



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2024 – 01:59 am BST

PDB ID : 5COJ
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

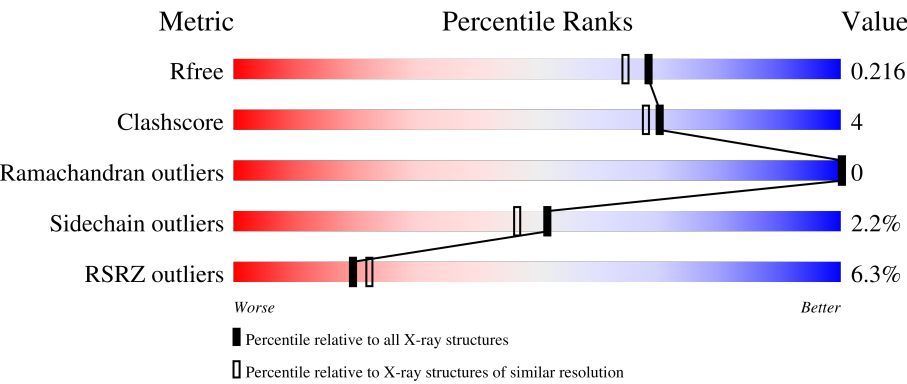
1 Overall quality at a glance i

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>83%6%•9%</div></div>
1	B	277	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>85%•10%</div></div>
1	C	277	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>84%5%10%</div></div>
1	E	277	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>84%6%•9%</div></div>
1	F	277	<div><div>13%</div><div><div></div><div></div><div></div><div></div></div><div>73%10%••13%</div></div>

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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

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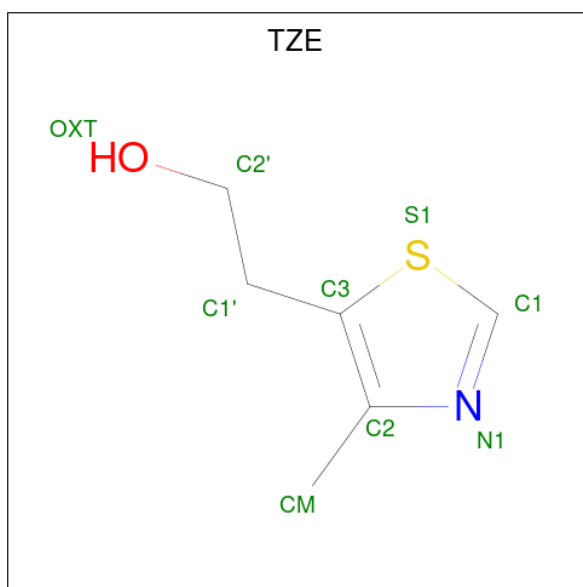
Chain	Residue	Modelled	Actual	Comment	Reference
B	267	TYR	-	expression tag	UNP Q6GEY3
B	268	PHE	-	expression tag	UNP Q6GEY3
B	269	GLN	-	expression tag	UNP Q6GEY3
B	270	SER	-	expression tag	UNP Q6GEY3
B	271	GLY	-	expression tag	UNP Q6GEY3
B	272	HIS	-	expression tag	UNP Q6GEY3
B	273	HIS	-	expression tag	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

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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 (three-letter code: 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 (three-letter code: 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.

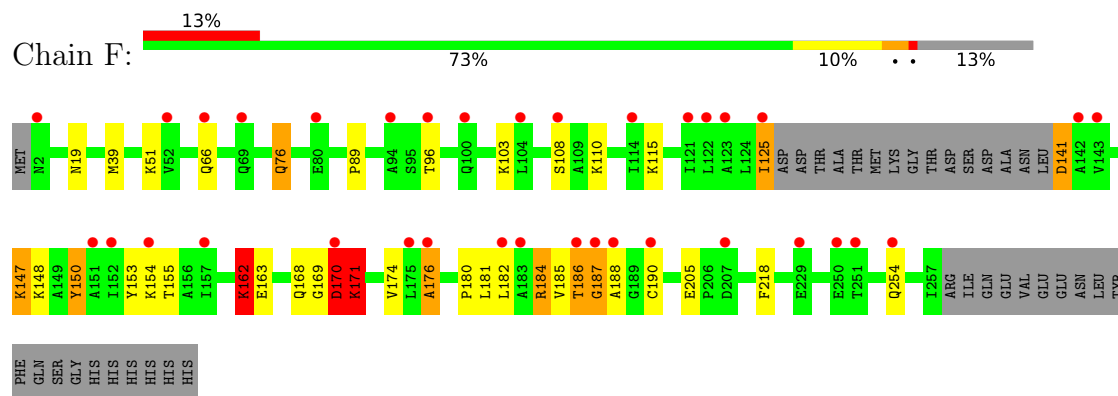
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total 85	O 85	0	0
4	B	107	Total 107	O 107	0	0
4	C	123	Total 123	O 123	0	0
4	E	24	Total 24	O 24	0	0
4	F	18	Total 18	O 18	0	0
4	H	14	Total 14	O 14	0	0

i

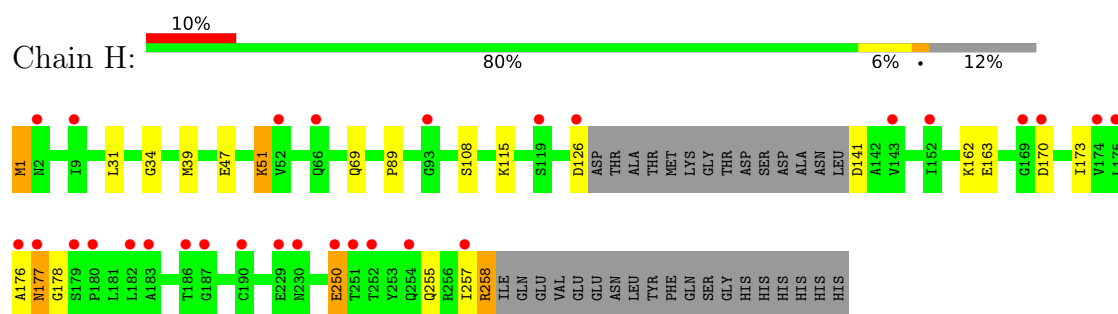
- Molecule 1: Hydroxyethylthiazole kinase



● Molecule 1: Hydroxyethylthiazole kinase



● Molecule 1: Hydroxyethylthiazole kinase



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 19.55 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-1.90) 97.7 (19.55-1.90)	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 (5.02%)	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 , 52.5	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 [i](#)

5.1 Standard geometry [i](#)

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	1.50	8/1920 (0.4%)	1.58	10/2611 (0.4%)
1	B	1.27	4/1883 (0.2%)	1.00	9/2560 (0.4%)
1	C	1.29	4/1891 (0.2%)	0.88	3/2572 (0.1%)
1	E	0.78	5/1920 (0.3%)	0.84	8/2612 (0.3%)
1	F	2.74	21/1825 (1.2%)	1.63	34/2482 (1.4%)
1	H	1.18	10/1853 (0.5%)	1.43	21/2520 (0.8%)
All	All	1.57	52/11292 (0.5%)	1.27	85/15357 (0.6%)

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

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	76	GLN	CD-OE1	66.66	2.70	1.24
1	F	66	GLN	CG-CD	59.59	2.88	1.51
1	A	258	ARG	CZ-NH1	-33.97	0.88	1.33
1	C	100	GLN	CD-OE1	31.58	1.93	1.24
1	B	260	GLN	CD-NE2	-30.68	0.56	1.32
1	A	258	ARG	NE-CZ	27.91	1.69	1.33
1	F	76	GLN	CD-NE2	27.16	2.00	1.32
1	F	171	LYS	N-CA	25.63	1.97	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	150	TYR	CB-CG	23.95	1.87	1.51
1	F	180	PRO	N-CD	-23.71	1.14	1.47
1	F	108	SER	CA-CB	22.58	1.86	1.52
1	A	258	ARG	CZ-NH2	20.92	1.60	1.33
1	H	170	ASP	CA-CB	19.68	1.97	1.53
1	H	141	ASP	CA-CB	18.33	1.94	1.53
1	F	176	ALA	C-N	-15.98	0.97	1.34
1	H	178	GLY	C-N	15.95	1.70	1.34
1	F	170	ASP	N-CA	15.92	1.78	1.46
1	H	51	LYS	CB-CG	-15.57	1.10	1.52
1	F	76	GLN	CG-CD	15.55	1.86	1.51
1	C	100	GLN	CD-NE2	-13.50	0.99	1.32
1	F	168	GLN	C-N	13.39	1.57	1.33
1	F	254	GLN	CA-CB	-13.28	1.24	1.53
1	B	162	LYS	CA-CB	-13.15	1.25	1.53
1	C	100	GLN	CG-CD	12.92	1.80	1.51
1	A	69	GLN	CG-CD	12.53	1.79	1.51
1	F	125	ILE	CA-CB	12.29	1.83	1.54
1	H	47	GLU	CA-CB	-12.07	1.27	1.53
1	E	47	GLU	CA-CB	-11.86	1.27	1.53
1	E	107	LYS	CA-CB	-11.60	1.28	1.53
1	F	162	LYS	CA-CB	-11.50	1.28	1.53
1	H	162	LYS	CA-CB	-10.82	1.30	1.53
1	H	1	MET	SD-CE	-10.45	1.19	1.77
1	F	141	ASP	CA-CB	-10.08	1.31	1.53
1	H	250	GLU	CG-CD	-9.76	1.37	1.51
1	F	51	LYS	CB-CG	-8.37	1.29	1.52
1	A	250	GLU	CD-OE2	8.32	1.34	1.25
1	F	174	VAL	CA-CB	-8.25	1.37	1.54
1	H	69	GLN	CA-CB	-8.20	1.35	1.53
1	F	147	LYS	CB-CG	8.13	1.74	1.52
1	A	154	LYS	CB-CG	-8.01	1.30	1.52
1	F	170	ASP	CA-C	-7.86	1.32	1.52
1	H	177	ASN	C-N	-7.07	1.20	1.33
1	B	260	GLN	CA-CB	6.76	1.68	1.53
1	B	190	CYS	CB-SG	6.35	1.93	1.82
1	F	148	LYS	CA-CB	-6.33	1.40	1.53
1	E	51	LYS	CA-CB	-6.32	1.40	1.53
1	E	258	ARG	CA-CB	-6.25	1.40	1.53
1	C	10	GLU	CD-OE2	-6.00	1.19	1.25
1	F	96	THR	CA-CB	-5.96	1.37	1.53
1	A	103	LYS	CG-CD	-5.65	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	126	ASP	CB-CG	-5.22	1.40	1.51
1	A	261	GLU	CA-CB	5.12	1.65	1.53

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ARG	NE-CZ-NH2	-60.67	89.97	120.30
1	H	141	ASP	N-CA-CB	-40.15	38.32	110.60
1	F	125	ILE	CB-CA-C	-34.98	41.65	111.60
1	H	177	ASN	O-C-N	-29.13	73.67	123.20
1	A	258	ARG	NE-CZ-NH1	23.50	132.05	120.30
1	F	76	GLN	OE1-CD-NE2	20.45	168.94	121.90
1	F	66	GLN	CG-CD-OE1	20.21	162.03	121.60
1	F	66	GLN	CG-CD-NE2	-18.77	71.65	116.70
1	F	76	GLN	CG-CD-OE1	-16.58	88.45	121.60
1	A	258	ARG	NH1-CZ-NH2	16.26	137.29	119.40
1	F	176	ALA	O-C-N	-13.40	101.27	122.70
1	B	260	GLN	OE1-CD-NE2	-13.01	91.99	121.90
1	F	168	GLN	O-C-N	12.32	144.15	123.20
1	F	170	ASP	CA-C-O	-12.13	94.63	120.10
1	H	177	ASN	CA-C-N	11.70	139.60	116.20
1	H	170	ASP	N-CA-CB	-11.67	89.59	110.60
1	H	162	LYS	N-CA-CB	11.55	131.40	110.60
1	H	176	ALA	N-CA-CB	11.53	126.24	110.10
1	F	141	ASP	CB-CA-C	11.34	133.07	110.40
1	B	260	GLN	N-CA-CB	-11.29	90.28	110.60
1	F	163	GLU	N-CA-CB	-11.04	90.74	110.60
1	F	150	TYR	CA-CB-CG	-10.77	92.95	113.40
1	B	260	GLN	CG-CD-NE2	10.24	141.27	116.70
1	F	171	LYS	N-CA-CB	10.24	129.03	110.60
1	H	170	ASP	CB-CA-C	-10.19	90.03	110.40
1	F	168	GLN	CA-C-N	-10.17	95.86	116.20
1	B	162	LYS	N-CA-CB	9.96	128.54	110.60
1	E	107	LYS	CB-CA-C	9.74	129.88	110.40
1	F	171	LYS	N-CA-C	-9.72	84.76	111.00
1	H	69	GLN	N-CA-CB	8.73	126.31	110.60
1	F	147	LYS	CB-CG-CD	8.44	133.54	111.60
1	F	169	GLY	O-C-N	8.25	135.90	122.70
1	E	256	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	H	1	MET	CG-SD-CE	8.17	113.27	100.20
1	F	170	ASP	C-N-CA	-8.11	101.42	121.70
1	F	66	GLN	CB-CG-CD	-7.94	90.95	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	171	LYS	CB-CA-C	7.78	125.95	110.40
1	F	147	LYS	CA-CB-CG	-7.77	96.32	113.40
1	H	47	GLU	N-CA-CB	7.75	124.56	110.60
1	F	148	LYS	CB-CA-C	7.72	125.84	110.40
1	F	76	GLN	CB-CG-CD	-7.42	92.30	111.60
1	F	108	SER	N-CA-CB	-7.30	99.56	110.50
1	A	69	GLN	OE1-CD-NE2	7.24	138.55	121.90
1	F	180	PRO	CA-CB-CG	-7.24	90.25	104.00
1	F	76	GLN	CG-CD-NE2	-7.22	99.37	116.70
1	B	126	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	E	266	LEU	CA-CB-CG	7.12	131.68	115.30
1	A	258	ARG	CD-NE-CZ	-7.07	113.70	123.60
1	F	103	LYS	CA-CB-CG	-6.89	98.24	113.40
1	F	169	GLY	CA-C-N	-6.82	102.20	117.20
1	A	69	GLN	CG-CD-NE2	-6.77	100.46	116.70
1	F	125	ILE	CA-CB-CG2	6.67	124.24	110.90
1	E	256	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	F	150	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	F	176	ALA	CA-C-N	6.51	131.52	117.20
1	C	256	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	103	LYS	CB-CG-CD	6.41	128.27	111.60
1	E	47	GLU	CB-CA-C	6.31	123.03	110.40
1	H	258	ARG	CB-CG-CD	6.20	127.71	111.60
1	H	177	ASN	C-N-CA	6.17	135.26	122.30
1	E	258	ARG	CB-CA-C	6.15	122.71	110.40
1	H	162	LYS	CA-CB-CG	6.14	126.91	113.40
1	E	140	LEU	CA-CB-CG	-6.13	101.20	115.30
1	B	20	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	H	178	GLY	O-C-N	-5.97	113.14	122.70
1	F	170	ASP	N-CA-CB	5.91	121.24	110.60
1	H	173	ILE	CA-CB-CG1	-5.89	99.81	111.00
1	F	254	GLN	N-CA-CB	5.78	121.00	110.60
1	H	51	LYS	CA-CB-CG	5.68	125.90	113.40
1	F	169	GLY	C-N-CA	-5.67	107.53	121.70
1	H	163	GLU	CB-CA-C	5.41	121.22	110.40
1	A	182	LEU	CB-CA-C	5.40	120.46	110.20
1	F	162	LYS	N-CA-CB	5.39	120.30	110.60
1	B	256	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	162	LYS	CA-CB-CG	5.31	125.09	113.40
1	B	126	ASP	N-CA-C	5.30	125.32	111.00
1	C	100	GLN	CG-CD-NE2	-5.28	104.03	116.70
1	B	190	CYS	CB-CA-C	5.28	120.95	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	173	ILE	CG1-CB-CG2	-5.19	99.98	111.40
1	H	173	ILE	CA-CB-CG2	-5.18	100.55	110.90
1	H	176	ALA	CB-CA-C	5.14	117.81	110.10
1	E	140	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	C	20	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	154	LYS	CA-CB-CG	5.09	124.60	113.40
1	H	257	ILE	CB-CA-C	-5.04	101.52	111.60

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

All (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
1	F	176	ALA	Mainchain
1	F	186	THR	Peptide
1	F	187	GLY	Peptide
1	H	177	ASN	Mainchain

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	1896	0	1935	25	1
1	B	1859	0	1898	2	0
1	C	1867	0	1908	18	0
1	E	1896	0	1934	7	0
1	F	1802	0	1840	27	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1829	0	1870	4	0
2	A	18	0	18	9	0
2	C	9	0	9	6	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
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	79	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.

All (79) 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:C:39:MET:HE1	2:C:301:TZE:H3M	1.31	1.13
1:F:188:ALA:HB1	1:F:218:PHE:HZ	0.99	1.11
1:C:39:MET:CE	2:C:301:TZE:H3M	1.81	1.10
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
1:A:39:MET:HE1	2:A:301:TZE:H3M	1.35	1.06
1:A:39:MET:CE	2:A:301:TZE:H3M	1.85	1.05
1:F:190:CYS:SG	2:F:301:TZE:OXT	2.13	1.04
1:F:182:LEU:HD22	1:F:188:ALA:CB	1.90	1.00
1:C:100:GLN:CG	1:C:100:GLN:NE2	2.26	0.99
1:F:182:LEU:HD22	1:F:188:ALA:HB3	1.47	0.96
1:A:69:GLN:CG	1:A:69:GLN:NE2	2.34	0.91
1:F:190:CYS:SG	2:F:301:TZE:C2'	2.61	0.88
1:E:190:CYS:SG	4:E:402:HOH:O	2.26	0.86
1:C:175:LEU:CD2	1:C:259:ILE:CG2	2.58	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:LYS:C	1:F:171:LYS:N	2.35	0.79
1:A:258:ARG:NE	1:A:258:ARG:NH2	2.32	0.77
1:C:187:GLY:HA2	4:C:459:HOH:O	1.85	0.77
1:C:175:LEU:HD23	1:C:259:ILE:HG22	1.69	0.75
1:C:190:CYS:SG	4:C:459:HOH:O	2.30	0.74
1:A:258:ARG:NE	1:A:258:ARG:NH1	2.37	0.72
1:C:175:LEU:HD22	1:C:259:ILE:CG2	2.16	0.71
1:F:153:TYR:O	1:F:155:THR:HG23	1.94	0.68
1:A:187:GLY:HA2	4:A:474:HOH:O	1.95	0.66
1:C:39:MET:HE2	2:C:301:TZE:H3M	1.77	0.63
1:C:39:MET:CE	2:C:301:TZE:CM	2.70	0.63
1:A:190:CYS:SG	2:A:302:TZE:H22'	2.39	0.62
1:F:190:CYS:SG	2:F:301:TZE:H21'	2.38	0.61
1:A:39:MET:CE	2:A:301:TZE:CM	2.73	0.60
1:E:190:CYS:SG	2:E:301:TZE:H21'	2.42	0.60
1:F:182:LEU:HD22	1:F:188:ALA:HB2	1.82	0.60
1:A:39:MET:HE2	2:A:301:TZE:H3M	1.78	0.59
1:F:185:VAL:HG12	1:F:187:GLY:HA3	1.85	0.57
1:A:265:ASN:OD1	4:A:401:HOH:O	2.18	0.56
1:A:190:CYS:SG	4:A:474:HOH:O	2.47	0.56
1:C:39:MET:HE2	2:C:301:TZE:C2	2.37	0.55
1:F:182:LEU:CD2	1:F:188:ALA:CB	2.76	0.55
1:A:39:MET:HE2	2:A:301:TZE:C2	2.36	0.55
1:F:184:ARG:HH12	1:H:34:GLY:HA2	1.74	0.53
1:F:170:ASP:N	1:F:170:ASP:C	2.62	0.52
1:F:184:ARG:O	1:H:31:LEU:HD13	2.10	0.52
1:A:39:MET:HE2	2:A:301:TZE:CM	2.40	0.51
1:F:154:LYS:HD2	1:F:154:LYS:C	2.29	0.51
1:F:19:ASN:HD21	2:F:301:TZE:H22'	1.75	0.51
1:F:110:LYS:NZ	1:F:155:THR:HG22	2.26	0.50
1:A:69:GLN:HG3	1:F:205:GLU:HB3	1.94	0.49
1:E:122:LEU:O	1:E:125:ILE:O	2.30	0.49
1:C:39:MET:HE2	2:C:301:TZE:CM	2.41	0.48
1:A:265:ASN:CG	4:A:401:HOH:O	2.52	0.47
1:F:182:LEU:CD2	1:F:188:ALA:HB2	2.43	0.46
1:A:69:GLN:CG	1:A:69:GLN:HE21	2.23	0.45
1:E:125:ILE:O	1:E:126:ASP:C	2.54	0.45
1:A:173:ILE:HD11	1:A:259:ILE:HG23	1.98	0.45
1:F:154:LYS:O	1:F:154:LYS:HG3	2.17	0.44
1:H:1:MET:HB2	1:H:250:GLU:HG2	1.98	0.44
1:A:69:GLN:HG3	1:F:205:GLU:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:LYS:O	1:F:154:LYS:CG	2.63	0.43
1:A:125:ILE:O	1:A:126:ASP:HB2	2.18	0.43
1:F:171:LYS:N	1:F:171:LYS:O	2.52	0.43
1:F:184:ARG:HA	1:F:184:ARG:HE	1.82	0.43
1:C:89:PRO:HD2	1:C:115:LYS:O	2.18	0.43
1:C:27:ALA:HB2	1:C:39:MET:HE3	2.02	0.42
1:A:39:MET:HE2	2:A:301:TZE:N1	2.34	0.42
1:F:76:GLN:OE1	1:F:76:GLN:HB2	2.20	0.42
1:B:125:ILE:O	1:B:126:ASP:HB2	2.20	0.42
1:C:100:GLN:CG	1:C:100:GLN:HE21	2.23	0.42
1:H:89:PRO:HD2	1:H:115:LYS:O	2.20	0.42
1:C:1:MET:HB2	1:C:250:GLU:HG3	2.02	0.41
1:A:1:MET:HB2	1:A:250:GLU:HG2	2.02	0.41
1:A:89:PRO:HD2	1:A:115:LYS:O	2.19	0.41
1:F:89:PRO:HD2	1:F:115:LYS:O	2.21	0.41
1:A:69:GLN:CG	1:A:69:GLN:OE1	2.67	0.41
1:A:190:CYS:SG	2:A:302:TZE:C2'	3.08	0.41
1:E:116:GLY:O	1:E:159:ILE:HA	2.21	0.41
1:A:185:VAL:HG21	1:A:237:PHE:HD2	1.86	0.41
1:B:22:VAL:CG1	1:B:187:GLY:HA3	2.51	0.40
1:E:89:PRO:HD2	1:E:115:LYS:O	2.21	0.40

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 ⓘ

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	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%)	198 (98%)	4 (2%)	55	51
1	B	197/223 (88%)	194 (98%)	3 (2%)	65	62
1	C	198/223 (89%)	197 (100%)	1 (0%)	88	89
1	E	202/223 (91%)	200 (99%)	2 (1%)	76	76
1	F	191/223 (86%)	181 (95%)	10 (5%)	23	14
1	H	194/223 (87%)	188 (97%)	6 (3%)	40	32
All	All	1184/1338 (88%)	1158 (98%)	26 (2%)	52	47

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	ASP
1	A	260	GLN
1	A	261	GLU
1	A	265	ASN
1	B	39	MET
1	B	107	LYS
1	B	261	GLU

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Mol	Chain	Res	Type
1	C	260	GLN
1	E	39	MET
1	E	266	LEU
1	F	39	MET
1	F	125	ILE
1	F	141	ASP
1	F	147	LYS
1	F	162	LYS
1	F	170	ASP
1	F	171	LYS
1	F	181	LEU
1	F	184	ARG
1	F	186	THR
1	H	39	MET
1	H	51	LYS
1	H	108	SER
1	H	126	ASP
1	H	255	GLN
1	H	258	ARG

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

Mol	Chain	Res	Type
1	B	69	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 monosaccharides in this entry.

5.6 Ligand geometry

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	E	301	-	5,9,9	1.55	1 (20%)	3,11,11	1.15	0
2	TZE	H	301	-	5,9,9	0.73	0	3,11,11	1.27	0
2	TZE	F	301	-	5,9,9	1.48	1 (20%)	3,11,11	2.30	1 (33%)
2	TZE	C	301	-	5,9,9	5.85	1 (20%)	3,11,11	1.29	0
2	TZE	A	301	-	5,9,9	2.75	2 (40%)	3,11,11	0.49	0
2	TZE	A	302	-	5,9,9	1.66	2 (40%)	3,11,11	2.23	1 (33%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	TZE	C1'-C3	12.88	1.56	1.50
2	A	301	TZE	C1'-C3	5.69	1.53	1.50
2	F	301	TZE	C1'-C3	3.04	1.52	1.50
2	E	301	TZE	C1'-C3	2.82	1.52	1.50
2	A	302	TZE	C1'-C3	2.47	1.52	1.50
2	A	301	TZE	CM-C2	2.04	1.53	1.50
2	A	302	TZE	CM-C2	2.00	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	TZE	C1'-C3-C2	-3.53	124.60	127.43
2	A	302	TZE	C1'-C3-C2	3.51	130.25	127.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	TZE	1	0
2	F	301	TZE	4	0
2	C	301	TZE	6	0
2	A	301	TZE	7	0
2	A	302	TZE	2	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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	176:ALA	C	177:ASN	N	0.97

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	252/277 (90%)	0.04	8 (3%)	47	50	13, 28, 50, 72	12 (4%)
1	B	248/277 (89%)	-0.19	1 (0%)	92	93	13, 23, 42, 68	8 (3%)
1	C	249/277 (89%)	-0.15	2 (0%)	86	87	12, 24, 42, 72	9 (3%)
1	E	252/277 (90%)	0.51	18 (7%)	16	17	34, 48, 68, 78	10 (3%)
1	F	238/277 (85%)	0.80	35 (14%)	2	2	33, 56, 79, 91	28 (11%)
1	H	243/277 (87%)	0.63	29 (11%)	4	5	33, 54, 76, 93	19 (7%)
All	All	1482/1662 (89%)	0.27	93 (6%)	20	22	12, 39, 71, 93	86 (5%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	187	GLY	5.9
1	F	186	THR	5.1
1	H	177	ASN	4.6
1	H	187	GLY	4.5
1	F	251	THR	4.5
1	F	183	ALA	4.4
1	E	229	GLU	4.2
1	H	66	GLN	4.1
1	A	187	GLY	4.0
1	H	2	ASN	3.9
1	H	176	ALA	3.9
1	C	140	LEU	3.8
1	H	126	ASP	3.7
1	F	125	ILE	3.7
1	E	187	GLY	3.6
1	E	140	LEU	3.6
1	E	9	ILE	3.5
1	H	229	GLU	3.5
1	H	169	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	175	LEU	3.4
1	E	250	GLU	3.4
1	E	96	THR	3.3
1	H	180	PRO	3.3
1	A	260	GLN	3.3
1	F	182	LEU	3.3
1	E	266	LEU	3.2
1	H	257	ILE	3.2
1	F	142	ALA	3.2
1	H	251	THR	3.2
1	E	251	THR	3.1
1	H	179	SER	3.1
1	E	65	ALA	3.1
1	H	254	GLN	3.1
1	H	250	GLU	3.0
1	H	252	THR	3.0
1	E	52	VAL	3.0
1	H	119	SER	2.9
1	E	255	GLN	2.9
1	F	104	LEU	2.9
1	F	100	GLN	2.8
1	A	265	ASN	2.8
1	F	114	ILE	2.8
1	F	170	ASP	2.8
1	F	229	GLU	2.8
1	A	1	MET	2.8
1	H	170	ASP	2.8
1	F	94	ALA	2.7
1	F	152	ILE	2.7
1	H	52	VAL	2.7
1	E	69	GLN	2.7
1	F	69	GLN	2.7
1	F	52	VAL	2.7
1	H	190	CYS	2.7
1	F	108	SER	2.6
1	F	207	ASP	2.6
1	F	157	ILE	2.6
1	F	122	LEU	2.6
1	H	143	VAL	2.6
1	F	175	LEU	2.5
1	E	126	ASP	2.5
1	E	56	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	93	GLY	2.5
1	F	121	ILE	2.5
1	A	262	VAL	2.5
1	E	162	LYS	2.5
1	E	254	GLN	2.4
1	F	154	LYS	2.4
1	F	2	ASN	2.4
1	F	176	ALA	2.4
1	F	250	GLU	2.4
1	C	170	ASP	2.4
1	H	152	ILE	2.3
1	F	80	GLU	2.3
1	B	1	MET	2.3
1	F	66	GLN	2.3
1	F	143	VAL	2.3
1	A	264	GLU	2.3
1	F	151	ALA	2.3
1	A	188	ALA	2.3
1	A	184	ARG	2.2
1	F	123	ALA	2.2
1	H	93	GLY	2.2
1	F	188	ALA	2.2
1	H	186	THR	2.2
1	F	190	CYS	2.2
1	H	174	VAL	2.2
1	F	96	THR	2.1
1	E	83	LEU	2.1
1	F	254	GLN	2.1
1	H	182	LEU	2.1
1	H	230	ASN	2.0
1	H	183	ALA	2.0
1	H	9	ILE	2.0

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	TZE	F	301	9/9	0.85	0.20	39,52,66,67	6
2	TZE	E	301	9/9	0.87	0.22	45,49,54,54	2
2	TZE	C	301	9/9	0.90	0.15	18,28,31,35	0
3	MG	A	303	1/1	0.90	0.12	50,50,50,50	1
2	TZE	A	301	9/9	0.91	0.17	23,32,44,52	0
2	TZE	H	301	9/9	0.92	0.18	39,43,46,56	7
2	TZE	A	302	9/9	0.93	0.15	25,40,52,53	3
3	MG	E	302	1/1	0.93	0.17	48,48,48,48	0
3	MG	C	302	1/1	0.97	0.13	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.