



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:21 am BST

PDB ID : 4YGE
Title : Crystal structure of ERGIC-53/MCFD2, trigonal 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 : 3.05 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 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

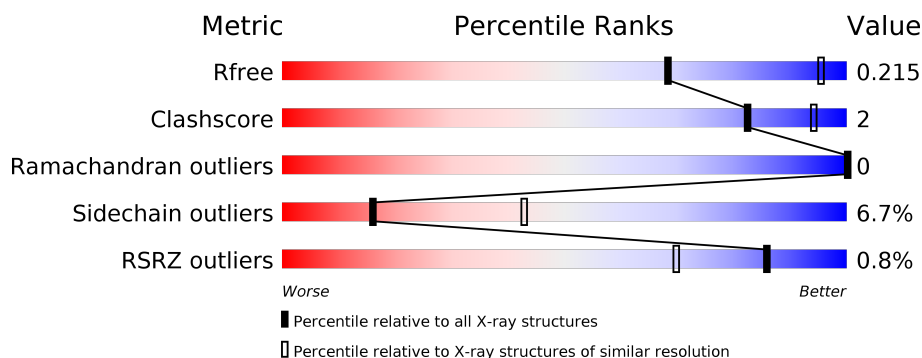
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 ≥ 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	
1	C	246	
1	E	246	
2	B	143	
2	D	143	
2	F	143	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6911 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	223	Total	C	N	O	S	0	0	0
			1753	1115	308	326	4			
1	E	223	Total	C	N	O	S	0	0	0
			1750	1115	308	323	4			

There are 21 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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	66	Total 532	C 331	N 85	O 113	S 3	0	0	0
2	D	66	Total 532	C 331	N 85	O 113	S 3	0	0	0
2	F	67	Total 540	C 337	N 86	O 114	S 3	0	0	0

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	MET	-	expression tag	UNP Q8NI22
B	5	GLY	-	expression tag	UNP Q8NI22
B	6	HIS	-	expression tag	UNP Q8NI22
B	7	HIS	-	expression tag	UNP Q8NI22
B	8	HIS	-	expression tag	UNP Q8NI22
B	9	HIS	-	expression tag	UNP Q8NI22
B	10	HIS	-	expression tag	UNP Q8NI22
B	11	HIS	-	expression tag	UNP Q8NI22
B	12	HIS	-	expression tag	UNP Q8NI22
B	13	HIS	-	expression tag	UNP Q8NI22
B	14	HIS	-	expression tag	UNP Q8NI22
B	15	HIS	-	expression tag	UNP Q8NI22
B	16	SER	-	expression tag	UNP Q8NI22
B	17	SER	-	expression tag	UNP Q8NI22
B	18	GLY	-	expression tag	UNP Q8NI22
B	19	HIS	-	expression tag	UNP Q8NI22
B	20	ILE	-	expression tag	UNP Q8NI22
B	21	GLU	-	expression tag	UNP Q8NI22
B	22	GLY	-	expression tag	UNP Q8NI22
B	23	ARG	-	expression tag	UNP Q8NI22
B	24	HIS	-	expression tag	UNP Q8NI22
B	25	MET	-	expression tag	UNP Q8NI22
B	26	LEU	-	expression tag	UNP Q8NI22
D	4	MET	-	expression tag	UNP Q8NI22
D	5	GLY	-	expression tag	UNP Q8NI22
D	6	HIS	-	expression tag	UNP Q8NI22
D	7	HIS	-	expression tag	UNP Q8NI22
D	8	HIS	-	expression tag	UNP Q8NI22
D	9	HIS	-	expression tag	UNP Q8NI22
D	10	HIS	-	expression tag	UNP Q8NI22
D	11	HIS	-	expression tag	UNP Q8NI22
D	12	HIS	-	expression tag	UNP Q8NI22
D	13	HIS	-	expression tag	UNP Q8NI22

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Chain	Residue	Modelled	Actual	Comment	Reference
D	14	HIS	-	expression tag	UNP Q8NI22
D	15	HIS	-	expression tag	UNP Q8NI22
D	16	SER	-	expression tag	UNP Q8NI22
D	17	SER	-	expression tag	UNP Q8NI22
D	18	GLY	-	expression tag	UNP Q8NI22
D	19	HIS	-	expression tag	UNP Q8NI22
D	20	ILE	-	expression tag	UNP Q8NI22
D	21	GLU	-	expression tag	UNP Q8NI22
D	22	GLY	-	expression tag	UNP Q8NI22
D	23	ARG	-	expression tag	UNP Q8NI22
D	24	HIS	-	expression tag	UNP Q8NI22
D	25	MET	-	expression tag	UNP Q8NI22
D	26	LEU	-	expression tag	UNP Q8NI22
F	4	MET	-	expression tag	UNP Q8NI22
F	5	GLY	-	expression tag	UNP Q8NI22
F	6	HIS	-	expression tag	UNP Q8NI22
F	7	HIS	-	expression tag	UNP Q8NI22
F	8	HIS	-	expression tag	UNP Q8NI22
F	9	HIS	-	expression tag	UNP Q8NI22
F	10	HIS	-	expression tag	UNP Q8NI22
F	11	HIS	-	expression tag	UNP Q8NI22
F	12	HIS	-	expression tag	UNP Q8NI22
F	13	HIS	-	expression tag	UNP Q8NI22
F	14	HIS	-	expression tag	UNP Q8NI22
F	15	HIS	-	expression tag	UNP Q8NI22
F	16	SER	-	expression tag	UNP Q8NI22
F	17	SER	-	expression tag	UNP Q8NI22
F	18	GLY	-	expression tag	UNP Q8NI22
F	19	HIS	-	expression tag	UNP Q8NI22
F	20	ILE	-	expression tag	UNP Q8NI22
F	21	GLU	-	expression tag	UNP Q8NI22
F	22	GLY	-	expression tag	UNP Q8NI22
F	23	ARG	-	expression tag	UNP Q8NI22
F	24	HIS	-	expression tag	UNP Q8NI22
F	25	MET	-	expression tag	UNP Q8NI22
F	26	LEU	-	expression tag	UNP Q8NI22

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Ca 2	0	0
3	D	2	Total 2	Ca 2	0	0
3	C	1	Total 1	Ca 1	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	A	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total 5	O 5	0	0
5	C	2	Total 2	O 2	0	0
5	E	2	Total 2	O 2	0	0
5	F	1	Total 1	O 1	0	0

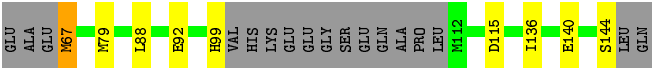
- Molecule 1: Protein ERGIC-53

Amino Acid	Percentage (%)
MET	~1.5
ASN	~1.5
HIS	~1.5
LYS	~1.5
VAL	~1.5
HIS	~1.5
MET	~1.5
ASP	~1.5
GLY	~1.5
VAL	~1.5
GLY	~1.5
ASP	~1.5
PRO	~1.5
ALA	~1.5
VAL	~1.5
ALA	~1.5
LEU	~1.5
P42	~1.5
V58	~1.5
P75	~1.5
S76	~1.5
V106	~1.5
T113	~1.5
G114	~1.5
R115	~1.5
A120	~1.5
D121	~1.5
E134	~1.5
S140	~1.5
L143	~1.5
D157	~1.5
M180	~1.5
K197	~1.5
R202	~1.5
I205	~1.5
Q209	~1.5
R210	~1.5
T211	~1.5
N218	~1.5
G219	~1.5
F220	~1.5
N225	~1.5

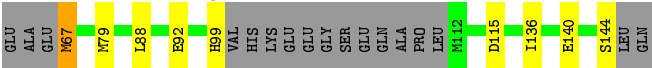
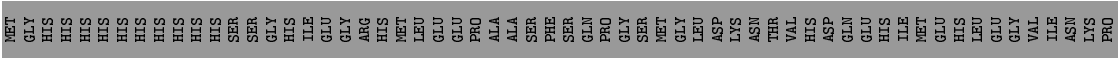
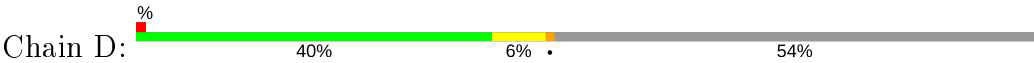
D177	H178	Q179	A186		D193	K197	E202	I205	Q209	X210	T211	L212	N218	G219	F220	K232	L267	T268	GLU																									
MET	ASN	HIS	LYS	VAL	HIS	MET	ASP	GLY	VAL	GLY	GLY	ASP	PRO	ALA	VAL	ALA	LEU	P42	R43	R44	K49	V88	P75	S76	K98	V106	T113	A120	D121	L133	E134	S140	L143	D152	D155	ASN	ASP	GLY	LYS	K160	H161	I168	Q173	V176

T268	
GLU	
MET	
ASN	
HIS	
LYS	
VAL	
HIS	
MET	
ASP	
GLY	
VAL	
GLY	
GLY	
ASP	
PRO	
ALA	
VAL	
ALA	
LEU	
P42	
H43	
R44	
T113	
G114	
R115	
S140	
D152	
D155	
ASN	
ASP	
G158	
K159	
K160	
F161	
I168	
D177	
H178	
Q179	
ASN	
ASP	
G182	
Q185	
A186	
R202	
Q209	
N210	
T211	
L212	
N218	
V232	

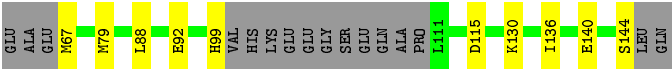
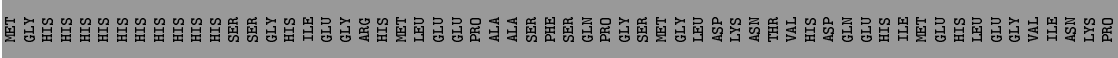
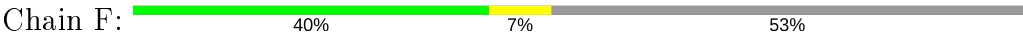
NET	GLY	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	ILE	GLU	GLY	ARG	ALA	ALA	SER	PHE	GLN	GLY	GLY	SER	NET	GLY	GLY	LEU	GLU	GLU	PRO	PRO	ALA	ALA	SER	ASN	THR	VAL	HIS	ASP	GLN	GLY	HIS	ILE	NET	GLU	HIS	LEU	GLU	GLY	VAL	ILE	ASN	LYS	PRO
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● Molecule 2: Multiple coagulation factor deficiency protein 2



● Molecule 2: Multiple coagulation factor deficiency protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.13Å 113.13Å 157.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.05 19.80 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.05) 99.9 (19.80-3.05)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.39 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.173 , 0.211 0.177 , 0.215	Depositor DCC
R_{free} test set	1156 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6911	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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: 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	0.70	0/1832	0.85	2/2487 (0.1%)
1	C	0.72	0/1802	0.89	3/2446 (0.1%)
1	E	0.69	0/1798	0.83	0/2437
2	B	0.57	0/540	0.77	1/727 (0.1%)
2	D	0.59	0/540	0.76	1/727 (0.1%)
2	F	0.65	0/548	0.73	0/738
All	All	0.68	0/7060	0.84	7/9562 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	67	MET	CB-CG-SD	7.16	133.88	112.40
1	C	143	LEU	CA-CB-CG	6.41	130.03	115.30
1	C	58	VAL	CB-CA-C	-5.68	100.60	111.40
2	B	67	MET	CA-CB-CG	5.58	122.79	113.30
1	A	58	VAL	CB-CA-C	-5.57	100.82	111.40
1	C	193	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	115	ARG	NE-CZ-NH2	-5.07	117.76	120.30

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	7	0
1	C	1753	0	1663	12	0
1	E	1750	0	1668	7	0
2	B	532	0	488	3	0
2	D	532	0	488	2	0
2	F	540	0	499	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	F	2	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	5	0	0	0	0
5	C	2	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
All	All	6911	0	6496	33	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.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:VAL:HG22	1:C:76:SER:O	1.98	0.63
1:A:58:VAL:HG22	1:A:76:SER:O	1.97	0.63
1:E:152:ASP:OD2	1:E:178:HIS:HE1	1.87	0.58
1:C:152:ASP:OD2	1:C:178:HIS:HE1	1.88	0.56
1:A:237:ILE:HG22	1:E:185:GLN:HB3	1.88	0.56
1:C:98:LYS:HE3	2:F:130:LYS:O	2.05	0.55
1:A:58:VAL:HG13	1:A:75:PRO:HB2	1.90	0.53
1:C:58:VAL:HG13	1:C:75:PRO:HB2	1.89	0.53
1:A:157:ASP:HB3	1:A:180:ASN:HA	1.91	0.52
1:E:177:ASP:OD2	1:E:179:GLN:HB3	2.10	0.51
1:E:179:GLN:HG2	1:E:179:GLN:O	2.11	0.50
1:C:152:ASP:OD2	1:C:178:HIS:CE1	2.68	0.47
1:E:152:ASP:OD2	1:E:178:HIS:CE1	2.69	0.45
2:F:88:LEU:HA	2:F:92:GLU:OE1	2.16	0.45
1:C:133:LEU:HB3	1:C:134:GLU:H	1.63	0.44
2:D:88:LEU:HA	2:D:92:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:CG2	1:A:205:ILE:HB	2.49	0.43
1:A:197:LYS:HE3	1:A:220:PHE:CZ	2.54	0.43
2:F:136:ILE:HA	2:F:140:GLU:OE1	2.19	0.43
2:B:88:LEU:HA	2:B:92:GLU:OE1	2.18	0.42
2:B:136:ILE:HA	2:B:140:GLU:OE1	2.19	0.42
2:D:136:ILE:HA	2:D:140:GLU:OE1	2.20	0.42
1:C:168:ILE:HD13	1:C:186:ALA:HA	2.01	0.42
1:C:197:LYS:HE3	1:C:220:PHE:CZ	2.55	0.42
1:E:168:ILE:HD13	1:E:186:ALA:HA	2.02	0.42
1:A:120:ALA:HB1	1:A:121:ASP:HA	2.02	0.42
2:B:136:ILE:HG21	2:B:136:ILE:HD13	1.87	0.41
1:C:120:ALA:HB1	1:C:121:ASP:HA	2.03	0.41
1:C:106:VAL:CG2	1:C:205:ILE:HB	2.51	0.41
2:F:136:ILE:HG21	2:F:136:ILE:HD13	1.87	0.41
1:E:212:LEU:O	1:E:232:LYS:HA	2.21	0.40
1:C:176:TYR:CE2	1:C:178:HIS:HA	2.57	0.40
1:C:212:LEU:O	1:C:232:LYS:HA	2.22	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	225/246 (92%)	216 (96%)	9 (4%)	0	100	100
1	C	219/246 (89%)	210 (96%)	9 (4%)	0	100	100
1	E	217/246 (88%)	206 (95%)	11 (5%)	0	100	100
2	B	62/143 (43%)	59 (95%)	3 (5%)	0	100	100
2	D	62/143 (43%)	59 (95%)	3 (5%)	0	100	100
2	F	63/143 (44%)	60 (95%)	3 (5%)	0	100	100
All	All	848/1167 (73%)	810 (96%)	38 (4%)	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%)	174 (94%)	11 (6%)	19	47
1	C	182/199 (92%)	168 (92%)	14 (8%)	13	38
1	E	181/199 (91%)	172 (95%)	9 (5%)	24	54
2	B	59/125 (47%)	54 (92%)	5 (8%)	10	34
2	D	59/125 (47%)	54 (92%)	5 (8%)	10	34
2	F	60/125 (48%)	55 (92%)	5 (8%)	11	35
All	All	726/972 (75%)	677 (93%)	49 (7%)	16	43

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	VAL
1	A	113	THR
1	A	134	GLU
1	A	140	SER
1	A	143	LEU
1	A	202	ARG
1	A	209	GLN
1	A	211	THR
1	A	218	ASN
1	A	232	LYS
1	A	237	ILE
2	B	67	MET
2	B	79	MET
2	B	99	HIS
2	B	115	ASP
2	B	144	SER
1	C	44	ARG
1	C	49	LYS
1	C	58	VAL

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Mol	Chain	Res	Type
1	C	113	THR
1	C	140	SER
1	C	173	GLN
1	C	179	GLN
1	C	202	ARG
1	C	209	GLN
1	C	211	THR
1	C	218	ASN
1	C	232	LYS
1	C	267	LEU
1	C	268	THR
2	D	67	MET
2	D	79	MET
2	D	99	HIS
2	D	115	ASP
2	D	144	SER
1	E	44	ARG
1	E	113	THR
1	E	115	ARG
1	E	140	SER
1	E	179	GLN
1	E	202	ARG
1	E	209	GLN
1	E	211	THR
1	E	218	ASN
2	F	67	MET
2	F	79	MET
2	F	99	HIS
2	F	115	ASP
2	F	144	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	225	ASN
1	A	243	HIS
1	A	266	GLN
2	B	119	ASN
1	C	178	HIS
1	C	218	ASN
1	C	225	ASN

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Mol	Chain	Res	Type
1	C	266	GLN
2	D	119	ASN
1	E	178	HIS
1	E	218	ASN
1	E	225	ASN
1	E	266	GLN
2	F	119	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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 ⓘ

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	227/246 (92%)	-0.61	1 (0%) 92 82	17, 31, 56, 70	0
1	C	223/246 (90%)	-0.57	1 (0%) 92 82	18, 32, 58, 85	0
1	E	223/246 (90%)	-0.57	4 (1%) 68 45	20, 32, 63, 97	0
2	B	66/143 (46%)	-0.24	0 100 100	32, 53, 80, 100	0
2	D	66/143 (46%)	-0.24	1 (1%) 73 51	28, 50, 74, 102	0
2	F	67/143 (46%)	-0.46	0 100 100	23, 37, 60, 73	0
All	All	872/1167 (74%)	-0.53	7 (0%) 86 70	17, 34, 67, 102	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	179	GLN	2.6
1	E	159	LYS	2.4
1	E	160	LYS	2.4
1	C	161	ASN	2.3
1	E	161	ASN	2.1
2	D	99	HIS	2.1
1	A	225	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 [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	CA	D	502	1/1	0.86	0.06	45,45,45,45	0
4	CL	C	502	1/1	0.88	0.34	51,51,51,51	0
3	CA	B	501	1/1	0.91	0.06	59,59,59,59	0
4	CL	A	503	1/1	0.92	0.21	58,58,58,58	0
3	CA	C	501	1/1	0.93	0.14	56,56,56,56	0
3	CA	A	501	1/1	0.95	0.09	31,31,31,31	0
3	CA	A	502	1/1	0.96	0.08	49,49,49,49	0
4	CL	E	501	1/1	0.96	0.19	38,38,38,38	0
3	CA	F	502	1/1	0.96	0.06	32,32,32,32	0
3	CA	B	502	1/1	0.97	0.06	38,38,38,38	0
3	CA	D	501	1/1	0.98	0.07	28,28,28,28	0
3	CA	F	501	1/1	0.98	0.07	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.