



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:47 PM UTC

PDB ID : 5COJ / pdb_00005coj
Title : Structure of Hydroxyethylthiazole kinase ThiM from Staphylococcus aureus in complex with native substrate 2-(4-methyl-1,3-thiazol-5-yl)ethanol.
Authors : Drebes, J.; Kuenz, M.; Eberle, R.J.; Oberthuer, D.; Cang, H.; Wrenger, C.; Betzel, C.
Deposited on : 2015-07-20
Resolution : 1.90 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

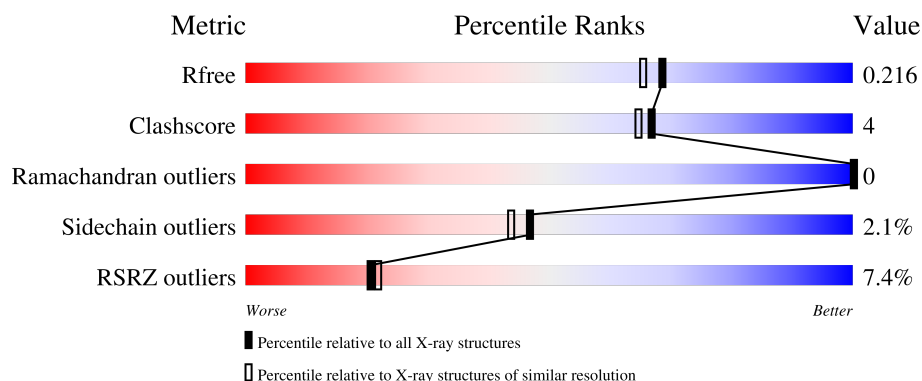
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	277	5% 82% 7% 9%
1	B	277	% 84% 5% 10%
1	C	277	2% 84% 5% 10%
1	E	277	5% 85% 5% 9%
1	F	277	16% 72% 10% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	277	

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	TZE	A	301	-	-	X	-
2	TZE	C	301	-	-	X	-
2	TZE	F	301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11578 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 Hydroxyethylthiazole kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	27	0	0
			1896	1208	310	372	6			
1	B	248	Total	C	N	O	S	9	0	0
			1859	1185	305	363	6			
1	C	249	Total	C	N	O	S	4	0	0
			1867	1191	306	364	6			
1	E	252	Total	C	N	O	S	33	0	0
			1896	1209	310	372	5			
1	F	241	Total	C	N	O	S	116	0	0
			1802	1152	294	351	5			
1	H	244	Total	C	N	O	S	77	0	0
			1829	1167	300	356	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLU	-	expression tag	UNP Q6GEY3
A	265	ASN	-	expression tag	UNP Q6GEY3
A	266	LEU	-	expression tag	UNP Q6GEY3
A	267	TYR	-	expression tag	UNP Q6GEY3
A	268	PHE	-	expression tag	UNP Q6GEY3
A	269	GLN	-	expression tag	UNP Q6GEY3
A	270	SER	-	expression tag	UNP Q6GEY3
A	271	GLY	-	expression tag	UNP Q6GEY3
A	272	HIS	-	expression tag	UNP Q6GEY3
A	273	HIS	-	expression tag	UNP Q6GEY3
A	274	HIS	-	expression tag	UNP Q6GEY3
A	275	HIS	-	expression tag	UNP Q6GEY3
A	276	HIS	-	expression tag	UNP Q6GEY3
A	277	HIS	-	expression tag	UNP Q6GEY3
B	264	GLU	-	expression tag	UNP Q6GEY3
B	265	ASN	-	expression tag	UNP Q6GEY3
B	266	LEU	-	expression tag	UNP Q6GEY3

Continued on next page...

Continued from previous page...

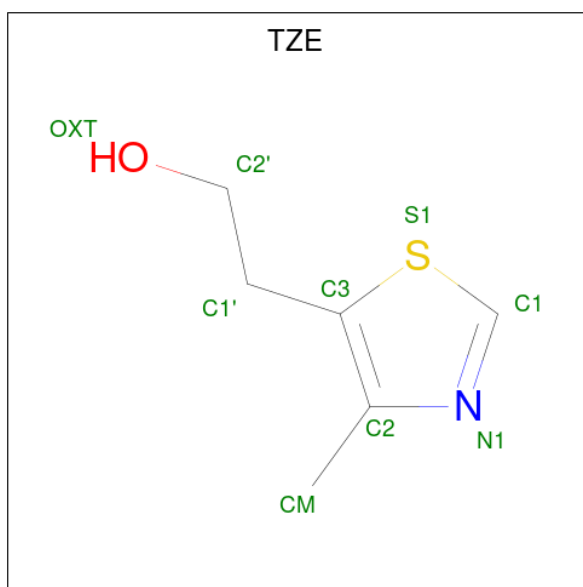
Chain	Residue	Modelled	Actual	Comment	Reference
B	267	TYR	-	expression tag	UNP Q6GEY3
B	268	PHE	-	expression tag	UNP Q6GEY3
B	269	GLN	-	expression tag	UNP Q6GEY3
B	270	SER	-	expression tag	UNP Q6GEY3
B	271	GLY	-	expression tag	UNP Q6GEY3
B	272	HIS	-	expression tag	UNP Q6GEY3
B	273	HIS	-	expression tag	UNP Q6GEY3
B	274	HIS	-	expression tag	UNP Q6GEY3
B	275	HIS	-	expression tag	UNP Q6GEY3
B	276	HIS	-	expression tag	UNP Q6GEY3
B	277	HIS	-	expression tag	UNP Q6GEY3
C	264	GLU	-	expression tag	UNP Q6GEY3
C	265	ASN	-	expression tag	UNP Q6GEY3
C	266	LEU	-	expression tag	UNP Q6GEY3
C	267	TYR	-	expression tag	UNP Q6GEY3
C	268	PHE	-	expression tag	UNP Q6GEY3
C	269	GLN	-	expression tag	UNP Q6GEY3
C	270	SER	-	expression tag	UNP Q6GEY3
C	271	GLY	-	expression tag	UNP Q6GEY3
C	272	HIS	-	expression tag	UNP Q6GEY3
C	273	HIS	-	expression tag	UNP Q6GEY3
C	274	HIS	-	expression tag	UNP Q6GEY3
C	275	HIS	-	expression tag	UNP Q6GEY3
C	276	HIS	-	expression tag	UNP Q6GEY3
C	277	HIS	-	expression tag	UNP Q6GEY3
E	264	GLU	-	expression tag	UNP Q6GEY3
E	265	ASN	-	expression tag	UNP Q6GEY3
E	266	LEU	-	expression tag	UNP Q6GEY3
E	267	TYR	-	expression tag	UNP Q6GEY3
E	268	PHE	-	expression tag	UNP Q6GEY3
E	269	GLN	-	expression tag	UNP Q6GEY3
E	270	SER	-	expression tag	UNP Q6GEY3
E	271	GLY	-	expression tag	UNP Q6GEY3
E	272	HIS	-	expression tag	UNP Q6GEY3
E	273	HIS	-	expression tag	UNP Q6GEY3
E	274	HIS	-	expression tag	UNP Q6GEY3
E	275	HIS	-	expression tag	UNP Q6GEY3
E	276	HIS	-	expression tag	UNP Q6GEY3
E	277	HIS	-	expression tag	UNP Q6GEY3
F	264	GLU	-	expression tag	UNP Q6GEY3
F	265	ASN	-	expression tag	UNP Q6GEY3
F	266	LEU	-	expression tag	UNP Q6GEY3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	267	TYR	-	expression tag	UNP Q6GEY3
F	268	PHE	-	expression tag	UNP Q6GEY3
F	269	GLN	-	expression tag	UNP Q6GEY3
F	270	SER	-	expression tag	UNP Q6GEY3
F	271	GLY	-	expression tag	UNP Q6GEY3
F	272	HIS	-	expression tag	UNP Q6GEY3
F	273	HIS	-	expression tag	UNP Q6GEY3
F	274	HIS	-	expression tag	UNP Q6GEY3
F	275	HIS	-	expression tag	UNP Q6GEY3
F	276	HIS	-	expression tag	UNP Q6GEY3
F	277	HIS	-	expression tag	UNP Q6GEY3
H	264	GLU	-	expression tag	UNP Q6GEY3
H	265	ASN	-	expression tag	UNP Q6GEY3
H	266	LEU	-	expression tag	UNP Q6GEY3
H	267	TYR	-	expression tag	UNP Q6GEY3
H	268	PHE	-	expression tag	UNP Q6GEY3
H	269	GLN	-	expression tag	UNP Q6GEY3
H	270	SER	-	expression tag	UNP Q6GEY3
H	271	GLY	-	expression tag	UNP Q6GEY3
H	272	HIS	-	expression tag	UNP Q6GEY3
H	273	HIS	-	expression tag	UNP Q6GEY3
H	274	HIS	-	expression tag	UNP Q6GEY3
H	275	HIS	-	expression tag	UNP Q6GEY3
H	276	HIS	-	expression tag	UNP Q6GEY3
H	277	HIS	-	expression tag	UNP Q6GEY3

- Molecule 2 is 2-(4-METHYL-THIAZOL-5-YL)-ETHANOL (CCD ID: TZE) (formula: C₆H₉NOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			9	6	1	1	1		
2	A	1	Total	C	N	O	S	0	0
			9	6	1	1	1		
2	C	1	Total	C	N	O	S	0	0
			9	6	1	1	1		
2	E	1	Total	C	N	O	S	0	0
			9	6	1	1	1		
2	F	1	Total	C	N	O	S	0	0
			9	6	1	1	1		
2	H	1	Total	C	N	O	S	0	0
			9	6	1	1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

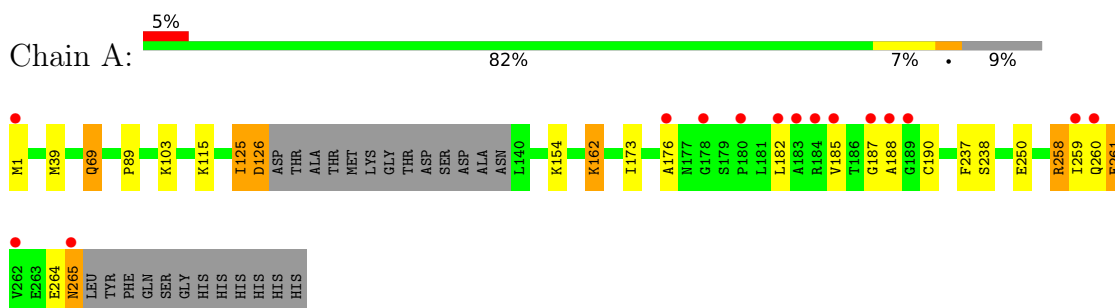
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total 85	O 85	0	0
4	B	107	Total 107	O 107	0	0
4	C	123	Total 123	O 123	0	0
4	E	24	Total 24	O 24	0	0
4	F	18	Total 18	O 18	0	0
4	H	14	Total 14	O 14	0	0

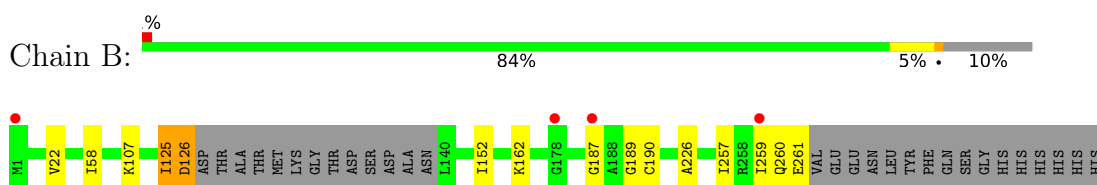
3 Residue-property plots

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.

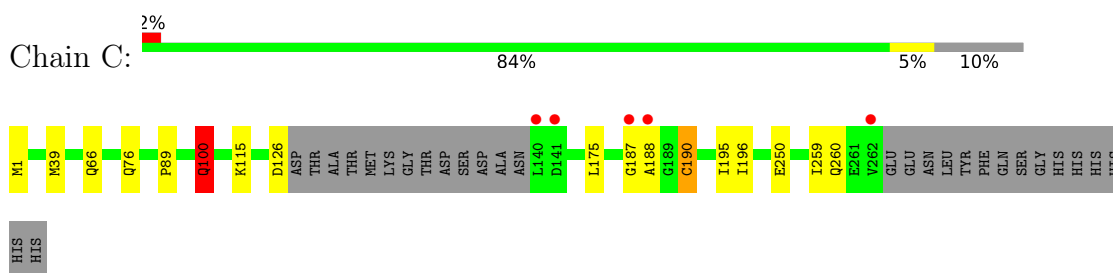
• Molecule 1: Hydroxyethylthiazole kinase



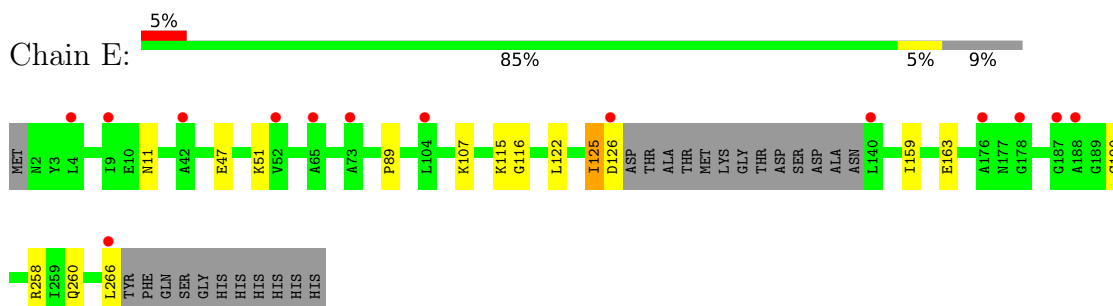
• Molecule 1: Hydroxyethylthiazole kinase



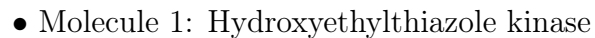
• Molecule 1: Hydroxyethylthiazole kinase



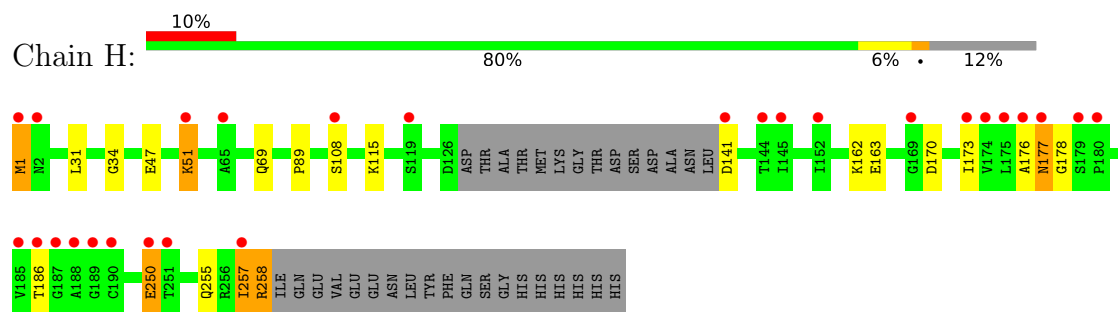
• Molecule 1: Hydroxyethylthiazole kinase



Chain F:



Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.55Å 62.74Å 108.46Å 92.18° 91.44° 101.32°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.91	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-1.90) 97.6 (20.00-1.91)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.186 , 0.210 0.195 , 0.216	Depositor DCC
R_{free} test set	6189 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l 0.027 for k,h,-l 0.032 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11578	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: TZE, MG

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	1.73	10/1920 (0.5%)	1.33	11/2611 (0.4%)
1	B	1.64	7/1883 (0.4%)	1.33	14/2560 (0.5%)
1	C	1.64	8/1891 (0.4%)	1.08	2/2572 (0.1%)
1	E	1.09	6/1920 (0.3%)	0.98	4/2612 (0.2%)
1	F	3.09	22/1825 (1.2%)	2.15	47/2482 (1.9%)
1	H	1.60	13/1853 (0.7%)	1.75	24/2520 (1.0%)
All	All	1.89	66/11292 (0.6%)	1.48	102/15357 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	F	1	7
1	H	2	1
All	All	3	10

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	76	GLN	CD-OE1	77.40	2.70	1.23
1	F	66	GLN	CG-CD	54.43	2.88	1.52
1	F	171	LYS	N-CA	42.68	1.97	1.46
1	C	100	GLN	CD-OE1	36.77	1.93	1.23
1	B	260	GLN	CD-NE2	-36.72	0.56	1.33

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	76	GLN	OE1-CD-NE2	46.34	168.94	122.60
1	H	177	ASN	O-C-N	-46.20	73.67	122.64
1	H	141	ASP	N-CA-CB	-42.46	38.32	110.50
1	F	125	ILE	CB-CA-C	-34.98	41.65	111.60
1	A	258	ARG	NE-CZ-NH2	-32.48	89.97	119.20

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	141	ASP	CA
1	H	162	LYS	CA
1	H	176	ALA	CA

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ILE	Peptide
1	C	100	GLN	Sidechain
1	F	150	TYR	Sidechain
1	F	170	ASP	Peptide,Mainchain
1	F	171	LYS	Mainchain

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	1896	0	1935	25	1
1	B	1859	0	1898	2	0
1	C	1867	0	1908	20	0
1	E	1896	0	1934	8	0
1	F	1802	0	1840	27	1
1	H	1829	0	1870	4	0
2	A	18	0	18	9	0
2	C	9	0	9	8	0
2	E	9	0	9	1	0
2	F	9	0	9	4	0
2	H	9	0	9	0	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	85	0	0	4	0
4	B	107	0	0	0	0
4	C	123	0	0	2	0
4	E	24	0	0	1	0
4	F	18	0	0	0	0
4	H	14	0	0	0	0
All	All	11578	0	11439	82	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 4.

The worst 5 of 82 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:C:175:LEU:CD2	1:C:259:ILE:HG22	1.75	1.16
1:F:188:ALA:HB1	1:F:218:PHE:CZ	1.82	1.15
1:F:188:ALA:HB1	1:F:218:PHE:HZ	0.99	1.11
1:C:175:LEU:HD22	1:C:259:ILE:HG22	1.31	1.09
1:E:163:GLU:OE2	1:E:260:GLN:NE2	1.85	1.09

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:A:264:GLU:OE1	1:F:162:LYS:NZ[1_445]	1.04	1.16

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	248/277 (90%)	247 (100%)	1 (0%)	0	100	100
1	B	244/277 (88%)	243 (100%)	1 (0%)	0	100	100
1	C	245/277 (88%)	243 (99%)	2 (1%)	0	100	100
1	E	248/277 (90%)	245 (99%)	3 (1%)	0	100	100
1	F	235/277 (85%)	231 (98%)	4 (2%)	0	100	100
1	H	240/277 (87%)	236 (98%)	4 (2%)	0	100	100
All	All	1460/1662 (88%)	1445 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	202/223 (91%)	197 (98%)	5 (2%)	42	37
1	B	197/223 (88%)	195 (99%)	2 (1%)	68	70
1	C	198/223 (89%)	196 (99%)	2 (1%)	68	70
1	E	202/223 (91%)	201 (100%)	1 (0%)	81	84
1	F	191/223 (86%)	180 (94%)	11 (6%)	18	10
1	H	194/223 (87%)	190 (98%)	4 (2%)	47	44
All	All	1184/1338 (88%)	1159 (98%)	25 (2%)	47	44

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	147	LYS
1	F	173	ILE
1	H	258	ARG
1	F	171	LYS
1	F	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	GLN
1	C	6	ASN
1	C	76	GLN
1	H	2	ASN
1	H	230	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
2	TZE	C	301	-	8,9,9	2.71	4 (50%)	8,11,11	4.32	5 (62%)
2	TZE	A	301	-	8,9,9	1.91	3 (37%)	8,11,11	3.77	4 (50%)
2	TZE	A	302	-	8,9,9	1.14	2 (25%)	8,11,11	3.24	3 (37%)
2	TZE	E	301	-	8,9,9	1.31	2 (25%)	8,11,11	5.28	4 (50%)
2	TZE	F	301	-	8,9,9	0.86	0	8,11,11	5.20	4 (50%)
2	TZE	H	301	-	8,9,9	1.05	0	8,11,11	5.47	4 (50%)

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	TZE	C	301	-	-	0/3/3/3	0/1/1/1
2	TZE	A	301	-	-	0/3/3/3	0/1/1/1
2	TZE	A	302	-	-	1/3/3/3	0/1/1/1
2	TZE	E	301	-	-	1/3/3/3	0/1/1/1
2	TZE	F	301	-	-	0/3/3/3	0/1/1/1
2	TZE	H	301	-	-	0/3/3/3	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	TZE	C2-N1	4.59	1.44	1.38
2	C	301	TZE	C1-N1	3.87	1.40	1.30
2	A	301	TZE	C2-N1	3.65	1.43	1.38
2	C	301	TZE	C1-S1	3.60	1.78	1.72
2	C	301	TZE	C1'-C3	2.74	1.56	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	TZE	S1-C1-N1	-11.52	106.18	116.08
2	E	301	TZE	S1-C1-N1	-10.91	106.70	116.08
2	F	301	TZE	S1-C1-N1	-10.35	107.18	116.08
2	C	301	TZE	S1-C1-N1	-9.14	108.22	116.08
2	H	301	TZE	C1-S1-C3	8.24	98.13	89.55

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	TZE	C3-C1'-C2'-OXT
2	A	302	TZE	C3-C1'-C2'-OXT

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	TZE	8	0
2	A	301	TZE	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	TZE	2	0
2	E	301	TZE	1	0
2	F	301	TZE	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	2
1	H	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	178:GLY	C	179:SER	N	2.24
1	H	178:GLY	C	179:SER	N	1.70
1	H	177:ASN	C	178:GLY	N	1.20
1	F	176:ALA	C	177:ASN	N	0.97

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	252/277 (90%)	-0.05	15 (5%) 27 29	13, 27, 50, 70	12 (4%)
1	B	248/277 (89%)	-0.35	4 (1%) 70 74	13, 23, 39, 67	8 (3%)
1	C	249/277 (89%)	-0.36	5 (2%) 65 69	12, 24, 40, 72	8 (3%)
1	E	252/277 (90%)	0.68	14 (5%) 30 32	18, 46, 67, 77	10 (3%)
1	F	238/277 (85%)	1.12	44 (18%) 3 3	26, 52, 74, 91	27 (11%)
1	H	243/277 (87%)	0.93	27 (11%) 10 11	26, 51, 72, 92	19 (7%)
All	All	1482/1662 (89%)	0.32	109 (7%) 20 22	12, 37, 68, 92	84 (5%)

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	ALA	6.9
1	A	187	GLY	5.3
1	F	176	ALA	5.3
1	F	257	ILE	5.2
1	F	187	GLY	5.1

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	MG	A	303	1/1	0.86	0.10	50,50,50,50	1
2	TZE	H	301	9/9	0.88	0.17	39,43,46,56	7
2	TZE	F	301	9/9	0.88	0.14	39,52,66,67	6
2	TZE	E	301	9/9	0.89	0.14	45,49,54,54	2
2	TZE	A	301	9/9	0.91	0.12	23,32,44,52	0
2	TZE	A	302	9/9	0.91	0.12	25,40,52,53	3
2	TZE	C	301	9/9	0.92	0.12	18,28,31,35	0
3	MG	E	302	1/1	0.93	0.09	48,48,48,48	0
3	MG	C	302	1/1	0.94	0.12	35,35,35,35	0
3	MG	B	301	1/1	0.97	0.10	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.