



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:24 AM UTC

PDB ID : 5CGE / pdb_00005cge
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 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:

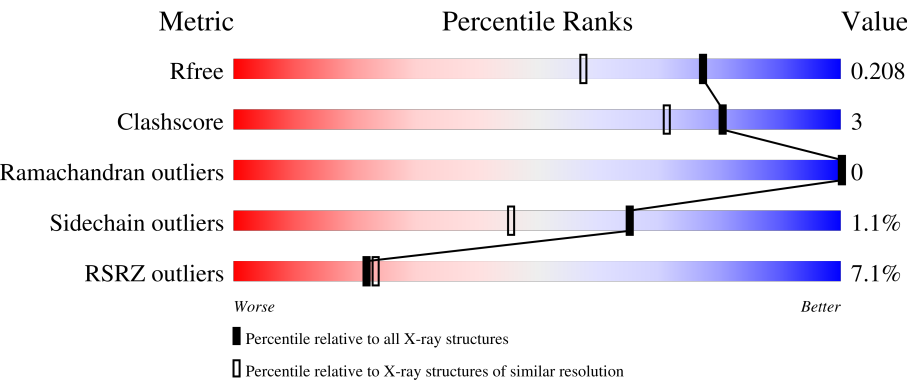
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance 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))
R _{free}	180053	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (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 $\leq 5\%$. 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	4% 82% 8% • 8%
1	B	277	3% 84% 9% 5%
1	C	277	3% 82% 7% • 10%
1	D	277	17% 81% 8% 12%
1	E	277	5% 89% 7% • •

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Mol	Chain	Length	Quality of chain
1	F	277	 9% 84% 7% 8%

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	51F	C	301	-	X	-	-

2 Entry composition

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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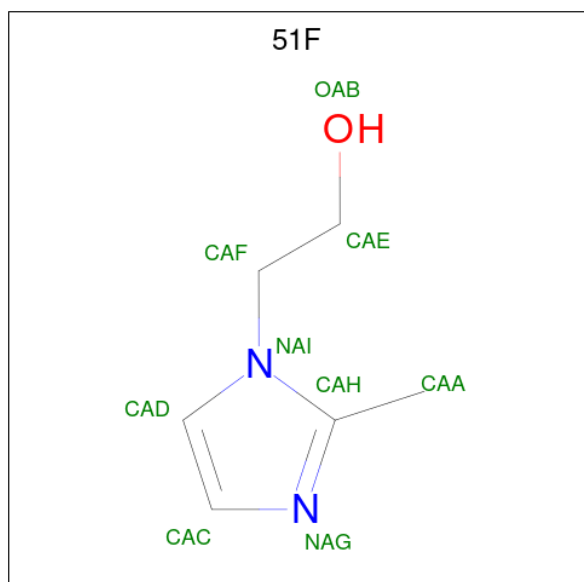
Chain	Residue	Modelled	Actual	Comment	Reference
B	267	TYR	-	expression tag	UNP Q6GEY3
B	268	PHE	-	expression tag	UNP Q6GEY3
B	269	GLN	-	expression tag	UNP Q6GEY3
B	270	SER	-	expression tag	UNP Q6GEY3
B	271	GLY	-	expression tag	UNP Q6GEY3
B	272	HIS	-	expression tag	UNP Q6GEY3
B	273	HIS	-	expression tag	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 (CCD ID: 51F) (formula: C₆H₁₀N₂O).



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

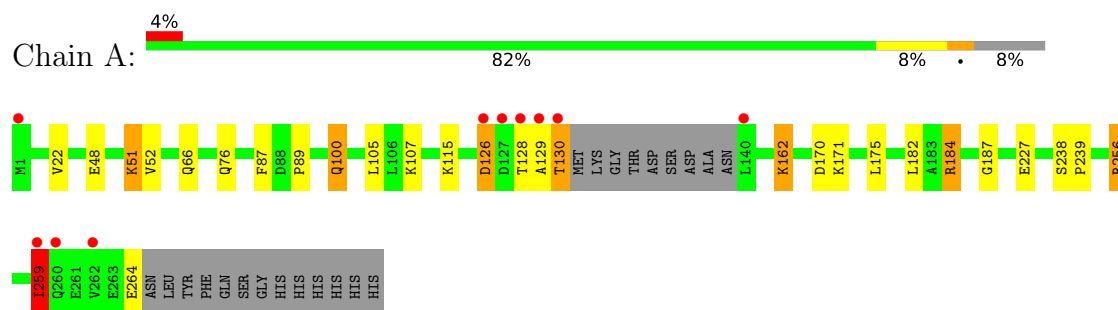
- Molecule 4 is water.

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

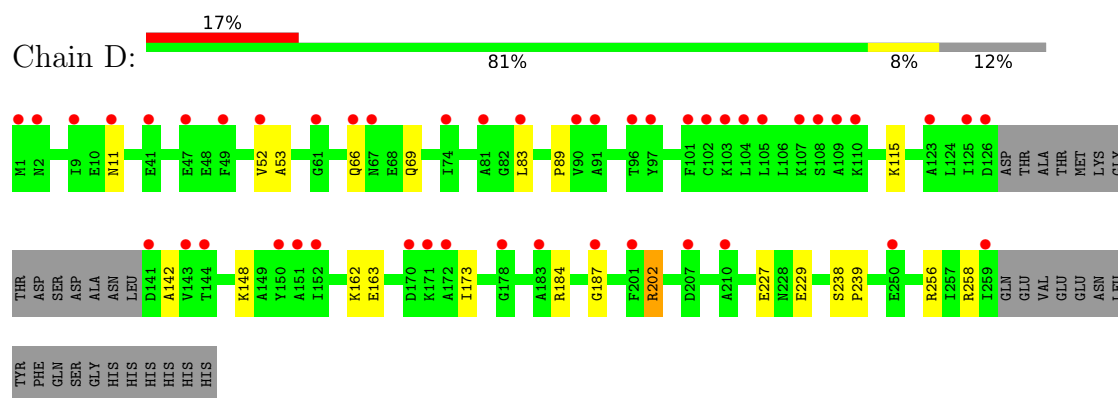
3 Residue-property plots [i](#)

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.

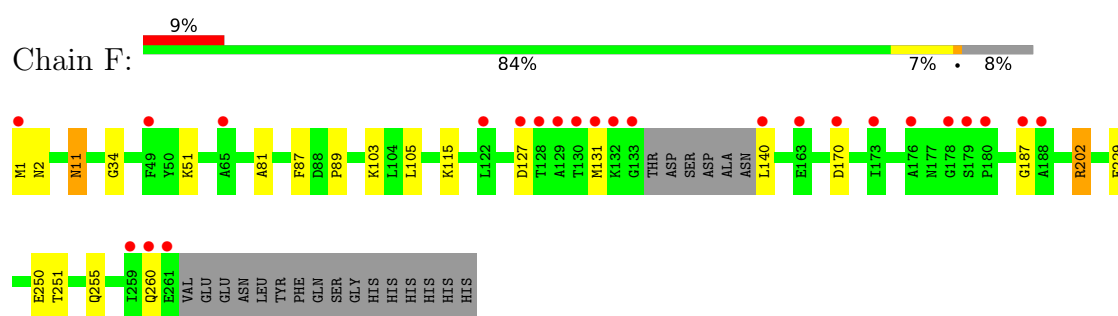
• Molecule 1: Hydroxyethylthiazole kinase



● Molecule 1: Hydroxyethylthiazole kinase



● Molecule 1: Hydroxyethylthiazole kinase



4 Data and refinement statistics

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 30.00 – 1.62	Depositor EDS
% Data completeness (in resolution range)	93.2 (30.00-1.62) 93.2 (30.00-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.00 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.182 , 0.203 0.191 , 0.208	Depositor DCC
R_{free} test set	9530 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
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.*

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: 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	1.33	6/1925 (0.3%)	1.27	16/2620 (0.6%)
1	B	1.36	6/1979 (0.3%)	1.20	9/2693 (0.3%)
1	C	1.48	11/1902 (0.6%)	1.19	4/2587 (0.2%)
1	D	1.37	9/1841 (0.5%)	0.99	3/2506 (0.1%)
1	E	1.02	3/2032 (0.1%)	1.05	6/2764 (0.2%)
1	F	1.14	5/1921 (0.3%)	0.96	4/2613 (0.2%)
All	All	1.29	40/11600 (0.3%)	1.12	42/15783 (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

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	184	ARG	CD-NE	-31.91	1.01	1.46
1	F	140	LEU	CB-CG	-25.64	1.02	1.53
1	C	51	LYS	CE-NZ	-18.64	0.93	1.49
1	B	261	GLU	CG-CD	-18.13	1.06	1.52
1	D	148	LYS	CG-CD	16.57	2.02	1.52
1	C	184	ARG	CZ-NH2	-14.76	1.14	1.33
1	A	107	LYS	CG-CD	14.72	1.96	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	142	ALA	CA-CB	-13.50	1.32	1.53
1	A	184	ARG	CD-NE	-12.64	1.28	1.46
1	A	184	ARG	CZ-NH2	11.16	1.48	1.33
1	E	52	VAL	CA-CB	-10.36	1.40	1.54
1	E	51	LYS	CD-CE	-10.29	1.21	1.52
1	D	162	LYS	CA-CB	-10.09	1.37	1.53
1	C	47	GLU	CD-OE1	-9.73	1.06	1.25
1	B	66	GLN	CB-CG	-9.48	1.24	1.52
1	F	131	MET	CA-CB	-7.79	1.43	1.52
1	C	47	GLU	CD-OE2	7.47	1.39	1.25
1	B	188	ALA	N-CA	7.23	1.54	1.46
1	A	22	VAL	N-CA	7.03	1.52	1.46
1	D	163	GLU	CG-CD	-6.97	1.34	1.52
1	D	66	GLN	CB-CG	-6.82	1.32	1.52
1	D	52	VAL	CA-CB	-6.74	1.46	1.54
1	A	162	LYS	CG-CD	-6.49	1.32	1.52
1	F	11	ASN	CA-CB	6.47	1.57	1.52
1	C	36	SER	N-CA	-6.33	1.40	1.46
1	F	229	GLU	CB-CG	-6.26	1.33	1.52
1	F	170	ASP	CA-CB	-6.12	1.44	1.53
1	C	1	MET	C-N	-6.10	1.26	1.33
1	A	51	LYS	CG-CD	-5.42	1.36	1.52
1	C	219	ASN	CG-ND2	-5.39	1.22	1.33
1	B	2	ASN	N-CA	-5.34	1.40	1.46
1	E	238	SER	CA-C	5.32	1.59	1.52
1	C	200	LEU	N-CA	5.29	1.52	1.46
1	C	40	SER	N-CA	5.21	1.52	1.46
1	D	229	GLU	CB-CG	-5.21	1.36	1.52
1	C	11	ASN	CA-C	5.20	1.57	1.53
1	B	36	SER	N-CA	-5.19	1.41	1.46
1	B	219	ASN	CG-ND2	-5.11	1.22	1.33
1	D	11	ASN	C-O	-5.10	1.21	1.23
1	C	103	LYS	CD-CE	-5.08	1.37	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	GLU	CB-CG-CD	17.42	142.22	112.60
1	E	51	LYS	CG-CD-CE	17.00	150.40	111.30
1	D	184	ARG	CG-CD-NE	16.46	148.20	112.00
1	A	100	GLN	OE1-CD-NE2	-15.92	106.68	122.60
1	C	51	LYS	CD-CE-NZ	14.11	157.05	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	LYS	CB-CG-CD	-13.99	79.13	111.30
1	A	259	ILE	CB-CA-C	-12.45	95.44	111.25
1	C	184	ARG	NE-CZ-NH2	-11.23	109.09	119.20
1	A	51	LYS	CG-CD-CE	11.01	136.62	111.30
1	A	184	ARG	NH1-CZ-NH2	-10.16	106.09	119.30
1	D	184	ARG	CD-NE-CZ	9.78	138.10	124.40
1	A	107	LYS	CG-CD-CE	9.24	132.56	111.30
1	A	184	ARG	NE-CZ-NH1	9.19	130.69	121.50
1	A	162	LYS	CB-CG-CD	8.90	131.78	111.30
1	E	258	ARG	NE-CZ-NH2	-8.77	111.31	119.20
1	E	258	ARG	NE-CZ-NH1	8.49	129.99	121.50
1	B	260	GLN	CA-CB-CG	8.37	130.83	114.10
1	F	131	MET	N-CA-CB	-8.24	97.47	110.49
1	A	66	GLN	CB-CG-CD	-7.85	99.25	112.60
1	F	140	LEU	CA-CB-CG	7.64	143.03	116.30
1	B	128	THR	N-CA-CB	-7.50	97.94	110.39
1	E	162	LYS	CG-CD-CE	7.32	128.13	111.30
1	A	51	LYS	CB-CG-CD	7.26	127.99	111.30
1	E	51	LYS	CD-CE-NZ	6.84	133.79	111.90
1	A	184	ARG	NE-CZ-NH2	-6.53	113.33	119.20
1	B	152	ILE	N-CA-C	6.40	116.55	110.53
1	F	140	LEU	CB-CG-CD2	6.14	129.12	110.70
1	B	2	ASN	N-CA-C	6.05	117.56	110.97
1	E	184	ARG	CB-CG-CD	-6.01	97.47	111.30
1	D	162	LYS	N-CA-CB	5.87	118.68	109.94
1	F	2	ASN	N-CA-C	-5.79	105.23	112.93
1	C	28	ASN	N-CA-C	5.71	117.51	111.28
1	A	171	LYS	CB-CG-CD	-5.66	98.29	111.30
1	A	126	ASP	N-CA-C	5.59	117.37	111.28
1	B	186	THR	CA-C-N	-5.57	110.50	121.41
1	B	186	THR	C-N-CA	-5.57	110.50	121.41
1	A	256	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	B	162	LYS	CA-CB-CG	-5.29	103.52	114.10
1	C	100	GLN	OE1-CD-NE2	5.28	127.88	122.60
1	B	260	GLN	CB-CG-CD	5.24	121.51	112.60
1	A	182	LEU	N-CA-C	5.12	117.52	111.33
1	A	162	LYS	CG-CD-CE	-5.08	99.60	111.30

There are no chirality outliers.

All (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
1	F	260	GLN	Peptide

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	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	8	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
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	59	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 3.

All (59) 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
1:C:173:ILE:HD13	1:C:261:GLU:HA	1.82	0.61
1:A:175:LEU:CD2	1:A:259:ILE:HD12	2.31	0.60
1:D:83:LEU:HD13	1:D:202:ARG:HH12	1.66	0.60
1:C:187:GLY:HA2	4:C:501:HOH:O	2.04	0.58
1:A:187:GLY:HA2	4:A:484:HOH:O	2.06	0.55
1:F:103:LYS:HE3	1:F:127:ASP:OD2	2.06	0.55
1:A:48:GLU:O	1:A:51:LYS:HG2	2.07	0.54
1:F:81:ALA:O	1:F:202:ARG:NH2	2.40	0.52
1:A:51:LYS:HG3	1:A:52:VAL:HG13	1.90	0.52
1:D:227:GLU:OE1	1:D:256:ARG:NH2	2.43	0.51
1:E:54:GLN:HE21	1:E:201:PHE:HA	1.75	0.51
1:B:128:THR:HG22	1:B:130:THR:H	1.74	0.51
1:B:87:PHE:CE1	1:B:105:LEU:HD23	2.47	0.50
1:B:261:GLU:HG3	1:B:262:VAL:HG23	1.95	0.48
1:E:119:SER:N	1:E:135:ASP:OD1	2.37	0.48
1:A:175:LEU:HD23	1:A:259:ILE:HD12	1.95	0.48
1:E:120:GLU:HG3	1:E:131:MET:HE1	1.96	0.47
1:B:128:THR:CG2	1:B:130:THR:OG1	2.63	0.47
1:F:103:LYS:CE	1:F:127:ASP:OD2	2.62	0.47
1:D:187:GLY:HA2	4:D:421:HOH:O	2.14	0.46
1:F:187:GLY:HA2	4:F:335:HOH:O	2.16	0.46
1:B:25:PHE:HD2	1:B:187:GLY:HA3	1.81	0.46
1:A:87:PHE:CE1	1:A:105:LEU:HD23	2.51	0.46
1:E:1:MET:HE2	1:E:5:ASN:OD1	2.16	0.45
1:F:87:PHE:CE1	1:F:105:LEU:HD23	2.53	0.44
1:A:259:ILE:O	1:A:259:ILE:HG22	2.09	0.44
1:F:251:THR:HG22	1:F:255:GLN:NE2	2.32	0.44
1:B:258:ARG:NH1	4:B:407:HOH:O	2.49	0.44
1:D:89:PRO:HD2	1:D:115:LYS:O	2.18	0.44
1:E:1:MET:CE	1:E:5:ASN:OD1	2.66	0.43
1:C:89:PRO:HD2	1:C:115:LYS:O	2.17	0.43
1:A:89:PRO:HD2	1:A:115:LYS:O	2.18	0.43
1:B:89:PRO:HD2	1:B:115:LYS:O	2.19	0.43
1:F:89:PRO:HD2	1:F:115:LYS:O	2.19	0.43
1:F:1:MET:HG3	1:F:250:GLU:HA	2.00	0.43
1:B:128:THR:HG23	1:B:130:THR:HG23	2.01	0.43
1:C:103:LYS:O	1:C:107:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:OE1	1:A:256:ARG:NH2	2.53	0.42
1:E:238:SER:HB3	1:E:239:PRO:HD3	2.02	0.42
1:A:129:ALA:O	1:A:130:THR:HG22	2.19	0.42
1:B:160:THR:HA	1:B:164:ASP:OD1	2.19	0.42
1:E:89:PRO:HD2	1:E:115:LYS:O	2.19	0.42
1:B:173:ILE:CD1	1:B:175:LEU:HG	2.50	0.42
1:B:69:GLN:HG2	4:B:423:HOH:O	2.19	0.42
4:A:474:HOH:O	1:C:184:ARG:CD	2.58	0.42
1:D:238:SER:HB3	1:D:239:PRO:HD3	2.02	0.41
1:B:11:ASN:HA	1:B:34:GLY:O	2.20	0.41
1:C:87:PHE:CE1	1:C:105:LEU:HD23	2.55	0.41
1:A:238:SER:HB3	1:A:239:PRO:HD3	2.01	0.41
1:A:170:ASP:O	1:A:264:GLU:HB3	2.20	0.41
1:B:261:GLU:HG3	1:B:262:VAL:N	2.36	0.41
1:C:11:ASN:HA	1:C:34:GLY:O	2.21	0.41
1:F:11:ASN:HA	1:F:34:GLY:O	2.21	0.41
1:E:87:PHE:CE1	1:E:105:LEU:HD23	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	196 (98%)	4 (2%)	48	24
1	B	207/223 (93%)	205 (99%)	2 (1%)	68	50
1	C	200/223 (90%)	200 (100%)	0	100	100
1	D	189/223 (85%)	186 (98%)	3 (2%)	55	32
1	E	213/223 (96%)	211 (99%)	2 (1%)	70	54
1	F	199/223 (89%)	197 (99%)	2 (1%)	68	50
All	All	1208/1338 (90%)	1195 (99%)	13 (1%)	65	46

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	ASP
1	A	130	THR
1	A	162	LYS
1	A	259	ILE
1	B	128	THR
1	B	140	LEU
1	E	107	LYS
1	E	162	LYS
1	D	69	GLN
1	D	173	ILE
1	D	202	ARG
1	F	51	LYS
1	F	202	ARG

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

Mol	Chain	Res	Type
1	A	67	ASN

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Mol	Chain	Res	Type
1	B	6	ASN
1	C	67	ASN
1	E	54	GLN
1	E	254	GLN
1	F	24	ASN
1	F	67	ASN
1	F	255	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	301	-	9,9,9	0.90	1 (11%)	9,11,11	3.58	4 (44%)
2	51F	D	302	-	9,9,9	0.90	0	9,11,11	2.28	3 (33%)
2	51F	B	301	-	9,9,9	1.58	2 (22%)	9,11,11	2.73	6 (66%)
2	51F	E	301	-	9,9,9	0.71	0	9,11,11	2.20	3 (33%)
2	51F	D	301	-	9,9,9	1.29	1 (11%)	9,11,11	1.50	2 (22%)
2	51F	C	301	-	9,9,9	2.85	6 (66%)	9,11,11	4.71	5 (55%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	51F	CAD-CAC	3.97	1.44	1.35
2	C	301	51F	CAF-NAI	3.88	1.56	1.47
2	C	301	51F	CAH-NAI	3.81	1.44	1.36
2	C	301	51F	CAH-NAG	3.77	1.40	1.32
2	B	301	51F	CAC-NAG	-3.03	1.32	1.38
2	C	301	51F	CAD-NAI	-2.76	1.32	1.38
2	D	301	51F	CAC-NAG	-2.34	1.33	1.38
2	C	301	51F	CAA-CAH	-2.23	1.45	1.49
2	A	301	51F	CAA-CAH	2.15	1.52	1.49
2	B	301	51F	CAF-NAI	2.01	1.51	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	51F	CAC-NAG-CAH	8.89	117.82	105.86
2	A	301	51F	CAA-CAH-NAI	-8.65	114.60	123.50
2	C	301	51F	CAA-CAH-NAG	6.63	134.41	124.34
2	C	301	51F	CAD-CAC-NAG	-6.36	102.42	110.74
2	C	301	51F	CAA-CAH-NAI	5.35	129.01	123.50
2	D	302	51F	CAA-CAH-NAI	5.13	128.78	123.50
2	B	301	51F	CAC-CAD-NAI	4.27	110.67	106.22
2	B	301	51F	CAD-CAC-NAG	-3.97	105.55	110.74
2	A	301	51F	CAC-NAG-CAH	-3.95	100.54	105.86
2	E	301	51F	CAD-CAC-NAG	-3.92	105.60	110.74
2	A	301	51F	CAF-NAI-CAH	3.59	133.79	126.93
2	B	301	51F	CAA-CAH-NAI	3.24	126.83	123.50
2	A	301	51F	CAC-CAD-NAI	3.21	109.57	106.22
2	E	301	51F	CAC-CAD-NAI	3.13	109.48	106.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302	51F	CAD-CAC-NAG	-3.07	106.73	110.74
2	B	301	51F	CAE-CAF-NAI	-2.95	106.44	112.15
2	D	301	51F	CAE-CAF-NAI	-2.86	106.62	112.15
2	D	301	51F	CAA-CAH-NAI	2.71	126.30	123.50
2	E	301	51F	CAC-NAG-CAH	2.55	109.29	105.86
2	B	301	51F	CAC-NAG-CAH	2.46	109.17	105.86
2	C	301	51F	CAF-NAI-CAD	-2.39	118.94	124.93
2	D	302	51F	CAC-NAG-CAH	2.32	108.98	105.86
2	B	301	51F	OAB-CAE-CAF	-2.12	102.50	111.22

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

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	255/277 (92%)	0.07	10 (3%)	43	47	14, 20, 42, 71	14 (5%)
1	B	262/277 (94%)	-0.08	8 (3%)	51	55	13, 18, 33, 69	16 (6%)
1	C	250/277 (90%)	-0.14	7 (2%)	55	59	14, 18, 28, 71	19 (7%)
1	D	245/277 (88%)	1.34	47 (19%)	3	3	18, 42, 67, 85	13 (5%)
1	E	267/277 (96%)	0.38	13 (4%)	35	37	14, 29, 54, 67	10 (3%)
1	F	255/277 (92%)	0.80	24 (9%)	14	14	22, 39, 59, 76	8 (3%)
All	All	1534/1662 (92%)	0.39	109 (7%)	22	23	13, 25, 56, 85	80 (5%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	LEU	8.9
1	F	129	ALA	7.9
1	E	133	GLY	7.1
1	F	130	THR	5.5
1	D	143	VAL	5.1
1	B	262	VAL	4.6
1	A	140	LEU	4.3
1	D	104	LEU	4.3
1	F	127	ASP	4.2
1	D	259	ILE	4.0
1	E	129	ALA	4.0
1	E	134	THR	4.0
1	A	130	THR	3.9
1	C	127	ASP	3.9
1	D	126	ASP	3.9
1	F	140	LEU	3.9
1	B	138	ALA	3.7
1	D	52	VAL	3.6
1	D	101	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	170	ASP	3.6
1	C	1	MET	3.5
1	D	2	ASN	3.5
1	A	262	VAL	3.4
1	F	1	MET	3.4
1	F	163	GLU	3.4
1	F	133	GLY	3.3
1	D	11	ASN	3.3
1	D	41	GLU	3.3
1	F	131	MET	3.2
1	E	130	THR	3.2
1	D	102	CYS	3.2
1	C	261	GLU	3.2
1	E	1	MET	3.2
1	E	132	LYS	3.2
1	D	1	MET	3.1
1	F	187	GLY	3.1
1	B	129	ALA	3.0
1	A	127	ASP	3.0
1	C	262	VAL	3.0
1	E	127	ASP	2.9
1	A	128	THR	2.9
1	D	66	GLN	2.9
1	D	210	ALA	2.9
1	D	187	GLY	2.9
1	B	137	ASP	2.9
1	D	67	ASN	2.9
1	D	91	ALA	2.8
1	A	1	MET	2.8
1	D	152	ILE	2.8
1	A	259	ILE	2.8
1	D	107	LYS	2.7
1	E	52	VAL	2.7
1	D	125	ILE	2.7
1	F	132	LYS	2.6
1	D	150	TYR	2.6
1	A	260	GLN	2.6
1	D	151	ALA	2.6
1	F	65	ALA	2.6
1	D	171	LYS	2.6
1	D	61	GLY	2.6
1	F	128	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	269	GLN	2.6
1	F	173	ILE	2.6
1	D	123	ALA	2.6
1	E	258	ARG	2.6
1	F	259	ILE	2.5
1	B	139	ASN	2.5
1	A	129	ALA	2.5
1	D	9	ILE	2.5
1	D	183	ALA	2.5
1	E	51	LYS	2.5
1	D	103	LYS	2.4
1	F	49	PHE	2.4
1	F	122	LEU	2.4
1	D	250	GLU	2.4
1	B	187	GLY	2.4
1	D	49	PHE	2.4
1	B	170	ASP	2.4
1	F	178	GLY	2.4
1	D	141	ASP	2.4
1	D	90	VAL	2.4
1	C	187	GLY	2.3
1	B	261	GLU	2.3
1	D	207	ASP	2.3
1	D	110	LYS	2.3
1	D	97	TYR	2.3
1	A	126	ASP	2.3
1	E	128	THR	2.3
1	D	47	GLU	2.3
1	F	170	ASP	2.3
1	E	9	ILE	2.2
1	D	105	LEU	2.2
1	F	260	GLN	2.2
1	F	261	GLU	2.1
1	D	144	THR	2.1
1	D	81	ALA	2.1
1	D	172	ALA	2.1
1	F	188	ALA	2.1
1	D	109	ALA	2.1
1	D	178	GLY	2.1
1	F	176	ALA	2.1
1	D	96	THR	2.1
1	D	74	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	260	GLN	2.0
1	D	108	SER	2.0
1	D	83	LEU	2.0
1	F	180	PRO	2.0
1	D	201	PHE	2.0
1	F	179	SER	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 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	302	1/1	0.87	0.10	52,52,52,52	0
3	MG	B	302	1/1	0.87	0.11	45,45,45,45	0
2	51F	E	301	9/9	0.88	0.12	26,30,38,50	0
3	MG	C	302	1/1	0.89	0.22	45,45,45,45	0
3	MG	E	302	1/1	0.91	0.11	46,46,46,46	0
2	51F	C	301	9/9	0.94	0.08	11,13,17,29	0
2	51F	B	301	9/9	0.94	0.09	14,16,24,34	0
2	51F	D	301	9/9	0.94	0.09	23,25,35,50	0
2	51F	D	302	9/9	0.94	0.09	24,30,42,48	0
2	51F	A	301	9/9	0.96	0.08	11,13,25,34	0
3	MG	C	303	1/1	0.98	0.13	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.