



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:24 am BST

PDB ID : 4YGD  
Title : Crystal structure of ERGIC-53/MCFD2, monoclinic calcium-bound form 2  
Authors : Satoh, T.; Nishio, M.; Yagi-Utsumi, M.; Suzuki, K.; Anzai, T.; Mizushima, T.; Kamiya, Y.; Kato, K.  
Deposited on : 2015-02-26  
Resolution : 2.51 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

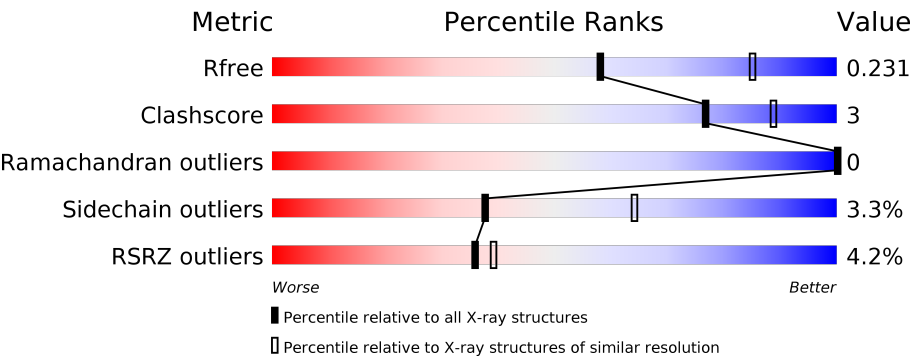
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	246	<div><div>4%</div><div>85%7%8%</div></div>
1	C	246	<div><div>4%</div><div>84%8%8%</div></div>
1	E	246	<div><div>4%</div><div>86%6%8%</div></div>
1	G	246	<div><div>4%</div><div>84%8%8%</div></div>
2	B	104	<div><div>2%</div><div>59%6%34%</div></div>
2	D	104	<div><div>%</div><div>49%9%40%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	104	<div><div></div><div>6%</div><div>50%</div><div>9%</div><div>39%</div></div>
2	H	104	<div><div></div><div>2%</div><div>59%</div><div>7%</div><div>33%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9564 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 Protein ERGIC-53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1782	1131	314	333	4			
1	C	227	Total	C	N	O	S	0	0	0
			1782	1131	314	333	4			
1	E	227	Total	C	N	O	S	0	0	0
			1782	1131	314	333	4			
1	G	227	Total	C	N	O	S	0	0	0
			1782	1131	314	333	4			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	expression tag	UNP P49257
A	25	ASN	-	expression tag	UNP P49257
A	26	HIS	-	expression tag	UNP P49257
A	27	LYS	-	expression tag	UNP P49257
A	28	VAL	-	expression tag	UNP P49257
A	29	HIS	-	expression tag	UNP P49257
A	30	MET	-	expression tag	UNP P49257
C	24	MET	-	expression tag	UNP P49257
C	25	ASN	-	expression tag	UNP P49257
C	26	HIS	-	expression tag	UNP P49257
C	27	LYS	-	expression tag	UNP P49257
C	28	VAL	-	expression tag	UNP P49257
C	29	HIS	-	expression tag	UNP P49257
C	30	MET	-	expression tag	UNP P49257
E	24	MET	-	expression tag	UNP P49257
E	25	ASN	-	expression tag	UNP P49257
E	26	HIS	-	expression tag	UNP P49257
E	27	LYS	-	expression tag	UNP P49257
E	28	VAL	-	expression tag	UNP P49257
E	29	HIS	-	expression tag	UNP P49257
E	30	MET	-	expression tag	UNP P49257

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Chain	Residue	Modelled	Actual	Comment	Reference
G	24	MET	-	expression tag	UNP P49257
G	25	ASN	-	expression tag	UNP P49257
G	26	HIS	-	expression tag	UNP P49257
G	27	LYS	-	expression tag	UNP P49257
G	28	VAL	-	expression tag	UNP P49257
G	29	HIS	-	expression tag	UNP P49257
G	30	MET	-	expression tag	UNP P49257

- Molecule 2 is a protein called Multiple coagulation factor deficiency protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	69	Total	C	N	O	S	0	0	0
			555	348	88	116	3			
2	D	62	Total	C	N	O	S	0	0	0
			502	314	79	107	2			
2	F	63	Total	C	N	O	S	0	0	0
			507	316	79	109	3			
2	H	70	Total	C	N	O	S	0	0	0
			560	351	89	117	3			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	43	MET	-	expression tag	UNP Q8NI22
B	44	GLY	-	expression tag	UNP Q8NI22
B	45	HIS	-	expression tag	UNP Q8NI22
B	46	HIS	-	expression tag	UNP Q8NI22
B	47	HIS	-	expression tag	UNP Q8NI22
B	48	HIS	-	expression tag	UNP Q8NI22
B	49	HIS	-	expression tag	UNP Q8NI22
B	50	HIS	-	expression tag	UNP Q8NI22
B	51	HIS	-	expression tag	UNP Q8NI22
B	52	HIS	-	expression tag	UNP Q8NI22
B	53	HIS	-	expression tag	UNP Q8NI22
B	54	HIS	-	expression tag	UNP Q8NI22
B	55	SER	-	expression tag	UNP Q8NI22
B	56	SER	-	expression tag	UNP Q8NI22
B	57	GLY	-	expression tag	UNP Q8NI22
B	58	HIS	-	expression tag	UNP Q8NI22
B	59	ILE	-	expression tag	UNP Q8NI22
B	60	GLU	-	expression tag	UNP Q8NI22
B	61	GLY	-	expression tag	UNP Q8NI22

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Chain	Residue	Modelled	Actual	Comment	Reference
B	62	ARG	-	expression tag	UNP Q8NI22
B	63	HIS	-	expression tag	UNP Q8NI22
B	64	MET	-	expression tag	UNP Q8NI22
B	65	LEU	-	expression tag	UNP Q8NI22
B	66	GLU	-	expression tag	UNP Q8NI22
D	43	MET	-	expression tag	UNP Q8NI22
D	44	GLY	-	expression tag	UNP Q8NI22
D	45	HIS	-	expression tag	UNP Q8NI22
D	46	HIS	-	expression tag	UNP Q8NI22
D	47	HIS	-	expression tag	UNP Q8NI22
D	48	HIS	-	expression tag	UNP Q8NI22
D	49	HIS	-	expression tag	UNP Q8NI22
D	50	HIS	-	expression tag	UNP Q8NI22
D	51	HIS	-	expression tag	UNP Q8NI22
D	52	HIS	-	expression tag	UNP Q8NI22
D	53	HIS	-	expression tag	UNP Q8NI22
D	54	HIS	-	expression tag	UNP Q8NI22
D	55	SER	-	expression tag	UNP Q8NI22
D	56	SER	-	expression tag	UNP Q8NI22
D	57	GLY	-	expression tag	UNP Q8NI22
D	58	HIS	-	expression tag	UNP Q8NI22
D	59	ILE	-	expression tag	UNP Q8NI22
D	60	GLU	-	expression tag	UNP Q8NI22
D	61	GLY	-	expression tag	UNP Q8NI22
D	62	ARG	-	expression tag	UNP Q8NI22
D	63	HIS	-	expression tag	UNP Q8NI22
D	64	MET	-	expression tag	UNP Q8NI22
D	65	LEU	-	expression tag	UNP Q8NI22
D	66	GLU	-	expression tag	UNP Q8NI22
F	43	MET	-	expression tag	UNP Q8NI22
F	44	GLY	-	expression tag	UNP Q8NI22
F	45	HIS	-	expression tag	UNP Q8NI22
F	46	HIS	-	expression tag	UNP Q8NI22
F	47	HIS	-	expression tag	UNP Q8NI22
F	48	HIS	-	expression tag	UNP Q8NI22
F	49	HIS	-	expression tag	UNP Q8NI22
F	50	HIS	-	expression tag	UNP Q8NI22
F	51	HIS	-	expression tag	UNP Q8NI22
F	52	HIS	-	expression tag	UNP Q8NI22
F	53	HIS	-	expression tag	UNP Q8NI22
F	54	HIS	-	expression tag	UNP Q8NI22
F	55	SER	-	expression tag	UNP Q8NI22

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Chain	Residue	Modelled	Actual	Comment	Reference
F	56	SER	-	expression tag	UNP Q8NI22
F	57	GLY	-	expression tag	UNP Q8NI22
F	58	HIS	-	expression tag	UNP Q8NI22
F	59	ILE	-	expression tag	UNP Q8NI22
F	60	GLU	-	expression tag	UNP Q8NI22
F	61	GLY	-	expression tag	UNP Q8NI22
F	62	ARG	-	expression tag	UNP Q8NI22
F	63	HIS	-	expression tag	UNP Q8NI22
F	64	MET	-	expression tag	UNP Q8NI22
F	65	LEU	-	expression tag	UNP Q8NI22
F	66	GLU	-	expression tag	UNP Q8NI22
H	43	MET	-	expression tag	UNP Q8NI22
H	44	GLY	-	expression tag	UNP Q8NI22
H	45	HIS	-	expression tag	UNP Q8NI22
H	46	HIS	-	expression tag	UNP Q8NI22
H	47	HIS	-	expression tag	UNP Q8NI22
H	48	HIS	-	expression tag	UNP Q8NI22
H	49	HIS	-	expression tag	UNP Q8NI22
H	50	HIS	-	expression tag	UNP Q8NI22
H	51	HIS	-	expression tag	UNP Q8NI22
H	52	HIS	-	expression tag	UNP Q8NI22
H	53	HIS	-	expression tag	UNP Q8NI22
H	54	HIS	-	expression tag	UNP Q8NI22
H	55	SER	-	expression tag	UNP Q8NI22
H	56	SER	-	expression tag	UNP Q8NI22
H	57	GLY	-	expression tag	UNP Q8NI22
H	58	HIS	-	expression tag	UNP Q8NI22
H	59	ILE	-	expression tag	UNP Q8NI22
H	60	GLU	-	expression tag	UNP Q8NI22
H	61	GLY	-	expression tag	UNP Q8NI22
H	62	ARG	-	expression tag	UNP Q8NI22
H	63	HIS	-	expression tag	UNP Q8NI22
H	64	MET	-	expression tag	UNP Q8NI22
H	65	LEU	-	expression tag	UNP Q8NI22
H	66	GLU	-	expression tag	UNP Q8NI22

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Ca 2 2	0	0
3	D	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total 2	Ca 2	0	0
3	H	2	Total 2	Ca 2	0	0
3	B	2	Total 2	Ca 2	0	0
3	C	2	Total 2	Ca 2	0	0
3	A	2	Total 2	Ca 2	0	0
3	F	2	Total 2	Ca 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Cl 1	0	0
4	A	2	Total 2	Cl 2	0	0

- Molecule 5 is water.

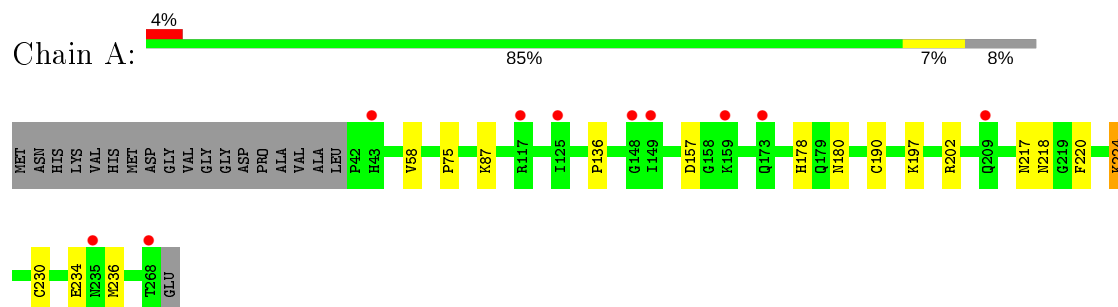
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	57	Total 57	O 57	0	0
5	B	27	Total 27	O 27	0	0
5	C	52	Total 52	O 52	0	0
5	D	17	Total 17	O 17	0	0
5	E	54	Total 54	O 54	0	0
5	F	13	Total 13	O 13	0	0
5	G	51	Total 51	O 51	0	0
5	H	22	Total 22	O 22	0	0



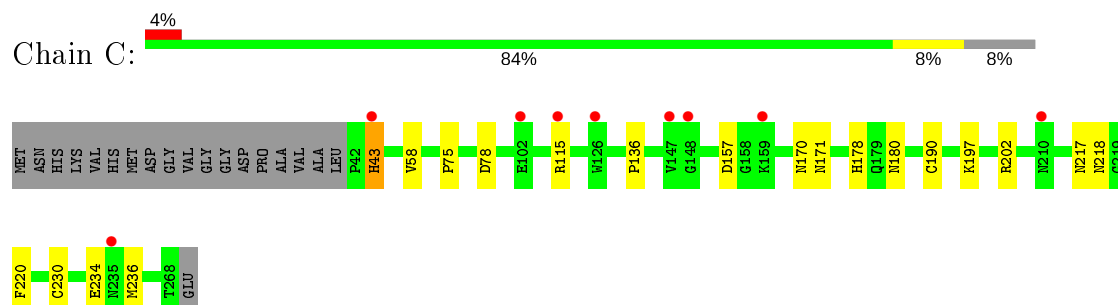
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

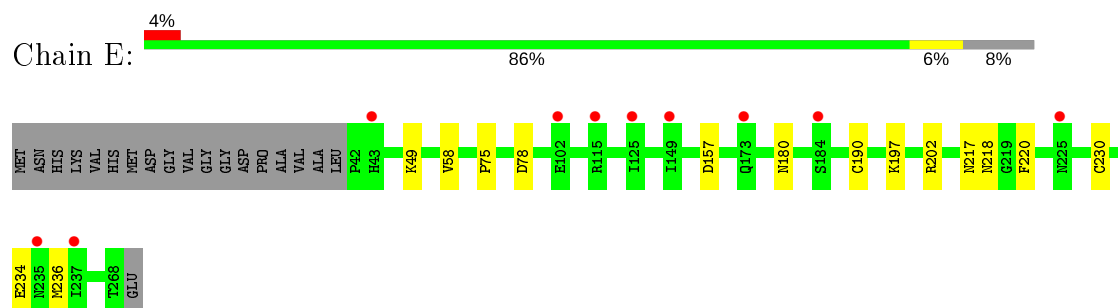
#### • Molecule 1: Protein ERGIC-53



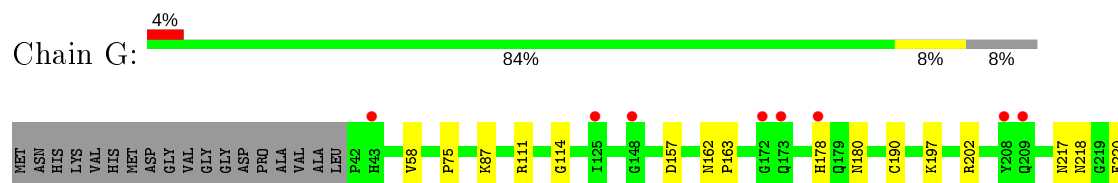
#### • Molecule 1: Protein ERGIC-53



#### • Molecule 1: Protein ERGIC-53



#### • Molecule 1: Protein ERGIC-53

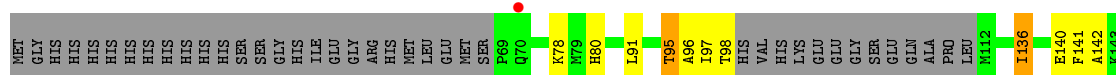




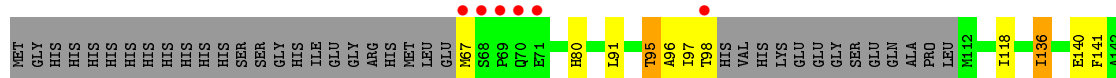
- Molecule 2: Multiple coagulation factor deficiency protein 2



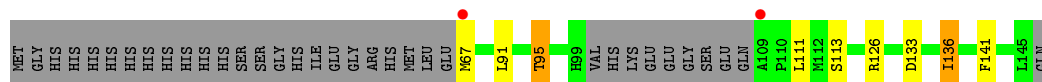
- Molecule 2: Multiple coagulation factor deficiency protein 2



- Molecule 2: Multiple coagulation factor deficiency protein 2



- Molecule 2: Multiple coagulation factor deficiency protein 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.06Å 58.77Å 119.39Å 90.00° 109.01° 90.00°	Depositor
Resolution (Å)	20.00 – 2.51 19.86 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.51) 98.7 (19.86-2.51)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	11.01 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.193 , 0.232 0.197 , 0.231	Depositor DCC
$R_{free}$ test set	2317 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0689e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, CL

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	0.68	0/1832	0.78	1/2487 (0.0%)
1	C	0.65	0/1832	0.77	1/2487 (0.0%)
1	E	0.67	0/1832	0.77	0/2487
1	G	0.68	0/1832	0.77	2/2487 (0.1%)
2	B	0.75	0/564	0.81	0/760
2	D	0.75	0/509	0.89	1/685 (0.1%)
2	F	0.76	0/514	0.85	0/693
2	H	0.76	0/569	0.87	1/768 (0.1%)
All	All	0.69	0/9484	0.79	6/12854 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	LYS	CA-CB-CG	5.53	125.56	113.40
1	C	115	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	G	224	LYS	CA-CB-CG	5.27	124.99	113.40
2	H	126	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	G	111	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	D	142	ALA	N-CA-C	5.07	124.69	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	1782	0	1690	8	0
1	C	1782	0	1690	10	0
1	E	1782	0	1690	8	0
1	G	1782	0	1690	9	0
2	B	555	0	518	3	0
2	D	502	0	463	8	0
2	F	507	0	463	8	0
2	H	560	0	522	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	2	0	0	0	0
4	G	1	0	0	0	0
5	A	57	0	0	0	0
5	B	27	0	0	0	0
5	C	52	0	0	0	0
5	D	17	0	0	0	0
5	E	54	0	0	0	0
5	F	13	0	0	0	0
5	G	51	0	0	0	1
5	H	22	0	0	1	1
All	All	9564	0	8726	54	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 (54) 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)
2:D:97:ILE:O	2:D:98:THR:OG1	2.02	0.76
2:F:97:ILE:O	2:F:98:THR:OG1	2.02	0.75
2:F:136:ILE:HD11	2:F:141:PHE:HB2	1.72	0.71
2:D:136:ILE:HD11	2:D:141:PHE:HB2	1.74	0.70
2:D:97:ILE:O	2:D:98:THR:CB	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:ILE:HD11	2:B:141:PHE:HB2	1.80	0.63
2:F:97:ILE:O	2:F:98:THR:CB	2.44	0.63
2:H:136:ILE:HD11	2:H:141:PHE:HB2	1.83	0.60
1:E:78:ASP:OD2	1:G:87:LYS:HE2	2.04	0.56
1:C:58:VAL:CG1	1:C:75:PRO:HB2	2.35	0.56
1:A:197:LYS:HE3	1:A:220:PHE:CZ	2.42	0.55
1:A:58:VAL:CG1	1:A:75:PRO:HB2	2.36	0.55
1:G:197:LYS:HE3	1:G:220:PHE:CZ	2.42	0.55
1:G:58:VAL:CG1	1:G:75:PRO:HB2	2.37	0.54
1:E:58:VAL:CG1	1:E:75:PRO:HB2	2.38	0.53
1:E:197:LYS:HE3	1:E:220:PHE:CZ	2.45	0.52
2:D:80:HIS:CD2	2:D:96:ALA:HB2	2.46	0.50
2:F:136:ILE:HD11	2:F:141:PHE:CB	2.42	0.49
1:C:58:VAL:HG11	1:C:75:PRO:HB2	1.95	0.49
1:E:202:ARG:HB2	1:E:217:ASN:HB3	1.95	0.48
2:H:133:ASP:OD2	5:H:605:HOH:O	2.20	0.48
1:C:197:LYS:HE3	1:C:220:PHE:CZ	2.49	0.48
2:F:80:HIS:CD2	2:F:96:ALA:HB2	2.49	0.47
1:A:136:PRO:O	1:A:178:HIS:HE1	1.96	0.47
1:A:58:VAL:HG11	1:A:75:PRO:HB2	1.96	0.47
1:G:58:VAL:HG11	1:G:75:PRO:HB2	1.97	0.47
1:E:58:VAL:HG11	1:E:75:PRO:HB2	1.97	0.46
1:C:136:PRO:O	1:C:178:HIS:HE1	1.98	0.46
1:A:190:CYS:HB3	1:A:230:CYS:O	2.16	0.45
2:D:136:ILE:HD11	2:D:141:PHE:CB	2.45	0.45
1:A:87:LYS:HE2	1:C:78:ASP:OD2	2.17	0.45
1:C:202:ARG:HB2	1:C:217:ASN:HB3	1.98	0.45
1:A:202:ARG:HB2	1:A:217:ASN:HB3	2.00	0.44
1:G:190:CYS:HB3	1:G:230:CYS:O	2.19	0.43
1:G:157:ASP:HB3	1:G:180:ASN:HA	2.01	0.43
1:C:190:CYS:HB3	1:C:230:CYS:O	2.19	0.43
2:D:136:ILE:HA	2:D:140:GLU:OE1	2.18	0.42
1:A:157:ASP:HB3	1:A:180:ASN:HA	2.01	0.42
2:D:136:ILE:CD1	2:D:141:PHE:HB2	2.48	0.42
1:C:157:ASP:HB3	1:C:180:ASN:HA	2.01	0.42
2:H:91:LEU:O	2:H:95:THR:HG23	2.19	0.42
1:E:157:ASP:HB3	1:E:180:ASN:HA	2.01	0.42
2:F:136:ILE:HA	2:F:140:GLU:OE1	2.19	0.42
2:B:136:ILE:HA	2:B:140:GLU:OE1	2.19	0.42
2:B:91:LEU:O	2:B:95:THR:HG23	2.19	0.42
1:G:162:ASN:HA	1:G:163:PRO:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:202:ARG:HB2	1:G:217:ASN:HB3	2.01	0.41
1:G:114:GLY:HA3	1:G:255:ASP:OD1	2.21	0.41
1:C:43:HIS:C	1:C:43:HIS:CD2	2.94	0.41
1:E:190:CYS:HB3	1:E:230:CYS:O	2.21	0.41
2:F:91:LEU:O	2:F:95:THR:HG23	2.20	0.41
2:D:91:LEU:O	2:D:95:THR:HG23	2.20	0.41
1:C:170:ASN:OD1	1:C:171:ASN:N	2.53	0.40
1:E:49:LYS:HD2	2:F:118:ILE:HD13	2.03	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)
5:G:606:HOH:O	5:H:603:HOH:O[2_454]	2.18	0.02

## 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	225/246 (92%)	217 (96%)	8 (4%)	0	100	100
1	C	225/246 (92%)	217 (96%)	8 (4%)	0	100	100
1	E	225/246 (92%)	218 (97%)	7 (3%)	0	100	100
1	G	225/246 (92%)	217 (96%)	8 (4%)	0	100	100
2	B	65/104 (62%)	64 (98%)	1 (2%)	0	100	100
2	D	58/104 (56%)	57 (98%)	1 (2%)	0	100	100
2	F	59/104 (57%)	58 (98%)	1 (2%)	0	100	100
2	H	66/104 (64%)	65 (98%)	1 (2%)	0	100	100
All	All	1148/1400 (82%)	1113 (97%)	35 (3%)	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	185/199 (93%)	181 (98%)	4 (2%)	52	77
1	C	185/199 (93%)	181 (98%)	4 (2%)	52	77
1	E	185/199 (93%)	182 (98%)	3 (2%)	62	84
1	G	185/199 (93%)	180 (97%)	5 (3%)	44	71
2	B	62/92 (67%)	57 (92%)	5 (8%)	11	23
2	D	55/92 (60%)	52 (94%)	3 (6%)	21	41
2	F	56/92 (61%)	53 (95%)	3 (5%)	22	42
2	H	62/92 (67%)	57 (92%)	5 (8%)	11	23
All	All	975/1164 (84%)	943 (97%)	32 (3%)	38	64

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	224	LYS
1	A	234	GLU
1	A	236	MET
2	B	67	MET
2	B	95	THR
2	B	111	LEU
2	B	113	SER
2	B	136	ILE
1	C	43	HIS
1	C	218	ASN
1	C	234	GLU
1	C	236	MET
2	D	78	LYS
2	D	95	THR
2	D	136	ILE

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Mol	Chain	Res	Type
1	E	218	ASN
1	E	234	GLU
1	E	236	MET
2	F	67	MET
2	F	95	THR
2	F	136	ILE
1	G	178	HIS
1	G	218	ASN
1	G	224	LYS
1	G	234	GLU
1	G	236	MET
2	H	67	MET
2	H	95	THR
2	H	111	LEU
2	H	113	SER
2	H	136	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
1	A	191	GLN
1	A	243	HIS
1	A	266	GLN
2	B	119	ASN
1	C	43	HIS
1	C	178	HIS
1	C	191	GLN
1	C	243	HIS
1	C	266	GLN
1	E	191	GLN
1	E	243	HIS
1	G	191	GLN
1	G	243	HIS
1	G	266	GLN
2	H	119	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 19 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	227/246 (92%)	-0.06	10 (4%) 34 37	18, 33, 61, 91	0
1	C	227/246 (92%)	0.08	9 (3%) 38 41	20, 38, 65, 79	0
1	E	227/246 (92%)	0.03	10 (4%) 34 37	18, 35, 62, 85	0
1	G	227/246 (92%)	0.02	9 (3%) 38 41	16, 35, 63, 88	0
2	B	69/104 (66%)	-0.14	2 (2%) 51 55	17, 32, 60, 80	0
2	D	62/104 (59%)	0.02	1 (1%) 72 74	23, 35, 59, 81	0
2	F	63/104 (60%)	0.05	6 (9%) 8 8	18, 33, 70, 90	0
2	H	70/104 (67%)	-0.16	2 (2%) 51 55	20, 32, 66, 89	0
All	All	1172/1400 (83%)	-0.00	49 (4%) 36 39	16, 35, 65, 91	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	67	MET	5.7
1	E	115	ARG	4.2
1	A	173	GLN	4.1
2	H	67	MET	3.9
1	E	43	HIS	3.8
1	C	115	ARG	3.7
2	H	109	ALA	3.5
2	D	70	GLN	3.3
1	E	173	GLN	3.2
1	A	159	LYS	3.1
1	A	43	HIS	2.9
1	G	43	HIS	2.9
2	B	67	MET	2.8
1	A	268	THR	2.7
2	F	68	SER	2.7
1	G	178	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	209	GLN	2.6
2	F	69	PRO	2.6
1	G	173	GLN	2.6
1	A	235	ASN	2.6
1	E	225	ASN	2.5
1	C	147	VAL	2.5
2	F	70	GLN	2.5
1	G	172	GLY	2.5
1	A	148	GLY	2.4
1	C	102	GLU	2.4
2	B	99	HIS	2.4
1	E	125	ILE	2.4
1	A	117	ARG	2.4
2	F	71	GLU	2.4
1	E	235	ASN	2.3
1	C	148	GLY	2.3
1	E	102	GLU	2.3
1	A	125	ILE	2.3
1	G	125	ILE	2.3
1	C	43	HIS	2.2
1	G	235	ASN	2.2
1	C	235	ASN	2.2
1	E	184	SER	2.2
1	A	149	ILE	2.1
1	G	148	GLY	2.1
1	G	209	GLN	2.1
1	E	149	ILE	2.1
1	C	159	LYS	2.1
1	C	126	TRP	2.1
1	E	237	ILE	2.1
2	F	98	THR	2.0
1	G	208	TYR	2.0
1	C	210	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	CL	G	503	1/1	0.83	0.32	55,55,55,55	0
3	CA	G	502	1/1	0.88	0.12	42,42,42,42	0
4	CL	A	504	1/1	0.90	0.36	61,61,61,61	0
3	CA	E	502	1/1	0.93	0.05	50,50,50,50	0
3	CA	C	502	1/1	0.95	0.07	49,49,49,49	0
4	CL	A	503	1/1	0.96	0.08	65,65,65,65	0
3	CA	E	501	1/1	0.96	0.04	41,41,41,41	0
3	CA	A	501	1/1	0.97	0.13	37,37,37,37	0
3	CA	C	501	1/1	0.97	0.07	38,38,38,38	0
3	CA	G	501	1/1	0.97	0.04	45,45,45,45	0
3	CA	F	502	1/1	0.98	0.03	32,32,32,32	0
3	CA	D	502	1/1	0.98	0.04	40,40,40,40	0
3	CA	D	501	1/1	0.98	0.06	25,25,25,25	0
3	CA	A	502	1/1	0.98	0.06	42,42,42,42	0
3	CA	H	502	1/1	0.98	0.05	25,25,25,25	0
3	CA	H	501	1/1	0.99	0.03	19,19,19,19	0
3	CA	F	501	1/1	0.99	0.05	22,22,22,22	0
3	CA	B	502	1/1	0.99	0.05	27,27,27,27	0
3	CA	B	501	1/1	1.00	0.06	22,22,22,22	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.