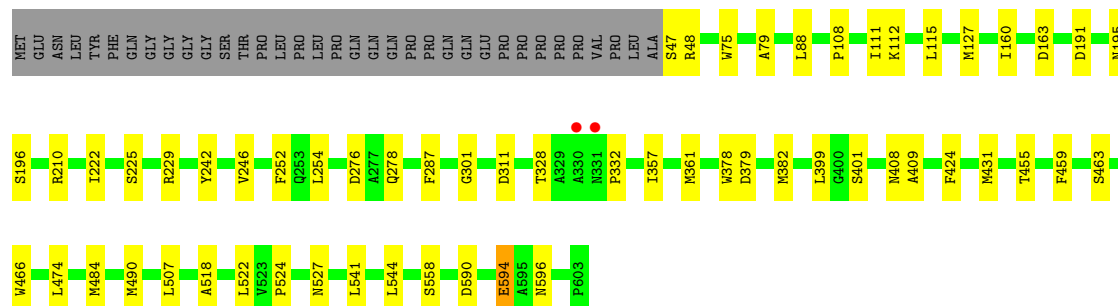
- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase





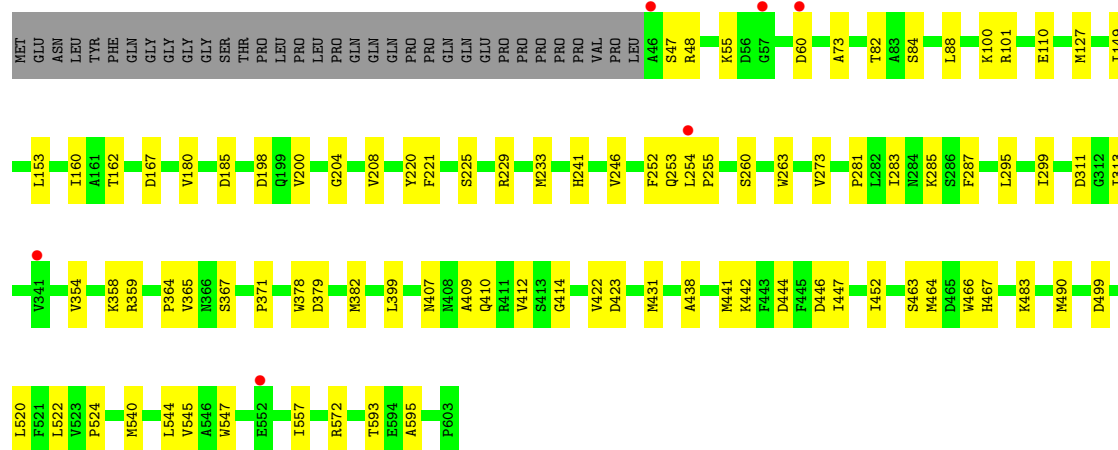
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain D: 84% 10% 6%



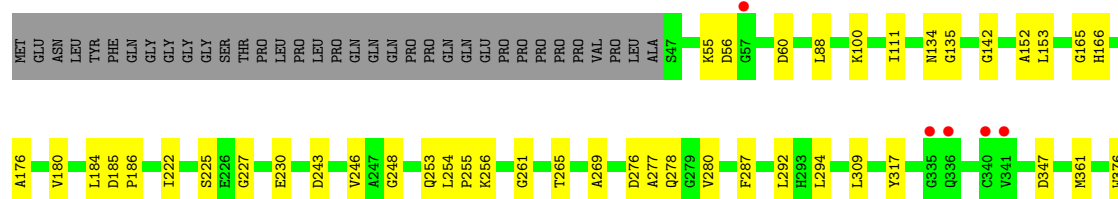
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

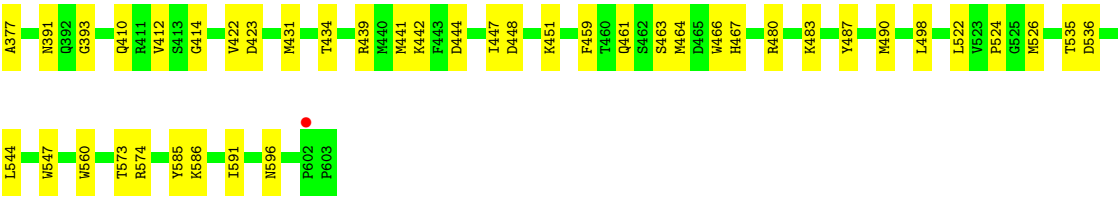
Chain E: 79% 15% 6%



• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain F: 80% 15% 6%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.97Å 120.51Å 126.29Å 90.44° 95.15° 90.20°	Depositor
Resolution (Å)	43.87 – 2.65 43.87 – 2.65	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.87-2.65) 96.0 (43.87-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.184 , 0.241 0.182 , 0.239	Depositor DCC
R_{free} test set	4887 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.004 for -h,k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25228	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PEG, SO4, CA, SEP

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	0.15	0/4226	0.32	2/5752 (0.0%)
1	B	0.10	0/4221	0.27	0/5745
1	C	0.12	0/4221	0.28	0/5745
1	D	0.10	0/4221	0.27	0/5745
1	E	0.11	0/4226	0.28	0/5752
1	F	0.11	0/4221	0.30	0/5745
All	All	0.12	0/25336	0.29	2/34484 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	VAL	N-CA-C	-5.52	107.06	111.81
1	A	180	VAL	N-CA-C	-5.33	107.28	112.29

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	4128	0	3903	36	0
1	B	4123	0	3898	61	0
1	C	4123	0	3898	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4123	0	3898	40	0
1	E	4128	0	3903	62	0
1	F	4123	0	3898	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	7	0	10	0	0
4	A	4	0	6	0	0
4	B	24	0	36	3	0
4	C	4	0	6	1	0
4	D	8	0	12	0	0
4	E	4	0	6	0	0
5	B	10	0	0	0	0
5	E	10	0	0	0	0
6	A	70	0	0	0	0
6	B	91	0	0	0	0
6	C	71	0	0	1	0
6	D	64	0	0	0	0
6	E	52	0	0	2	0
6	F	55	0	0	0	0
All	All	25228	0	23474	278	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 278 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:254:LEU:HD23	1:E:467:HIS:CD2	1.90	1.06
1:E:254:LEU:HD23	1:E:467:HIS:NE2	1.82	0.95
1:D:48:ARG:NH2	1:D:75:TRP:HD1	1.76	0.84
1:E:204:GLY:O	1:E:208:VAL:HG23	1.78	0.83
1:E:82:THR:HG22	1:E:84:SER:H	1.44	0.83

There are no symmetry-related clashes.

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	555/592 (94%)	529 (95%)	26 (5%)	0	100	100
1	B	554/592 (94%)	527 (95%)	27 (5%)	0	100	100
1	C	554/592 (94%)	530 (96%)	24 (4%)	0	100	100
1	D	554/592 (94%)	528 (95%)	25 (4%)	1 (0%)	43	60
1	E	555/592 (94%)	526 (95%)	29 (5%)	0	100	100
1	F	554/592 (94%)	527 (95%)	27 (5%)	0	100	100
All	All	3326/3552 (94%)	3167 (95%)	158 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	527	ASN

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	403/433 (93%)	401 (100%)	2 (0%)	81	91
1	B	403/433 (93%)	403 (100%)	0	100	100
1	C	403/433 (93%)	401 (100%)	2 (0%)	81	91
1	D	403/433 (93%)	401 (100%)	2 (0%)	81	91
1	E	403/433 (93%)	402 (100%)	1 (0%)	87	95
1	F	403/433 (93%)	403 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2418/2598 (93%)	2411 (100%)	7 (0%)	86	94

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	340	CYS
1	D	210	ARG
1	E	60	ASP
1	D	594	GLU
1	C	155	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	392	GLN
1	F	156	ASN
1	F	596	ASN
1	E	592	ASN
1	F	187	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	F	225	1	8,9,10	1.61	1 (12%)	7,12,14	1.15	1 (14%)
1	SEP	D	225	1	8,9,10	1.62	1 (12%)	7,12,14	1.31	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	A	225	1	8,9,10	1.62	1 (12%)	7,12,14	1.40	1 (14%)
1	SEP	E	225	1	8,9,10	1.63	1 (12%)	7,12,14	1.39	1 (14%)
1	SEP	B	225	1	8,9,10	0.59	0	7,12,14	0.72	0
1	SEP	C	225	1	8,9,10	1.62	1 (12%)	7,12,14	1.26	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	F	225	1	-	1/6/8/10	-
1	SEP	D	225	1	-	2/6/8/10	-
1	SEP	A	225	1	-	2/6/8/10	-
1	SEP	E	225	1	-	1/6/8/10	-
1	SEP	B	225	1	-	4/6/8/10	-
1	SEP	C	225	1	-	1/6/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	225	SEP	P-O1P	3.58	1.61	1.50
1	D	225	SEP	P-O1P	3.57	1.61	1.50
1	C	225	SEP	P-O1P	3.56	1.61	1.50
1	A	225	SEP	P-O1P	3.53	1.61	1.50
1	F	225	SEP	P-O1P	3.49	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	SEP	OG-CB-CA	3.17	111.23	108.14
1	E	225	SEP	OG-CB-CA	3.12	111.19	108.14
1	D	225	SEP	OG-CB-CA	2.82	110.89	108.14
1	C	225	SEP	OG-CB-CA	2.65	110.72	108.14
1	F	225	SEP	OG-CB-CA	2.31	110.39	108.14

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	225	SEP	CB-OG-P-O2P
1	B	225	SEP	CB-OG-P-O3P
1	B	225	SEP	CB-OG-P-O1P
1	A	225	SEP	CB-OG-P-O1P
1	A	225	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	$\# Z > 2$
5	SO4	E	703	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	E	702	-	4,4,4	0.23	0	6,6,6	0.07	0
4	EDO	B	707	-	3,3,3	0.42	0	2,2,2	0.40	0
4	EDO	B	706	-	3,3,3	0.42	0	2,2,2	0.37	0
4	EDO	B	708	-	3,3,3	0.42	0	2,2,2	0.37	0
5	SO4	B	703	-	4,4,4	0.24	0	6,6,6	0.08	0
4	EDO	B	709	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	A	703	-	3,3,3	0.41	0	2,2,2	0.33	0
3	PEG	A	702	-	6,6,6	0.11	0	5,5,5	0.12	0
4	EDO	B	705	-	3,3,3	0.42	0	2,2,2	0.35	0
4	EDO	C	702	-	3,3,3	0.43	0	2,2,2	0.34	0
4	EDO	D	702	-	3,3,3	0.11	0	2,2,2	0.03	0
4	EDO	E	704	-	3,3,3	0.42	0	2,2,2	0.41	0
4	EDO	B	704	-	3,3,3	0.42	0	2,2,2	0.38	0
5	SO4	B	702	-	4,4,4	0.23	0	6,6,6	0.08	0
4	EDO	D	703	-	3,3,3	0.42	0	2,2,2	0.38	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	EDO	B	707	-	-	1/1/1/1	-
4	EDO	B	706	-	-	0/1/1/1	-
4	EDO	B	708	-	-	0/1/1/1	-
4	EDO	B	709	-	-	0/1/1/1	-
4	EDO	A	703	-	-	1/1/1/1	-
3	PEG	A	702	-	-	0/4/4/4	-
4	EDO	B	705	-	-	0/1/1/1	-
4	EDO	C	702	-	-	0/1/1/1	-
4	EDO	D	702	-	-	1/1/1/1	-
4	EDO	E	704	-	-	0/1/1/1	-
4	EDO	B	704	-	-	0/1/1/1	-
4	EDO	D	703	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	EDO	O1-C1-C2-O2
4	B	707	EDO	O1-C1-C2-O2
4	D	703	EDO	O1-C1-C2-O2
4	D	702	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	706	EDO	1	0
4	B	705	EDO	1	0
4	C	702	EDO	1	0
4	B	704	EDO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	557/592 (94%)	-0.19	2 (0%) 88 87	34, 46, 66, 120	0
1	B	556/592 (93%)	-0.26	1 (0%) 91 90	30, 44, 66, 127	0
1	C	556/592 (93%)	-0.10	3 (0%) 87 85	33, 52, 80, 120	0
1	D	556/592 (93%)	-0.18	2 (0%) 88 87	34, 48, 73, 119	0
1	E	557/592 (94%)	0.01	6 (1%) 78 75	37, 59, 83, 111	0
1	F	556/592 (93%)	0.15	6 (1%) 78 75	39, 65, 97, 142	0
All	All	3338/3552 (93%)	-0.09	20 (0%) 85 83	30, 51, 84, 142	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	387	GLY	4.5
1	E	46	ALA	4.5
1	A	46	ALA	3.2
1	F	335	GLY	2.9
1	F	602	PRO	2.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	B	225	10/11	0.87	0.10	32,41,60,100	0
1	SEP	F	225	10/11	0.88	0.09	45,53,65,85	0
1	SEP	C	225	10/11	0.90	0.12	41,52,67,77	0
1	SEP	D	225	10/11	0.92	0.09	40,49,68,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	SEP	E	225	10/11	0.92	0.08	46,52,64,98	0
1	SEP	A	225	10/11	0.92	0.07	38,48,57,80	0

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($\text{\AA}^2$)	Q<0.9
5	SO4	B	702	5/5	0.50	0.11	111,112,123,132	0
4	EDO	B	705	4/4	0.71	0.20	38,44,45,49	4
5	SO4	B	703	5/5	0.73	0.09	99,101,105,125	0
5	SO4	E	703	5/5	0.73	0.10	102,102,109,133	0
4	EDO	D	702	4/4	0.75	0.14	44,45,62,64	0
4	EDO	C	702	4/4	0.79	0.20	57,63,68,68	0
4	EDO	E	704	4/4	0.82	0.13	59,63,64,67	0
4	EDO	B	704	4/4	0.85	0.12	48,51,54,59	0
3	PEG	A	702	7/7	0.87	0.16	44,63,68,70	0
4	EDO	A	703	4/4	0.87	0.20	38,38,48,49	4
4	EDO	B	706	4/4	0.88	0.15	48,51,53,58	0
4	EDO	B	709	4/4	0.89	0.11	49,55,61,62	0
4	EDO	D	703	4/4	0.89	0.15	52,59,62,63	0
5	SO4	E	702	5/5	0.90	0.15	46,54,64,65	5
4	EDO	B	708	4/4	0.90	0.14	40,45,46,49	4
4	EDO	B	707	4/4	0.91	0.10	54,55,56,60	0
2	CA	A	701	1/1	0.94	0.07	55,55,55,55	0
2	CA	C	701	1/1	0.95	0.07	58,58,58,58	0
2	CA	B	701	1/1	0.99	0.06	53,53,53,53	0
2	CA	D	701	1/1	0.99	0.06	60,60,60,60	0
2	CA	E	701	1/1	0.99	0.05	64,64,64,64	0
2	CA	F	701	1/1	0.99	0.05	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.