Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 01:05 pm BST

PDB ID	:	5CGA
Title	:	Structure of Hydroxyethylthiazole kinase ThiM from Staphylococcus aureus in complex with substrate analog 2-(1,3,5-trimethyl-1H-pyrazole-4-yl)ethanol
Authors	:	Kuenz, M.; Drebes, J.; Windshuegel, B.; Cang, H.; Wrenger, C.; Betzel, C.
Deposited on	:	2015-07-09
Resolution	:	1.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

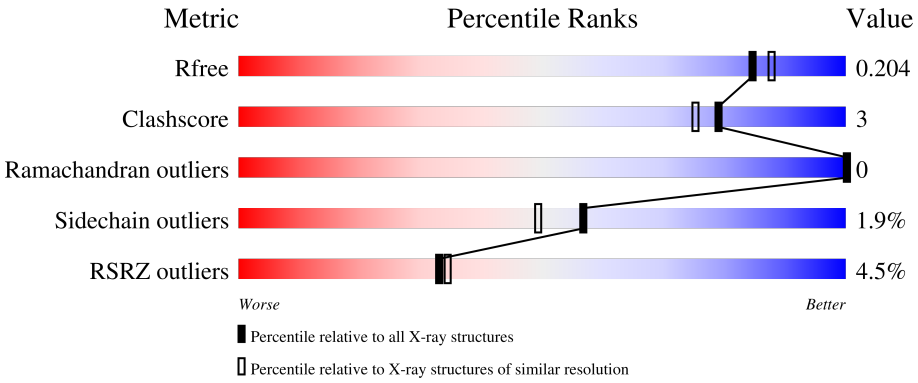
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 <=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	2% 81% 10% • 9%
1	B	277	% 79% 9% • 10%
1	C	277	% 81% 8% • 9%
1	E	277	5% 85% 6% • 8%
1	F	277	7% 80% 7% • 12%

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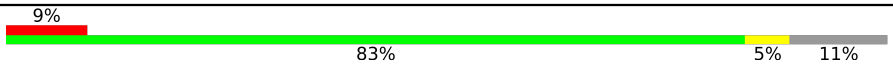
Mol	Chain	Length	Quality of chain
1	H	277	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11784 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	54	0	0
			1880	1200	309	365	6			
1	B	249	Total	C	N	O	S	34	0	0
			1862	1190	305	361	6			
1	C	251	Total	C	N	O	S	38	0	0
			1882	1199	308	369	6			
1	E	255	Total	C	N	O	S	69	0	0
			1925	1228	314	377	6			
1	F	245	Total	C	N	O	S	81	0	0
			1834	1171	301	357	5			
1	H	246	Total	C	N	O	S	34	0	0
			1845	1179	302	358	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	GLN	-	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	GLN	-	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	GLN	-	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	GLN	-	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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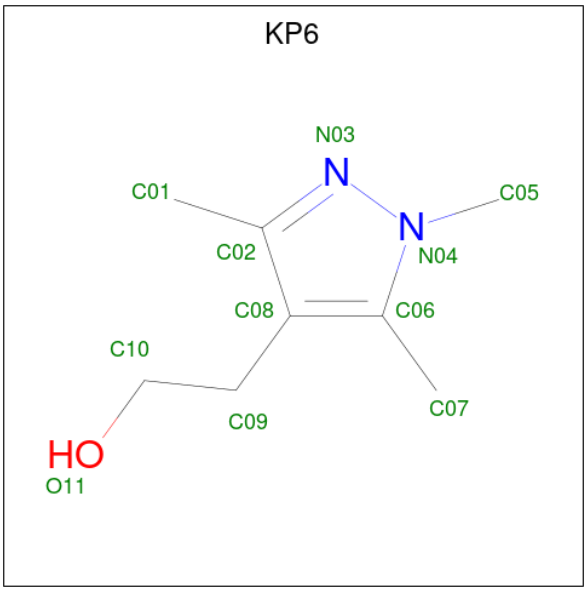
Chain	Residue	Modelled	Actual	Comment	Reference
F	267	TYR	-	expression tag	UNP Q6GEY3
F	268	GLN	-	expression tag	UNP Q6GEY3
F	269	GLN	-	expression tag	UNP Q6GEY3
F	270	SER	-	expression tag	UNP Q6GEY3
F	271	GLY	-	expression tag	UNP Q6GEY3
F	272	HIS	-	expression tag	UNP Q6GEY3
F	273	HIS	-	expression tag	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	GLN	-	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-(1,3,5-trimethyl-1H-pyrazol-4-yl)ethanol (three-letter code: KP6) (formula: $C_8H_{14}N_2O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 11 8 2 1	0	0
2	B	1	Total C N O 11 8 2 1	0	0
2	C	1	Total C N O 11 8 2 1	0	0
2	E	1	Total C N O 11 8 2 1	0	0
2	F	1	Total C N O 11 8 2 1	0	0
2	H	1	Total C N O 11 8 2 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

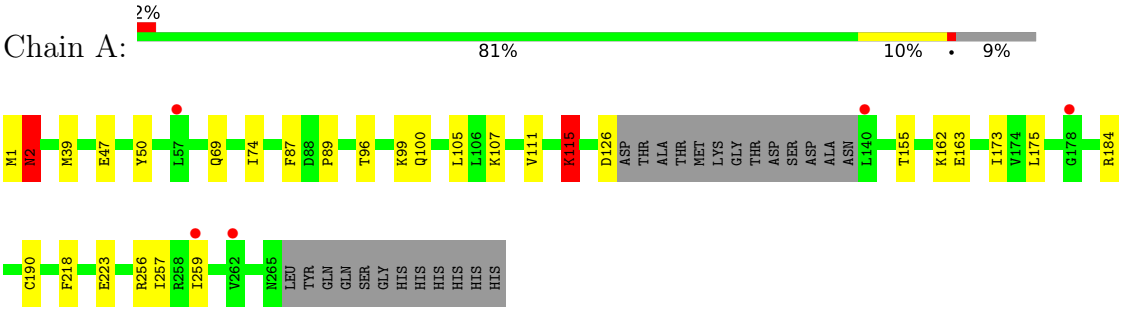
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	115	Total O 115 115	0	0
4	B	134	Total O 134 134	0	0
4	C	140	Total O 140 140	0	0
4	E	49	Total O 49 49	0	0
4	F	25	Total O 25 25	0	0
4	H	23	Total O 23 23	0	0

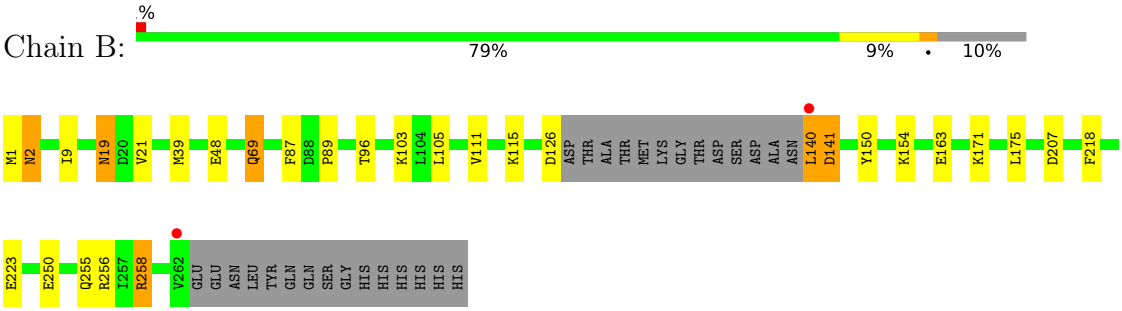
3 Residue-property plots (i)

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.

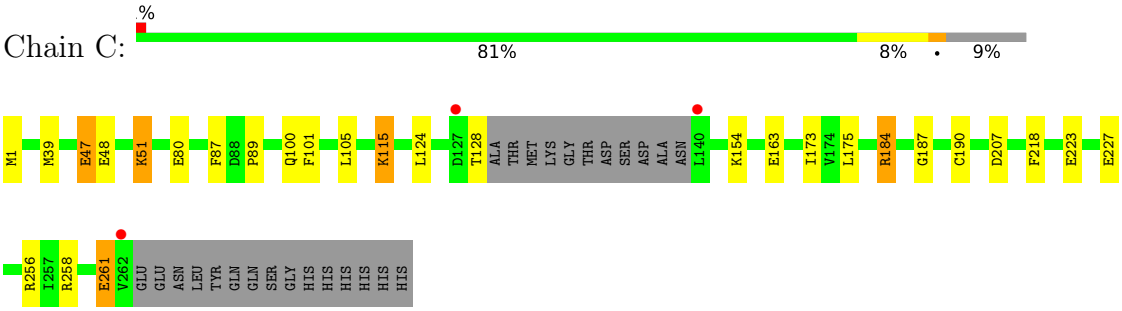
• Molecule 1: Hydroxyethylthiazole kinase



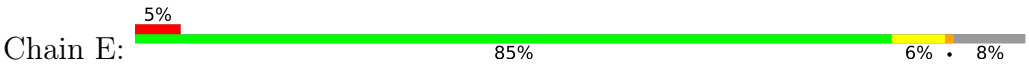
• Molecule 1: Hydroxyethylthiazole kinase

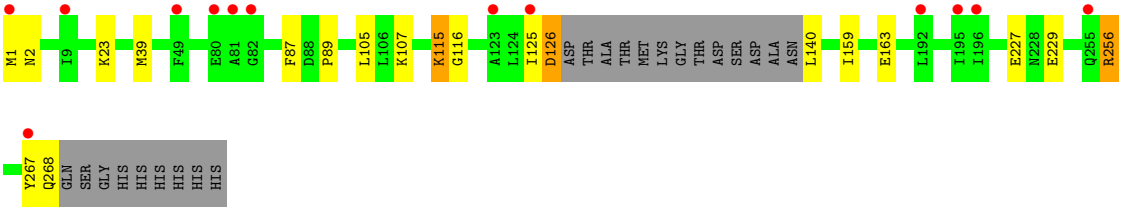


• Molecule 1: Hydroxyethylthiazole kinase

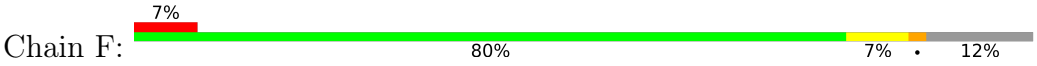


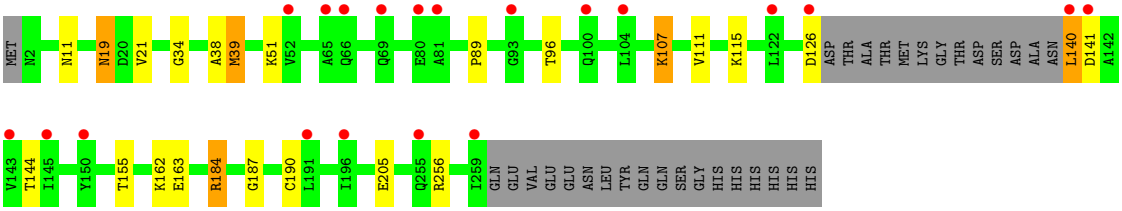
• Molecule 1: Hydroxyethylthiazole kinase



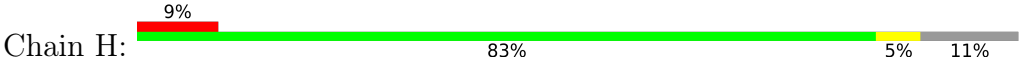


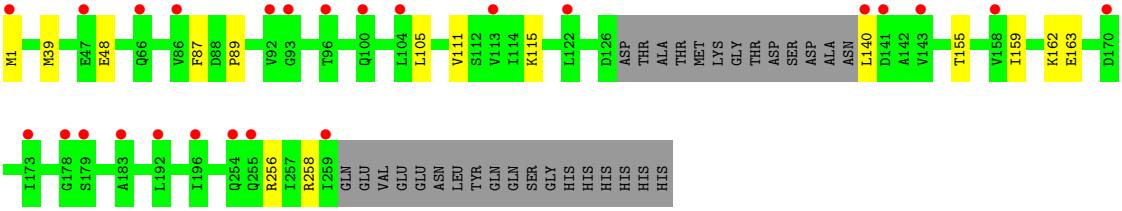
• Molecule 1: Hydroxyethylthiazole kinase





• Molecule 1: Hydroxyethylthiazole kinase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.03Å 62.36Å 108.32Å 92.59° 91.39° 101.28°	Depositor
Resolution (Å)	29.81 – 1.87 29.79 – 1.87	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.81-1.87) 95.9 (29.79-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.169 , 0.199 0.176 , 0.204	Depositor DCC
R_{free} test set	6337 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11784	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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: KP6, 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	1.48	13/1904 (0.7%)	1.20	13/2591 (0.5%)
1	B	1.26	9/1886 (0.5%)	1.36	14/2566 (0.5%)
1	C	1.53	11/1906 (0.6%)	1.66	15/2593 (0.6%)
1	E	1.15	8/1950 (0.4%)	1.07	13/2652 (0.5%)
1	F	1.39	6/1858 (0.3%)	3.33	10/2528 (0.4%)
1	H	1.05	3/1869 (0.2%)	1.30	5/2542 (0.2%)
All	All	1.32	50/11373 (0.4%)	1.81	70/15472 (0.5%)

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	B	0	4
1	C	0	2
1	E	0	1
1	F	0	1
All	All	0	9

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	184	ARG	NE-CZ	-37.92	0.83	1.33
1	A	184	ARG	CZ-NH2	-33.76	0.89	1.33
1	F	126	ASP	CA-C	31.07	2.33	1.52
1	C	258	ARG	NE-CZ	-28.20	0.96	1.33
1	H	258	ARG	CZ-NH1	-27.63	0.97	1.33
1	E	163	GLU	CG-CD	-24.41	1.15	1.51
1	C	184	ARG	CZ-NH2	-20.06	1.06	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	154	LYS	CE-NZ	-17.95	1.04	1.49
1	A	2	ASN	CG-ND2	-15.31	0.94	1.32
1	E	229	GLU	CG-CD	-15.17	1.29	1.51
1	C	261	GLU	CB-CG	-14.51	1.24	1.52
1	F	184	ARG	CZ-NH2	14.20	1.51	1.33
1	E	115	LYS	CE-NZ	-14.05	1.14	1.49
1	C	51	LYS	CG-CD	13.85	1.99	1.52
1	A	2	ASN	CG-OD1	13.72	1.54	1.24
1	A	184	ARG	CG-CD	-13.30	1.18	1.51
1	C	47	GLU	CD-OE2	-13.24	1.11	1.25
1	B	141	ASP	CG-OD2	13.20	1.55	1.25
1	H	258	ARG	CZ-NH2	13.03	1.50	1.33
1	A	100	GLN	CG-CD	-10.99	1.25	1.51
1	B	69	GLN	CD-NE2	-10.83	1.05	1.32
1	E	126	ASP	CA-CB	10.74	1.77	1.53
1	H	163	GLU	CG-CD	-8.67	1.39	1.51
1	E	23	LYS	CE-NZ	-8.40	1.28	1.49
1	B	163	GLU	CG-CD	-8.08	1.39	1.51
1	A	163	GLU	CG-CD	-7.92	1.40	1.51
1	B	2	ASN	CG-OD1	-7.14	1.08	1.24
1	A	218	PHE	CG-CD2	-6.82	1.28	1.38
1	F	163	GLU	CB-CG	6.70	1.64	1.52
1	B	141	ASP	CG-OD1	6.69	1.40	1.25
1	C	218	PHE	CG-CD2	-6.61	1.28	1.38
1	C	163	GLU	CG-CD	-6.31	1.42	1.51
1	F	51	LYS	CB-CG	-6.26	1.35	1.52
1	C	80	GLU	CD-OE2	-6.21	1.18	1.25
1	B	103	LYS	CD-CE	-6.11	1.35	1.51
1	E	2	ASN	CG-OD1	-6.11	1.10	1.24
1	B	223	GLU	CB-CG	-6.06	1.40	1.52
1	A	47	GLU	CD-OE1	-6.04	1.19	1.25
1	F	107	LYS	CB-CG	6.03	1.68	1.52
1	C	101	PHE	CG-CD2	-5.83	1.30	1.38
1	E	2	ASN	CG-ND2	5.74	1.47	1.32
1	B	150	TYR	CE1-CZ	-5.65	1.31	1.38
1	A	115	LYS	CE-NZ	-5.51	1.35	1.49
1	A	223	GLU	CB-CG	-5.51	1.41	1.52
1	A	107	LYS	CB-CG	-5.44	1.37	1.52
1	A	162	LYS	CB-CG	5.37	1.67	1.52
1	E	107	LYS	CB-CG	-5.31	1.38	1.52
1	B	218	PHE	CG-CD2	-5.25	1.30	1.38
1	C	223	GLU	CB-CG	-5.16	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	CYS	CB-SG	5.10	1.91	1.82

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	184	ARG	NE-CZ-NH1	-149.18	45.71	120.30
1	H	258	ARG	NE-CZ-NH2	-48.75	95.92	120.30
1	F	126	ASP	CA-C-O	-44.99	25.61	120.10
1	C	184	ARG	NE-CZ-NH2	-43.97	98.31	120.30
1	C	184	ARG	NE-CZ-NH1	-35.03	102.78	120.30
1	F	184	ARG	NE-CZ-NH2	28.14	134.37	120.30
1	F	184	ARG	NH1-CZ-NH2	-27.06	89.64	119.40
1	B	69	GLN	CG-CD-NE2	-26.11	54.02	116.70
1	A	184	ARG	NE-CZ-NH2	-25.07	107.77	120.30
1	F	184	ARG	CD-NE-CZ	22.02	154.43	123.60
1	B	69	GLN	OE1-CD-NE2	21.49	171.32	121.90
1	E	126	ASP	CB-CA-C	-20.26	69.89	110.40
1	C	258	ARG	CD-NE-CZ	19.02	150.22	123.60
1	C	51	LYS	CG-CD-CE	18.89	168.56	111.90
1	A	2	ASN	CB-CG-OD1	-18.37	84.85	121.60
1	B	258	ARG	NE-CZ-NH2	-18.08	111.26	120.30
1	H	258	ARG	NH1-CZ-NH2	16.09	137.09	119.40
1	C	258	ARG	NE-CZ-NH1	-15.42	112.59	120.30
1	C	258	ARG	NE-CZ-NH2	15.06	127.83	120.30
1	B	141	ASP	OD1-CG-OD2	-14.47	95.80	123.30
1	E	163	GLU	CB-CG-CD	13.27	150.02	114.20
1	B	258	ARG	NE-CZ-NH1	13.25	126.92	120.30
1	E	140	LEU	CB-CG-CD2	-13.09	88.75	111.00
1	C	51	LYS	CB-CG-CD	-10.58	84.09	111.60
1	F	107	LYS	CA-CB-CG	-10.57	90.15	113.40
1	A	184	ARG	NH1-CZ-NH2	10.45	130.89	119.40
1	C	184	ARG	NH1-CZ-NH2	-9.32	109.14	119.40
1	A	99	LYS	CB-CG-CD	9.06	135.17	111.60
1	E	229	GLU	CB-CG-CD	8.96	138.39	114.20
1	B	2	ASN	CB-CG-ND2	-8.77	95.64	116.70
1	A	256	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	E	23	LYS	CD-CE-NZ	8.55	131.37	111.70
1	C	256	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	E	229	GLU	CG-CD-OE1	-8.30	101.71	118.30
1	E	229	GLU	CG-CD-OE2	8.25	134.81	118.30
1	E	140	LEU	CB-CG-CD1	8.20	124.94	111.00
1	E	163	GLU	CG-CD-OE1	-8.06	102.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	GLU	CB-CG-CD	8.05	135.93	114.20
1	E	163	GLU	CG-CD-OE2	7.81	133.92	118.30
1	B	256	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	E	126	ASP	CA-CB-CG	7.00	128.81	113.40
1	F	256	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	B	141	ASP	CB-CG-OD2	6.88	124.50	118.30
1	C	256	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	H	256	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	B	171	LYS	CB-CG-CD	6.66	128.93	111.60
1	A	100	GLN	CG-CD-OE1	-6.41	108.78	121.60
1	H	258	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	E	140	LEU	CA-CB-CG	-6.13	101.20	115.30
1	A	163	GLU	CG-CD-OE1	-6.12	106.05	118.30
1	A	162	LYS	CA-CB-CG	-6.11	99.96	113.40
1	C	184	ARG	CD-NE-CZ	6.01	132.02	123.60
1	A	163	GLU	CG-CD-OE2	6.00	130.31	118.30
1	B	171	LYS	CG-CD-CE	5.87	129.50	111.90
1	A	47	GLU	CG-CD-OE2	-5.76	106.78	118.30
1	F	51	LYS	CA-CB-CG	5.76	126.07	113.40
1	F	256	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	256	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	F	107	LYS	CB-CG-CD	5.66	126.31	111.60
1	A	47	GLU	OE1-CD-OE2	5.62	130.04	123.30
1	B	256	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	207	ASP	CB-CG-OD1	5.39	123.15	118.30
1	C	100	GLN	OE1-CD-NE2	5.39	134.30	121.90
1	H	256	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	207	ASP	CB-CG-OD1	5.20	122.98	118.30
1	E	256	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	126	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	C	47	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	C	207	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	B	154	LYS	CD-CE-NZ	5.00	123.20	111.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ASN	Sidechain
1	B	141	ASP	Sidechain
1	B	2	ASN	Sidechain
1	B	255	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	B	258	ARG	Sidechain
1	C	184	ARG	Sidechain
1	C	47	GLU	Sidechain
1	E	125	ILE	Peptide
1	F	184	ARG	Sidechain

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	1880	0	1917	12	0
1	B	1862	0	1907	9	0
1	C	1882	0	1919	10	0
1	E	1925	0	1963	6	0
1	F	1834	0	1873	24	0
1	H	1845	0	1894	6	0
2	A	11	0	0	0	0
2	B	11	0	0	0	0
2	C	11	0	0	0	0
2	E	11	0	0	5	0
2	F	11	0	0	0	0
2	H	11	0	0	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	115	0	0	0	0
4	B	134	0	0	1	0
4	C	140	0	0	3	1
4	E	49	0	0	0	1
4	F	25	0	0	2	0
4	H	23	0	0	1	0
All	All	11784	0	11473	62	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.

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:MET:HE2	1:F:39:MET:N	1.45	1.28
1:F:38:ALA:C	1:F:39:MET:HE2	1.80	0.99
1:F:39:MET:N	1:F:39:MET:CE	2.28	0.96
1:F:39:MET:HE2	1:F:39:MET:H	1.44	0.82
1:A:175:LEU:CD2	1:A:259:ILE:HG22	2.10	0.81
1:A:175:LEU:HD22	1:A:259:ILE:HG22	1.66	0.77
1:F:187:GLY:HA2	4:F:401:HOH:O	1.90	0.71
1:B:1:MET:HB3	1:B:250:GLU:HG2	1.73	0.71
1:C:190:CYS:SG	4:C:429:HOH:O	2.01	0.68
1:C:187:GLY:HA2	4:C:429:HOH:O	1.96	0.66
1:F:190:CYS:SG	4:F:401:HOH:O	2.53	0.66
2:E:301:KP6:N03	1:F:39:MET:HE3	2.12	0.65
1:B:19:ASN:HD22	1:B:21:VAL:H	1.47	0.63
1:F:19:ASN:HD22	1:F:21:VAL:H	1.45	0.62
1:F:141:ASP:OD1	1:F:144:THR:OG1	2.18	0.62
1:F:38:ALA:CA	1:F:39:MET:HE2	2.28	0.62
1:E:227:GLU:OE2	1:E:256:ARG:NH2	2.34	0.61
1:A:69:GLN:HG3	1:F:205:GLU:HB3	1.83	0.60
1:E:267:TYR:O	1:E:268:GLN:HB2	2.02	0.59
1:F:39:MET:CE	1:F:39:MET:H	2.06	0.59
1:C:175:LEU:HD12	1:C:175:LEU:N	2.20	0.57
1:F:141:ASP:OD1	1:F:144:THR:CB	2.53	0.56
1:B:175:LEU:HD12	1:B:175:LEU:N	2.20	0.56
1:C:227:GLU:OE1	4:C:401:HOH:O	2.19	0.50
1:F:141:ASP:OD1	1:F:144:THR:N	2.37	0.50
1:B:96:THR:HG23	1:C:48:GLU:OE2	2.12	0.49
1:A:173:ILE:HD11	1:A:259:ILE:HB	1.97	0.47
2:E:301:KP6:C02	1:F:39:MET:HE3	2.44	0.47
1:H:159:ILE:HG22	4:H:407:HOH:O	2.16	0.46
1:A:257:ILE:HG12	1:A:259:ILE:HG23	1.96	0.46
1:A:96:THR:HG23	1:B:48:GLU:OE2	2.17	0.45
1:E:87:PHE:CE1	1:E:105:LEU:HD23	2.52	0.45
2:E:301:KP6:N03	1:F:39:MET:CE	2.79	0.45
1:B:140:LEU:N	4:B:405:HOH:O	2.50	0.45
1:A:1:MET:CG	1:A:1:MET:O	2.66	0.44
1:B:1:MET:CG	1:B:1:MET:O	2.64	0.44
1:C:87:PHE:CE1	1:C:105:LEU:HD23	2.52	0.44
1:E:1:MET:CG	1:E:1:MET:O	2.65	0.44
1:A:69:GLN:HG3	1:F:205:GLU:CB	2.47	0.44
1:E:89:PRO:HD2	1:E:115:LYS:O	2.18	0.44
1:H:1:MET:O	1:H:1:MET:CG	2.65	0.44
1:C:124:LEU:O	1:C:128:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:301:KP6:C01	1:F:39:MET:HE1	2.48	0.43
1:B:87:PHE:CE1	1:B:105:LEU:HD23	2.53	0.43
1:C:89:PRO:HD2	1:C:115:LYS:O	2.18	0.43
1:E:116:GLY:O	1:E:159:ILE:HA	2.18	0.43
1:H:87:PHE:CE1	1:H:105:LEU:HD23	2.54	0.43
1:C:1:MET:O	1:C:1:MET:CG	2.67	0.43
2:E:301:KP6:C01	1:F:39:MET:CE	2.97	0.42
1:H:89:PRO:HD2	1:H:115:LYS:O	2.20	0.42
1:F:111:VAL:HG23	1:F:155:THR:HG21	2.01	0.42
1:A:111:VAL:HG23	1:A:155:THR:HG21	2.01	0.42
1:C:173:ILE:HD13	1:C:261:GLU:HA	2.02	0.42
1:F:89:PRO:HD2	1:F:115:LYS:O	2.20	0.42
1:F:96:THR:HG23	1:H:48:GLU:OE2	2.19	0.42
1:A:87:PHE:CE1	1:A:105:LEU:HD23	2.54	0.42
1:F:11:ASN:HA	1:F:34:GLY:O	2.20	0.41
1:A:50:TYR:OH	1:A:74:ILE:HB	2.21	0.41
1:B:89:PRO:HD2	1:B:115:LYS:O	2.21	0.41
1:A:89:PRO:HD2	1:A:115:LYS:O	2.20	0.40
1:H:111:VAL:HG23	1:H:155:THR:HG21	2.02	0.40
1:F:140:LEU:HD12	1:F:144:THR:CG2	2.51	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)
4:C:426:HOH:O	4:E:413:HOH:O[1_556]	2.17	0.03

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%)	245 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	245/277 (88%)	243 (99%)	2 (1%)	0	100	100
1	C	247/277 (89%)	246 (100%)	1 (0%)	0	100	100
1	E	251/277 (91%)	248 (99%)	3 (1%)	0	100	100
1	F	241/277 (87%)	239 (99%)	2 (1%)	0	100	100
1	H	242/277 (87%)	240 (99%)	2 (1%)	0	100	100
All	All	1474/1662 (89%)	1461 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	198/223 (89%)	194 (98%)	4 (2%)	55	47
1	B	197/223 (88%)	191 (97%)	6 (3%)	41	30
1	C	200/223 (90%)	197 (98%)	3 (2%)	65	59
1	E	205/223 (92%)	203 (99%)	2 (1%)	76	73
1	F	194/223 (87%)	189 (97%)	5 (3%)	46	36
1	H	196/223 (88%)	193 (98%)	3 (2%)	65	59
All	All	1190/1338 (89%)	1167 (98%)	23 (2%)	57	49

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	39	MET
1	A	115	LYS
1	A	126	ASP
1	B	9	ILE
1	B	19	ASN
1	B	39	MET
1	B	69	GLN

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Mol	Chain	Res	Type
1	B	111	VAL
1	B	140	LEU
1	C	39	MET
1	C	51	LYS
1	C	115	LYS
1	E	39	MET
1	E	126	ASP
1	F	19	ASN
1	F	39	MET
1	F	107	LYS
1	F	140	LEU
1	F	162	LYS
1	H	39	MET
1	H	140	LEU
1	H	162	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	ASN
1	E	6	ASN
1	E	260	GLN
1	F	19	ASN
1	H	2	ASN
1	H	6	ASN
1	H	11	ASN
1	H	67	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 monosaccharides 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	KP6	F	301	-	10,11,11	2.48	2 (20%)	11,15,15	2.67	4 (36%)
2	KP6	E	301	-	10,11,11	2.63	4 (40%)	11,15,15	2.14	5 (45%)
2	KP6	C	301	-	10,11,11	2.50	4 (40%)	11,15,15	3.19	4 (36%)
2	KP6	H	301	-	10,11,11	2.62	3 (30%)	11,15,15	2.66	5 (45%)
2	KP6	A	301	-	10,11,11	2.57	3 (30%)	11,15,15	3.07	5 (45%)
2	KP6	B	301	-	10,11,11	2.57	3 (30%)	11,15,15	4.21	7 (63%)

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	KP6	F	301	-	-	1/3/3/3	0/1/1/1
2	KP6	E	301	-	-	1/3/3/3	0/1/1/1
2	KP6	C	301	-	-	0/3/3/3	0/1/1/1
2	KP6	H	301	-	-	1/3/3/3	0/1/1/1
2	KP6	A	301	-	-	0/3/3/3	0/1/1/1
2	KP6	B	301	-	-	0/3/3/3	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	KP6	C06-C08	5.94	1.51	1.39
2	H	301	KP6	C08-C02	5.93	1.49	1.39
2	F	301	KP6	C08-C02	5.83	1.49	1.39
2	E	301	KP6	C08-C02	5.46	1.48	1.39
2	C	301	KP6	C06-C08	5.36	1.50	1.39
2	A	301	KP6	C08-C02	5.34	1.48	1.39
2	A	301	KP6	C06-C08	5.05	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	KP6	C06-C08	4.88	1.49	1.39
2	F	301	KP6	C06-C08	4.67	1.48	1.39
2	H	301	KP6	C06-C08	4.45	1.48	1.39
2	C	301	KP6	C08-C02	4.14	1.46	1.39
2	B	301	KP6	C02-N03	4.03	1.41	1.33
2	E	301	KP6	C02-N03	3.14	1.39	1.33
2	B	301	KP6	C08-C02	3.06	1.44	1.39
2	C	301	KP6	C06-N04	-3.02	1.33	1.37
2	A	301	KP6	C02-N03	2.82	1.39	1.33
2	H	301	KP6	C02-N03	2.47	1.38	1.33
2	C	301	KP6	C02-N03	2.40	1.38	1.33
2	E	301	KP6	C06-N04	-2.08	1.34	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	KP6	C02-N03-N04	9.57	112.57	104.35
2	C	301	KP6	C02-N03-N04	7.99	111.21	104.35
2	F	301	KP6	C02-N03-N04	7.08	110.44	104.35
2	A	301	KP6	C02-N03-N04	6.75	110.15	104.35
2	B	301	KP6	C01-C02-N03	6.07	132.89	119.78
2	H	301	KP6	C02-N03-N04	5.08	108.72	104.35
2	B	301	KP6	C01-C02-C08	-4.74	119.14	129.47
2	C	301	KP6	C01-C02-N03	4.56	129.62	119.78
2	A	301	KP6	C01-C02-N03	4.44	129.38	119.78
2	H	301	KP6	C01-C02-N03	4.26	128.98	119.78
2	B	301	KP6	C08-C06-N04	3.67	109.72	106.79
2	B	301	KP6	C06-N04-N03	-3.64	107.67	112.10
2	A	301	KP6	C09-C08-C02	3.42	129.70	127.30
2	E	301	KP6	C02-N03-N04	3.37	107.25	104.35
2	C	301	KP6	C05-N04-C06	3.26	133.08	128.82
2	E	301	KP6	C09-C08-C02	3.14	129.50	127.30
2	H	301	KP6	C01-C02-C08	-3.13	122.64	129.47
2	E	301	KP6	C01-C02-N03	3.06	126.39	119.78
2	A	301	KP6	C01-C02-C08	-3.04	122.84	129.47
2	F	301	KP6	C05-N04-C06	3.02	132.77	128.82
2	F	301	KP6	C09-C08-C02	2.90	129.33	127.30
2	H	301	KP6	C08-C06-N04	2.68	108.94	106.79
2	E	301	KP6	C05-N04-C06	2.68	132.32	128.82
2	B	301	KP6	C09-C08-C02	2.47	129.03	127.30
2	C	301	KP6	C01-C02-C08	-2.40	124.24	129.47
2	A	301	KP6	C05-N04-C06	2.36	131.90	128.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	KP6	C06-C08-C02	-2.35	102.70	106.62
2	H	301	KP6	C06-C08-C02	-2.20	102.95	106.62
2	F	301	KP6	C01-C02-N03	2.16	124.45	119.78
2	E	301	KP6	C01-C02-C08	-2.11	124.86	129.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	KP6	C08-C09-C10-O11
2	F	301	KP6	C08-C09-C10-O11
2	H	301	KP6	C08-C09-C10-O11

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	KP6	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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%)	-0.15	5 (1%) 65 67	14, 27, 44, 62	26 (10%)
1	B	249/277 (89%)	-0.32	2 (0%) 86 87	13, 23, 37, 60	19 (7%)
1	C	251/277 (90%)	-0.23	3 (1%) 79 80	12, 24, 39, 74	24 (9%)
1	E	255/277 (92%)	0.12	13 (5%) 28 29	25, 40, 64, 75	25 (9%)
1	F	245/277 (88%)	0.54	20 (8%) 11 12	27, 51, 76, 103	22 (8%)
1	H	246/277 (88%)	0.49	25 (10%) 6 7	27, 48, 68, 89	11 (4%)
All	All	1498/1662 (90%)	0.07	68 (4%) 33 34	12, 34, 66, 103	127 (8%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	140	LEU	8.9
1	F	122	LEU	6.1
1	F	52	VAL	5.5
1	H	140	LEU	4.7
1	H	259	ILE	4.5
1	H	178	GLY	4.3
1	H	141	ASP	4.0
1	B	262	VAL	4.0
1	H	122	LEU	3.7
1	F	259	ILE	3.6
1	E	192	LEU	3.5
1	H	173	ILE	3.4
1	A	259	ILE	3.4
1	E	49	PHE	3.4
1	F	69	GLN	3.3
1	H	100	GLN	3.2
1	F	141	ASP	3.1
1	F	143	VAL	3.1
1	H	1	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	143	VAL	2.9
1	H	192	LEU	2.9
1	E	196	ILE	2.9
1	A	140	LEU	2.8
1	F	81	ALA	2.8
1	E	267	TYR	2.8
1	E	1	MET	2.7
1	H	196	ILE	2.7
1	H	66	GLN	2.6
1	H	254	GLN	2.6
1	H	93	GLY	2.6
1	H	113	VAL	2.6
1	H	255	GLN	2.6
1	C	127	ASP	2.5
1	F	191	LEU	2.5
1	H	170	ASP	2.5
1	E	125	ILE	2.5
1	E	9	ILE	2.5
1	F	126	ASP	2.5
1	C	262	VAL	2.4
1	H	86	VAL	2.4
1	H	92	VAL	2.4
1	H	158	VAL	2.4
1	F	150	TYR	2.4
1	H	183	ALA	2.4
1	H	47	GLU	2.4
1	F	145	ILE	2.4
1	F	100	GLN	2.4
1	F	196	ILE	2.3
1	C	140	LEU	2.3
1	F	65	ALA	2.3
1	H	179	SER	2.3
1	E	255	GLN	2.3
1	A	178	GLY	2.3
1	E	195	ILE	2.3
1	F	66	GLN	2.2
1	F	80	GLU	2.2
1	H	96	THR	2.2
1	E	123	ALA	2.2
1	E	81	ALA	2.2
1	F	93	GLY	2.2
1	E	82	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	255	GLN	2.1
1	E	80	GLU	2.1
1	A	57	LEU	2.1
1	H	104	LEU	2.1
1	F	104	LEU	2.1
1	A	262	VAL	2.0
1	B	140	LEU	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, 95^{th} 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	302	1/1	0.74	0.19	46,46,46,46	1
3	MG	C	302	1/1	0.80	0.10	43,43,43,43	1
3	MG	E	302	1/1	0.88	0.15	47,47,47,47	1
2	KP6	E	301	11/11	0.89	0.26	39,40,45,48	5
2	KP6	A	301	11/11	0.90	0.17	24,40,45,48	1
2	KP6	H	301	11/11	0.91	0.20	35,42,52,52	3
2	KP6	B	301	11/11	0.91	0.22	22,30,36,38	2
2	KP6	C	301	11/11	0.93	0.13	24,31,37,39	2
2	KP6	F	301	11/11	0.93	0.24	32,38,47,48	4
3	MG	B	302	1/1	0.94	0.08	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.