wwPDB X-ray Structure Validation Summary Report (i)

Apr 29, 2024 – 02:03 am BST

PDB ID	:	5CGE
Title	:	Structure of Hydroxyethylthiazole Kinase ThiM from Staphylococcus aureus in complex with substrate analog 2-(2-methyl-1H-imidazole-1-yl)ethanol
Authors	:	Kuenz, M.; Drebes, J.; Windshuegel, B.; Cang, H.; Wrenger, C.; Betzel, C.
Deposited on	:	2015-07-09
Resolution	:	1.62 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

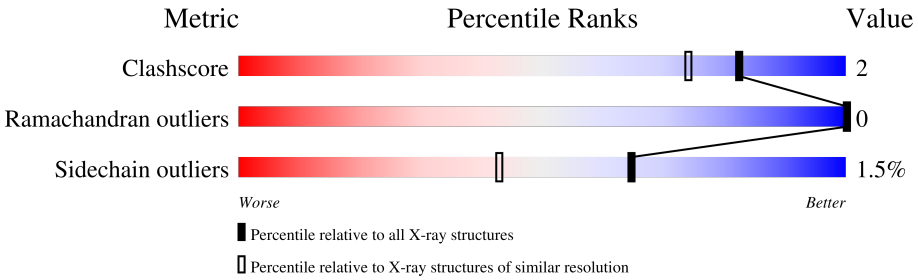
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (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 1.62 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))
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	277	82% 8% • 8%
1	B	277	85% 9% • 5%
1	C	277	83% 6% • 10%
1	D	277	81% 7% • 12%
1	E	277	89% 7% •
1	F	277	83% 8% • 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12018 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	255	Total	C	N	O	S	27	0	0
			1901	1211	312	372	6			
1	B	262	Total	C	N	O	S	31	0	0
			1954	1242	320	385	7			
1	C	250	Total	C	N	O	S	21	0	0
			1878	1198	307	367	6			
1	E	267	Total	C	N	O	S	29	0	0
			2006	1276	327	396	7			
1	D	245	Total	C	N	O	S	33	0	0
			1817	1164	299	348	6			
1	F	255	Total	C	N	O	S	19	0	0
			1897	1209	311	370	7			

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
D	264	GLU	-	expression tag	UNP Q6GEY3
D	265	ASN	-	expression tag	UNP Q6GEY3
D	266	LEU	-	expression tag	UNP Q6GEY3

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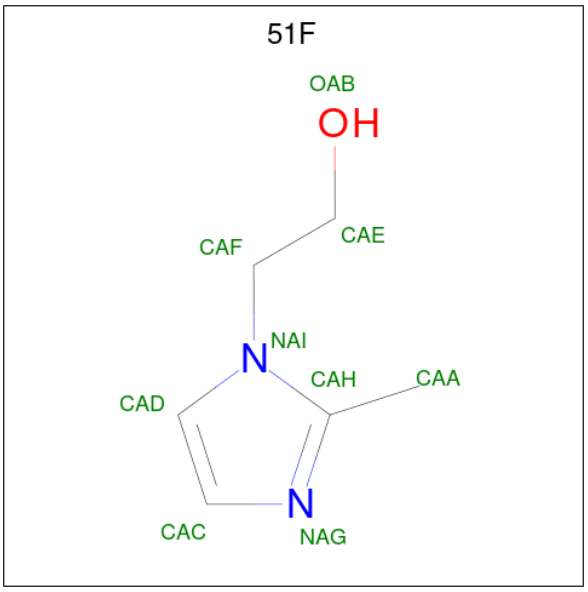
Chain	Residue	Modelled	Actual	Comment	Reference
D	267	TYR	-	expression tag	UNP Q6GEY3
D	268	PHE	-	expression tag	UNP Q6GEY3
D	269	GLN	-	expression tag	UNP Q6GEY3
D	270	SER	-	expression tag	UNP Q6GEY3
D	271	GLY	-	expression tag	UNP Q6GEY3
D	272	HIS	-	expression tag	UNP Q6GEY3
D	273	HIS	-	expression tag	UNP Q6GEY3
D	274	HIS	-	expression tag	UNP Q6GEY3
D	275	HIS	-	expression tag	UNP Q6GEY3
D	276	HIS	-	expression tag	UNP Q6GEY3
D	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
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

- Molecule 2 is 2-(2-methyl-1H-imidazol-1-yl)ethanol (three-letter code: 51F) (formula: $C_6H_{10}N_2O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 9 6 2 1	0	0
2	B	1	Total C N O 9 6 2 1	0	0
2	C	1	Total C N O 9 6 2 1	0	0
2	E	1	Total C N O 9 6 2 1	0	0
2	D	1	Total C N O 9 6 2 1	0	0
2	D	1	Total C N O 9 6 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	2	Total Mg 2 2	0	0
3	E	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	105	Total O 105 105	0	0
4	B	129	Total O 129 129	0	0
4	C	145	Total O 145 145	0	0
4	E	58	Total O 58 58	0	0
4	D	30	Total O 30 30	0	0
4	F	39	Total O 39 39	0	0

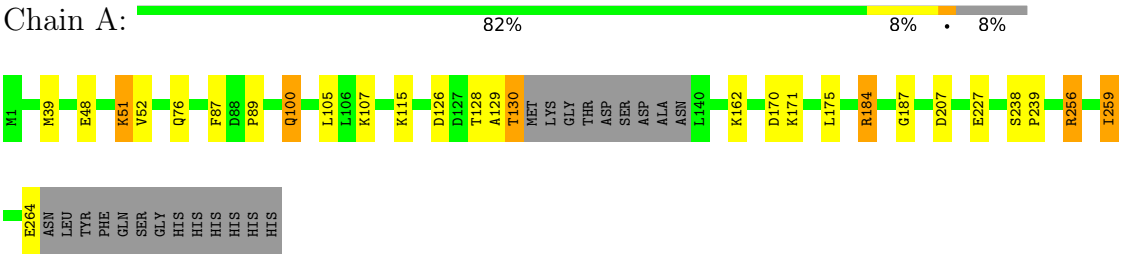
3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

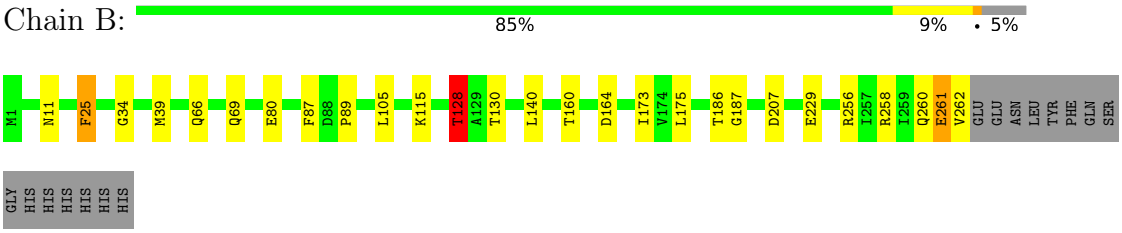
- Molecule 1: Hydroxyethylthiazole kinase

Chain A:



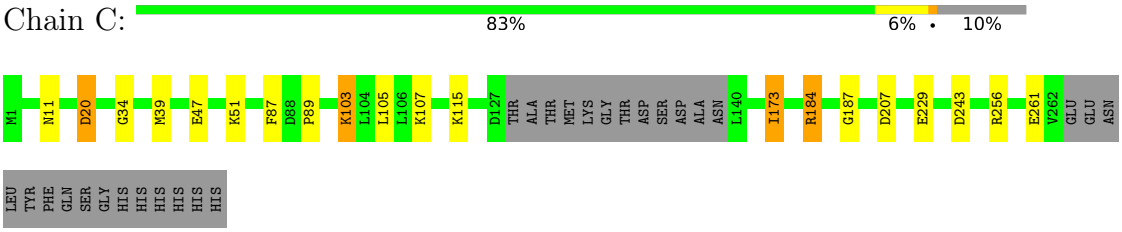
- Molecule 1: Hydroxyethylthiazole kinase

Chain B:



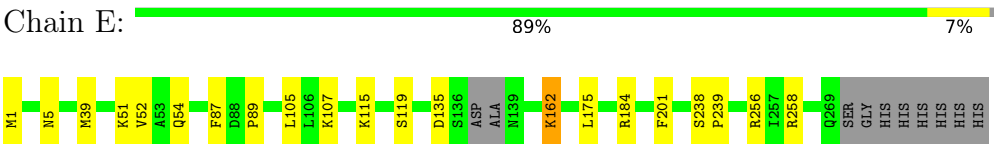
- Molecule 1: Hydroxyethylthiazole kinase

Chain C:



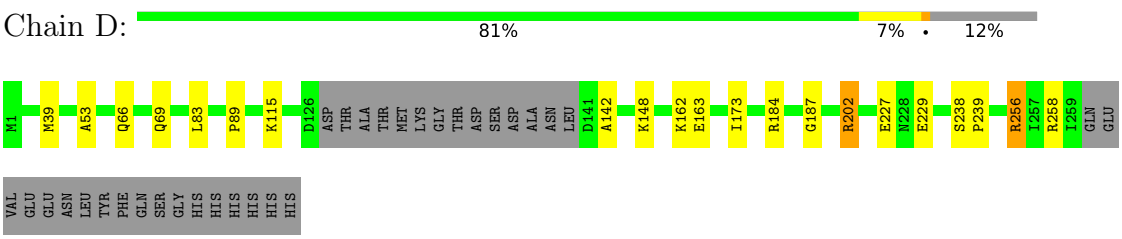
- Molecule 1: Hydroxyethylthiazole kinase

Chain E:



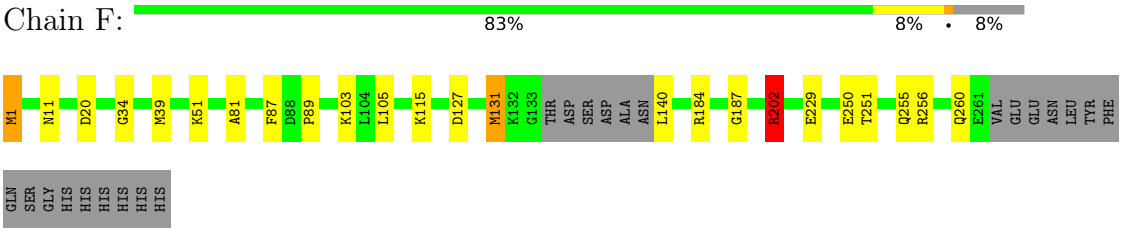
- Molecule 1: Hydroxyethylthiazole kinase

Chain D:



• Molecule 1: Hydroxyethylthiazole kinase

Chain F:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.34Å 62.48Å 109.17Å 92.64° 92.05° 101.46°	Depositor
Resolution (Å)	30.00 – 1.62	Depositor
% Data completeness (in resolution range)	93.2 (30.00-1.62)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.00 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.182 , 0.203	Depositor
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.562	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
Total number of atoms	12018	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 51F

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	1.03	4/1925 (0.2%)	1.17	14/2620 (0.5%)
1	B	1.22	3/1979 (0.2%)	1.06	9/2693 (0.3%)
1	C	1.29	6/1902 (0.3%)	1.18	11/2587 (0.4%)
1	D	1.09	7/1841 (0.4%)	0.89	4/2506 (0.2%)
1	E	0.80	2/2032 (0.1%)	1.01	8/2764 (0.3%)
1	F	0.81	2/1921 (0.1%)	0.89	9/2613 (0.3%)
All	All	1.06	24/11600 (0.2%)	1.04	55/15783 (0.3%)

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	2
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	261	GLU	CG-CD	-30.14	1.06	1.51
1	D	184	ARG	CD-NE	-26.40	1.01	1.46
1	C	51	LYS	CE-NZ	-22.25	0.93	1.49
1	F	140	LEU	CB-CG	-17.37	1.02	1.52
1	C	47	GLU	CD-OE1	-17.07	1.06	1.25

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	184	ARG	NE-CZ-NH2	-22.42	109.09	120.30
1	A	184	ARG	NE-CZ-NH1	20.78	130.69	120.30
1	C	51	LYS	CD-CE-NZ	19.72	157.05	111.70
1	E	258	ARG	NE-CZ-NH1	19.37	129.99	120.30
1	E	258	ARG	NE-CZ-NH2	-17.98	111.31	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLN	Sidechain
1	A	184	ARG	Sidechain
1	C	20	ASP	Sidechain
1	D	258	ARG	Peptide
1	E	175	LEU	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	1901	0	1933	14	0
1	B	1954	0	1991	13	0
1	C	1878	0	1921	8	0
1	D	1817	0	1858	7	0
1	E	2006	0	2029	6	0
1	F	1897	0	1930	9	0
2	A	9	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	0	0
2	D	18	0	0	0	0
2	E	9	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	E	1	0	0	0	0
4	A	105	0	0	4	0
4	B	129	0	0	2	0
4	C	145	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	30	0	0	1	0
4	E	58	0	0	0	0
4	F	39	0	0	1	0
All	All	12018	0	11662	57	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 2.

The worst 5 of 57 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:D:53:ALA:O	1:D:202:ARG:NH1	1.88	1.05
1:A:76:GLN:HG3	4:A:462:HOH:O	1.70	0.91
1:A:128:THR:O	1:A:130:THR:HB	1.86	0.75
4:A:474:HOH:O	1:C:184:ARG:HD2	1.90	0.71
1:D:83:LEU:HD13	1:D:202:ARG:NH1	2.13	0.64

There are no symmetry-related clashes.

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	251/277 (91%)	249 (99%)	2 (1%)	0	100	100
1	B	260/277 (94%)	259 (100%)	1 (0%)	0	100	100
1	C	246/277 (89%)	242 (98%)	4 (2%)	0	100	100
1	D	241/277 (87%)	240 (100%)	1 (0%)	0	100	100
1	E	263/277 (95%)	261 (99%)	2 (1%)	0	100	100
1	F	251/277 (91%)	249 (99%)	2 (1%)	0	100	100
All	All	1512/1662 (91%)	1500 (99%)	12 (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	200/223 (90%)	197 (98%)	3 (2%)	65	43
1	B	207/223 (93%)	204 (99%)	3 (1%)	67	46
1	C	200/223 (90%)	199 (100%)	1 (0%)	88	80
1	D	189/223 (85%)	185 (98%)	4 (2%)	53	27
1	E	213/223 (96%)	210 (99%)	3 (1%)	67	46
1	F	199/223 (89%)	195 (98%)	4 (2%)	55	29
All	All	1208/1338 (90%)	1190 (98%)	18 (2%)	65	43

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	39	MET
1	F	202	ARG
1	F	131	MET
1	E	107	LYS
1	D	202	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	67	ASN
1	F	67	ASN
1	F	255	GLN
1	E	11	ASN
1	B	6	ASN

5.3.3 RNA

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 11 ligands modelled in this entry, 5 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	51F	D	301	-	8,9,9	1.17	1 (12%)	6,11,11	1.12	0
2	51F	D	302	-	8,9,9	1.04	1 (12%)	6,11,11	0.60	0
2	51F	B	301	-	8,9,9	1.31	2 (25%)	6,11,11	2.38	2 (33%)
2	51F	E	301	-	8,9,9	0.62	0	6,11,11	1.44	0
2	51F	C	301	-	8,9,9	2.60	4 (50%)	6,11,11	4.10	4 (66%)
2	51F	A	301	-	8,9,9	0.81	0	6,11,11	3.94	1 (16%)

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	51F	D	301	-	-	0/3/3/3	0/1/1/1
2	51F	D	302	-	-	0/3/3/3	0/1/1/1
2	51F	B	301	-	-	0/3/3/3	0/1/1/1
2	51F	E	301	-	-	0/3/3/3	0/1/1/1
2	51F	C	301	-	-	0/3/3/3	0/1/1/1
2	51F	A	301	-	-	0/3/3/3	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	51F	CAF-NAI	4.91	1.56	1.48
2	C	301	51F	CAD-NAI	-4.14	1.32	1.38
2	D	301	51F	CAD-NAI	-2.90	1.34	1.38
2	D	302	51F	CAD-NAI	-2.82	1.34	1.38
2	B	301	51F	CAF-NAI	2.28	1.51	1.48

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	51F	CAD-NAI-CAH	-9.45	100.00	108.69
2	C	301	51F	CAD-NAI-CAH	8.26	116.29	108.69
2	B	301	51F	CAD-NAI-CAH	-4.78	104.29	108.69
2	C	301	51F	CAA-CAH-NAG	4.42	134.41	121.77
2	C	301	51F	CAD-CAC-NAG	-2.76	102.42	109.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.