Full wwPDB X-ray Structure Validation Report (i)

Aug 19, 2023 – 06:14 PM EDT

PDB ID	:	2GGE
Title	:	Crystal Structure of Mandelate Racemase/Muconate Lactonizing Enzyme from Bacillus Subtilis complexed with MG++ at 1.8 A
Authors	:	Malashkevich, V.N.; Sauder, J.M.; Schwinn, K.D.; Emtage, S.; Thompson, D.A.; Rutter, M.E.; Dickey, M.; Groshong, C.; Bain, K.T.; Adams, J.M.; Reyes, C.; Rooney, I.; Powell, A.; Boice, A.; Gheyi, T.; Ozyurt, S.; Atwell, S.; Wasserman, S.R.; Burley, S.K.; Sali, A.; Babbitt, P.; Pieper, U.; Gerlt, J.A.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2006-03-23
Resolution	:	1.89 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 (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 (1)) were used in the production of this report:

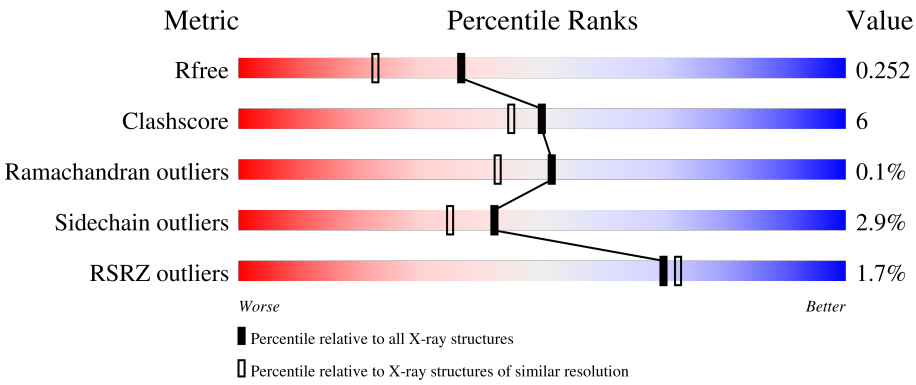
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

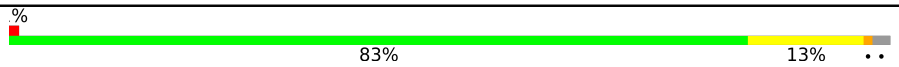
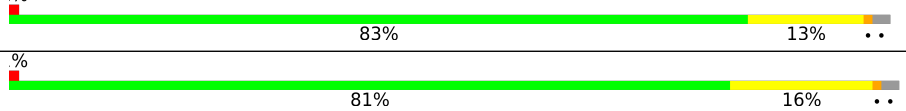
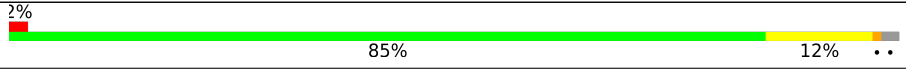
The reported resolution of this entry is 1.89 Å.

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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	382	
1	B	382	
1	C	382	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

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Mol	Chain	Length	Quality of chain
1	D	382	% 85% 12%
1	E	382	% 82% 14%
1	F	382	4% 85% 12%
1	G	382	2% 84% 13%
1	H	382	2% 81% 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25632 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 yitF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	373	2979	1907	516	540	16	0	0	0
1	B	374	2990	1913	518	543	16	0	1	0
1	C	374	2984	1910	517	541	16	0	0	0
1	D	376	3004	1921	522	545	16	0	1	0
1	E	373	2979	1907	516	540	16	0	0	0
1	F	373	2991	1913	518	544	16	0	2	0
1	G	374	2994	1916	520	542	16	0	1	0
1	H	374	2990	1913	518	543	16	0	1	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP O06741
A	2	ALA	-	cloning artifact	UNP O06741
A	3	LEU	-	cloning artifact	UNP O06741
A	4	VAL	-	cloning artifact	UNP O06741
A	375	GLU	-	cloning artifact	UNP O06741
A	376	GLY	-	cloning artifact	UNP O06741
A	377	HIS	-	expression tag	UNP O06741
A	378	HIS	-	expression tag	UNP O06741
A	379	HIS	-	expression tag	UNP O06741
A	380	HIS	-	expression tag	UNP O06741
A	381	HIS	-	expression tag	UNP O06741
A	382	HIS	-	expression tag	UNP O06741
B	1	MET	-	cloning artifact	UNP O06741

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ALA	-	cloning artifact	UNP O06741
B	3	LEU	-	cloning artifact	UNP O06741
B	4	VAL	-	cloning artifact	UNP O06741
B	375	GLU	-	cloning artifact	UNP O06741
B	376	GLY	-	cloning artifact	UNP O06741
B	377	HIS	-	expression tag	UNP O06741
B	378	HIS	-	expression tag	UNP O06741
B	379	HIS	-	expression tag	UNP O06741
B	380	HIS	-	expression tag	UNP O06741
B	381	HIS	-	expression tag	UNP O06741
B	382	HIS	-	expression tag	UNP O06741
C	1	MET	-	cloning artifact	UNP O06741
C	2	ALA	-	cloning artifact	UNP O06741
C	3	LEU	-	cloning artifact	UNP O06741
C	4	VAL	-	cloning artifact	UNP O06741
C	375	GLU	-	cloning artifact	UNP O06741
C	376	GLY	-	cloning artifact	UNP O06741
C	377	HIS	-	expression tag	UNP O06741
C	378	HIS	-	expression tag	UNP O06741
C	379	HIS	-	expression tag	UNP O06741
C	380	HIS	-	expression tag	UNP O06741
C	381	HIS	-	expression tag	UNP O06741
C	382	HIS	-	expression tag	UNP O06741
D	1	MET	-	cloning artifact	UNP O06741
D	2	ALA	-	cloning artifact	UNP O06741
D	3	LEU	-	cloning artifact	UNP O06741
D	4	VAL	-	cloning artifact	UNP O06741
D	375	GLU	-	cloning artifact	UNP O06741
D	376	GLY	-	cloning artifact	UNP O06741
D	377	HIS	-	expression tag	UNP O06741
D	378	HIS	-	expression tag	UNP O06741
D	379	HIS	-	expression tag	UNP O06741
D	380	HIS	-	expression tag	UNP O06741
D	381	HIS	-	expression tag	UNP O06741
D	382	HIS	-	expression tag	UNP O06741
E	1	MET	-	cloning artifact	UNP O06741
E	2	ALA	-	cloning artifact	UNP O06741
E	3	LEU	-	cloning artifact	UNP O06741
E	4	VAL	-	cloning artifact	UNP O06741
E	375	GLU	-	cloning artifact	UNP O06741
E	376	GLY	-	cloning artifact	UNP O06741
E	377	HIS	-	expression tag	UNP O06741

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Chain	Residue	Modelled	Actual	Comment	Reference
E	378	HIS	-	expression tag	UNP O06741
E	379	HIS	-	expression tag	UNP O06741
E	380	HIS	-	expression tag	UNP O06741
E	381	HIS	-	expression tag	UNP O06741
E	382	HIS	-	expression tag	UNP O06741
F	1	MET	-	cloning artifact	UNP O06741
F	2	ALA	-	cloning artifact	UNP O06741
F	3	LEU	-	cloning artifact	UNP O06741
F	4	VAL	-	cloning artifact	UNP O06741
F	375	GLU	-	cloning artifact	UNP O06741
F	376	GLY	-	cloning artifact	UNP O06741
F	377	HIS	-	expression tag	UNP O06741
F	378	HIS	-	expression tag	UNP O06741
F	379	HIS	-	expression tag	UNP O06741
F	380	HIS	-	expression tag	UNP O06741
F	381	HIS	-	expression tag	UNP O06741
F	382	HIS	-	expression tag	UNP O06741
G	1	MET	-	cloning artifact	UNP O06741
G	2	ALA	-	cloning artifact	UNP O06741
G	3	LEU	-	cloning artifact	UNP O06741
G	4	VAL	-	cloning artifact	UNP O06741
G	375	GLU	-	cloning artifact	UNP O06741
G	376	GLY	-	cloning artifact	UNP O06741
G	377	HIS	-	expression tag	UNP O06741
G	378	HIS	-	expression tag	UNP O06741
G	379	HIS	-	expression tag	UNP O06741
G	380	HIS	-	expression tag	UNP O06741
G	381	HIS	-	expression tag	UNP O06741
G	382	HIS	-	expression tag	UNP O06741
H	1	MET	-	cloning artifact	UNP O06741
H	2	ALA	-	cloning artifact	UNP O06741
H	3	LEU	-	cloning artifact	UNP O06741
H	4	VAL	-	cloning artifact	UNP O06741
H	375	GLU	-	cloning artifact	UNP O06741
H	376	GLY	-	cloning artifact	UNP O06741
H	377	HIS	-	expression tag	UNP O06741
H	378	HIS	-	expression tag	UNP O06741
H	379	HIS	-	expression tag	UNP O06741
H	380	HIS	-	expression tag	UNP O06741
H	381	HIS	-	expression tag	UNP O06741
H	382	HIS	-	expression tag	UNP O06741

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Cl 2 2	0	0
3	G	1	Total Cl 1 1	0	0

- Molecule 4 is water.

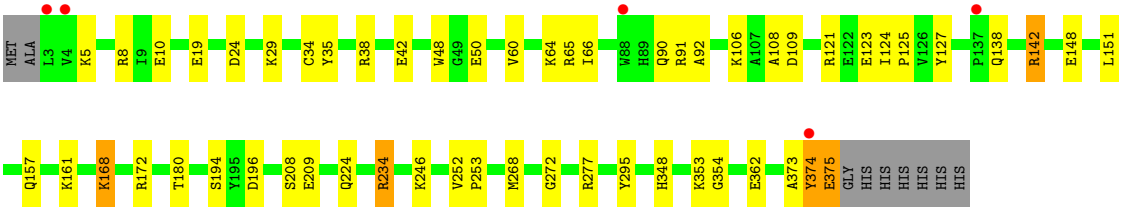
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	227	Total O 227 227	0	0
4	B	256	Total O 256 256	0	0
4	C	197	Total O 197 197	0	0
4	D	232	Total O 232 232	0	0
4	E	207	Total O 207 207	0	0
4	F	151	Total O 151 151	0	0
4	G	208	Total O 208 208	0	0
4	H	232	Total O 232 232	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

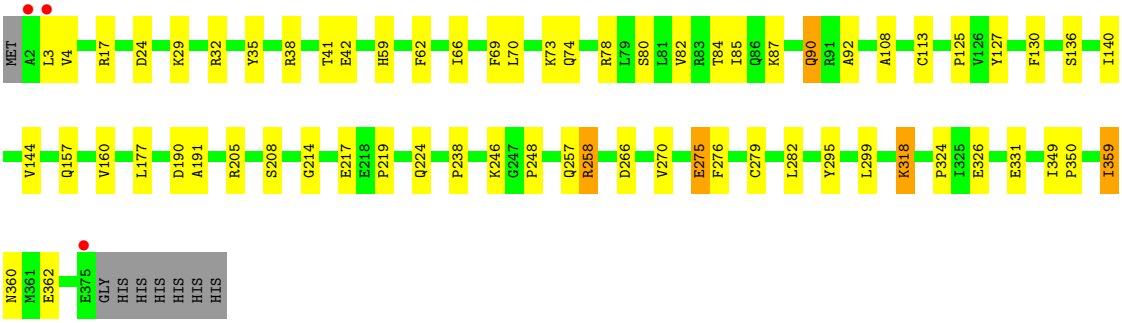
• Molecule 1: yitF

Chain A:



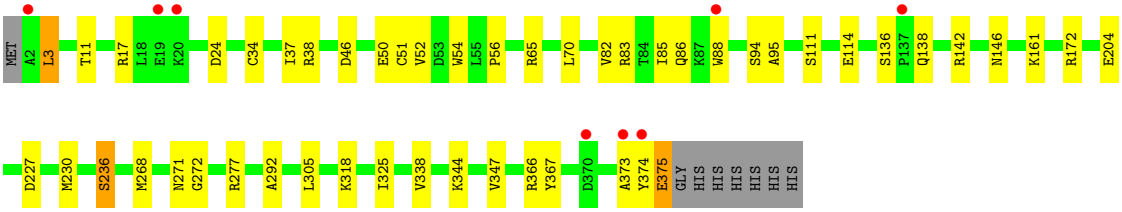
• Molecule 1: yitF

Chain B:



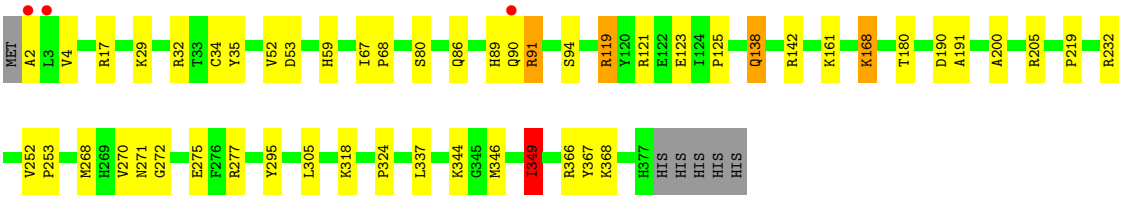
• Molecule 1: yitF

Chain C:



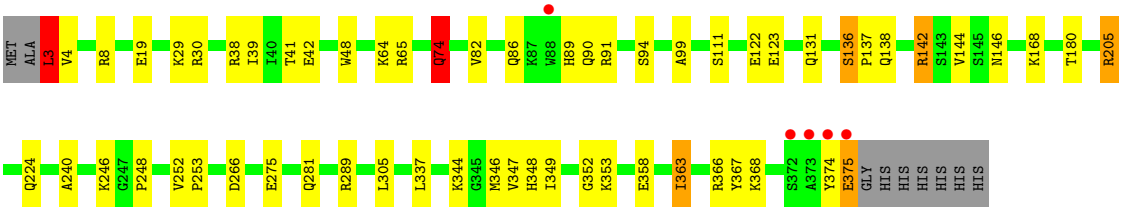
• Molecule 1: yitF

Chain D:



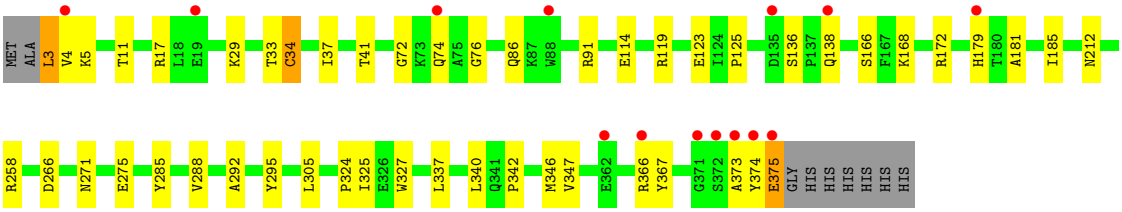
• Molecule 1: yitF

Chain E:



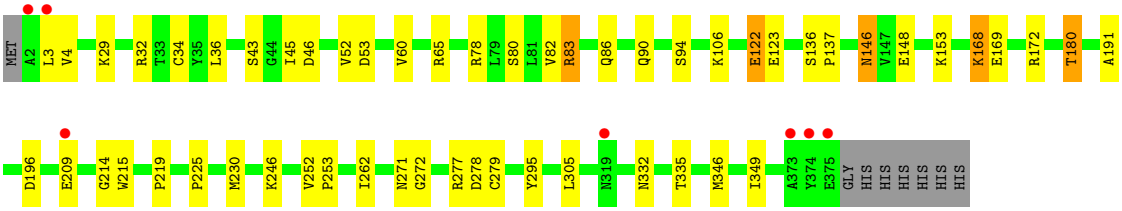
• Molecule 1: yitF

Chain F:



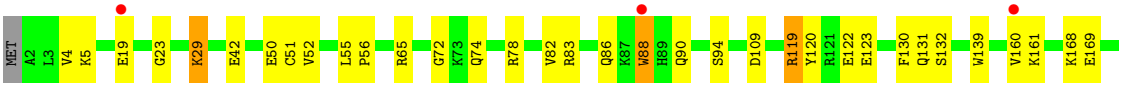
• Molecule 1: yitF

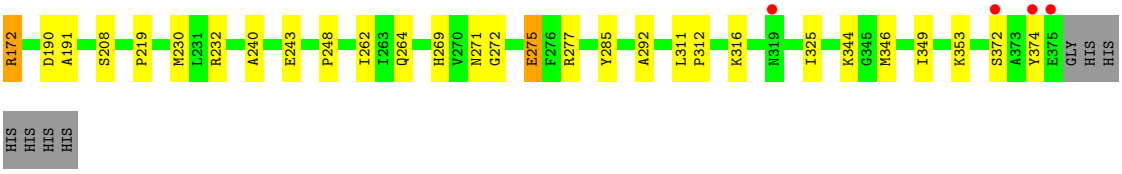
Chain G:



• Molecule 1: yitF

Chain H:




R172
D190
A191
S208
P219
M230
L231
R232
A240
E243
P248
I262
I263
Q264
H269
V270
N271
G272
E275
F276
R277
Y285
A292
L311
P312
K316
N319
I325
K344
G345
M346
I349
K353
S372
A373
Y374
E375
GLY
HIS
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	112.42Å 110.65Å 129.31Å 90.00° 105.77° 90.00°	Depositor
Resolution (Å)	27.95 – 1.89 27.95 – 1.88	Depositor EDS
% Data completeness (in resolution range)	85.7 (27.95-1.89) 85.3 (27.95-1.88)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 1.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.253 0.188 , 0.252	Depositor DCC
R_{free} test set	10531 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25632	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	1.15	3/3058 (0.1%)	0.97	5/4145 (0.1%)
1	B	1.12	2/3069 (0.1%)	0.96	6/4160 (0.1%)
1	C	1.04	1/3063 (0.0%)	0.91	4/4152 (0.1%)
1	D	1.14	5/3084 (0.2%)	1.02	12/4180 (0.3%)
1	E	1.05	2/3058 (0.1%)	0.92	4/4145 (0.1%)
1	F	0.92	2/3070 (0.1%)	0.85	2/4161 (0.0%)
1	G	1.09	6/3074 (0.2%)	0.95	8/4167 (0.2%)
1	H	1.05	3/3069 (0.1%)	0.92	6/4160 (0.1%)
All	All	1.07	24/24545 (0.1%)	0.94	47/33270 (0.1%)

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	H	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	CYS	CB-SG	-10.37	1.64	1.82
1	C	34	CYS	CB-SG	-8.49	1.67	1.82
1	G	34	CYS	CB-SG	-7.10	1.70	1.82
1	G	122	GLU	CB-CG	7.05	1.65	1.52
1	G	122	GLU	CG-CD	6.99	1.62	1.51
1	B	113	CYS	CB-SG	6.38	1.93	1.82
1	E	240	ALA	CA-CB	6.21	1.65	1.52
1	D	34	CYS	CB-SG	-6.00	1.72	1.82
1	G	246	LYS	CD-CE	5.92	1.66	1.51
1	A	35	TYR	CD2-CE2	5.73	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	209	GLU	CG-CD	5.62	1.60	1.51
1	H	160	VAL	CB-CG1	5.54	1.64	1.52
1	F	34	CYS	CB-SG	-5.47	1.72	1.81
1	G	279	CYS	CB-SG	-5.39	1.73	1.81
1	F	275	GLU	CG-CD	5.33	1.59	1.51
1	E	275	GLU	CG-CD	5.26	1.59	1.51
1	H	172	ARG	CG-CD	5.21	1.65	1.51
1	D	200	ALA	CA-CB	-5.16	1.41	1.52
1	D	344	LYS	CD-CE	5.14	1.64	1.51
1	D	275	GLU	CG-CD	5.14	1.59	1.51
1	B	130	PHE	CE2-CZ	5.11	1.47	1.37
1	H	130	PHE	CE1-CZ	5.09	1.47	1.37
1	A	121	ARG	CG-CD	5.04	1.64	1.51
1	D	275	GLU	CD-OE2	5.03	1.31	1.25

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	119	ARG	NE-CZ-NH1	9.59	125.10	120.30
1	H	78	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	277	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	G	277	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	G	83	ARG	NE-CZ-NH1	-7.31	116.65	120.30
1	A	234	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	D	91	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	B	32	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	266	ASP	CB-CG-OD1	6.77	124.39	118.30
1	B	282	LEU	CB-CG-CD1	-6.74	99.54	111.00
1	E	3	LEU	CA-CB-CG	6.64	130.57	115.30
1	D	119	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	E	205	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	D	232	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	D	344	LYS	CD-CE-NZ	6.24	126.04	111.70
1	B	258	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	H	119	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	3	LEU	CA-CB-CG	6.01	129.13	115.30
1	C	83	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	G	78	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	B	24	ASP	CB-CG-OD1	5.81	123.53	118.30
1	G	32	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	H	78	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	E	266	ASP	CB-CG-OD1	5.66	123.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	277	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	B	38	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	D	268	MET	CG-SD-CE	5.56	109.10	100.20
1	A	374	TYR	N-CA-C	-5.55	96.00	111.00
1	A	196	ASP	CB-CG-OD1	5.55	123.29	118.30
1	H	232	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	91	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	G	230	MET	CG-SD-CE	5.43	108.89	100.20
1	F	266	ASP	CB-CG-OD1	5.39	123.15	118.30
1	G	36	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	A	277	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	G	36	LEU	CB-CG-CD1	-5.28	102.03	111.00
1	D	121	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	38	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	G	196	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	E	289	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	D	349	ILE	CA-CB-CG2	5.09	121.09	110.90
1	C	277	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	17	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	32	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	F	266	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	H	230	MET	CG-SD-CE	5.03	108.25	100.20
1	H	119	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	374	TYR	Peptide

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	2979	0	2935	40	0
1	B	2990	0	2944	38	0
1	C	2984	0	2940	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3004	0	2954	32	0
1	E	2979	0	2935	54	0
1	F	2991	0	2943	38	0
1	G	2994	0	2946	29	0
1	H	2990	0	2944	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	D	2	0	0	0	0
3	G	1	0	0	0	0
4	A	227	0	0	7	0
4	B	256	0	0	1	0
4	C	197	0	0	3	0
4	D	232	0	0	7	0
4	E	207	0	0	14	0
4	F	151	0	0	3	0
4	G	208	0	0	6	0
4	H	232	0	0	5	0
All	All	25632	0	23541	275	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 6.

All (275) 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:E:90:GLN:HG2	4:E:559:HOH:O	1.50	1.08
1:F:172:ARG:HD2	4:F:528:HOH:O	1.53	1.05
1:A:142:ARG:HG3	1:A:142:ARG:NH1	1.59	1.04
1:C:172:ARG:HD2	4:C:559:HOH:O	1.59	1.02
1:A:142:ARG:HH11	1:A:142:ARG:CG	1.74	1.01
4:C:564:HOH:O	1:D:2:ALA:HB2	1.63	0.98
1:A:8:ARG:HD2	4:A:596:HOH:O	1.64	0.98
1:A:142:ARG:HG3	1:A:142:ARG:HH11	0.80	0.95
1:E:205:ARG:HD3	4:E:403:HOH:O	1.68	0.94
1:D:86:GLN:NE2	1:D:271:ASN:HB3	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:ARG:HG3	1:F:119:ARG:HH11	1.33	0.92
1:G:29:LYS:NZ	4:G:1912:HOH:O	2.09	0.86
1:G:122:GLU:HG2	4:G:1907:HOH:O	1.74	0.86
1:G:29:LYS:HD3	1:G:295:TYR:OH	1.78	0.84
1:E:136:SER:CB	1:E:142:ARG:NH2	2.45	0.79
1:A:29:LYS:HD3	1:A:295:TYR:OH	1.82	0.79
1:E:64:LYS:HE2	4:E:508:HOH:O	1.81	0.79
1:E:8:ARG:HD2	4:E:596:HOH:O	1.82	0.77
1:A:38:ARG:CZ	4:A:486:HOH:O	2.33	0.76
1:A:8:ARG:NH1	1:A:10:GLU:OE2	2.19	0.75
1:F:119:ARG:HG3	1:F:119:ARG:NH1	2.02	0.74
1:H:82:VAL:O	1:H:86:GLN:HG3	1.87	0.74
1:F:29:LYS:HD3	1:F:295:TYR:OH	1.88	0.73
1:E:374:TYR:HD2	1:E:375:GLU:HG3	1.52	0.72
1:D:305:LEU:HB3	1:D:349:ILE:HD11	1.71	0.71
1:G:278:ASP:OD2	1:H:285:TYR:OH	2.09	0.71
1:D:119:ARG:NE	4:D:1900:HOH:O	2.24	0.71
1:E:3:LEU:HD23	1:F:114:GLU:OE2	1.92	0.70
1:E:146:ASN:CG	4:E:601:HOH:O	2.29	0.70
1:E:374:TYR:HD2	1:E:375:GLU:CG	2.04	0.69
1:E:281:GLN:NE2	4:E:522:HOH:O	2.24	0.69
1:D:366:ARG:HD3	4:D:1940:HOH:O	1.91	0.69
1:A:168:LYS:HG3	1:A:172:ARG:HH12	1.58	0.69
1:A:168:LYS:CG	1:A:172:ARG:HH12	2.05	0.69
1:G:146:ASN:ND2	4:G:1926:HOH:O	2.27	0.68
1:D:86:GLN:CD	1:D:271:ASN:HB3	2.15	0.67
1:B:3:LEU:O	1:B:74:GLN:OE1	2.12	0.67
1:A:90:GLN:HG3	1:A:91:ARG:N	2.10	0.67
1:B:29:LYS:HD3	1:B:295:TYR:OH	1.95	0.67
1:D:52:VAL:HB	4:D:1978:HOH:O	1.94	0.66
1:E:136:SER:HB3	1:E:142:ARG:NH2	2.09	0.66
1:H:50:GLU:OE2	4:H:590:HOH:O	2.12	0.66
1:A:60:VAL:HG22	1:A:64:LYS:HG2	1.78	0.65
1:C:51:CYS:HB3	1:C:95:ALA:HB2	1.78	0.65
1:F:123:GLU:HB3	1:F:346:MET:CE	2.28	0.64
1:B:248:PRO:HD3	1:B:275:GLU:HG3	1.78	0.63
1:F:375:GLU:OE2	1:F:375:GLU:HA	1.98	0.63
1:A:123:GLU:OE2	1:A:348:HIS:CE1	2.51	0.63
1:A:38:ARG:HD2	1:A:48:TRP:CZ2	2.33	0.62
1:G:86:GLN:NE2	1:G:271:ASN:HB3	2.13	0.62
1:A:142:ARG:NH1	1:A:142:ARG:CG	2.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:ARG:NE	4:E:425:HOH:O	2.32	0.62
1:E:205:ARG:NH2	4:E:425:HOH:O	2.34	0.61
1:E:90:GLN:HE22	1:E:246:LYS:HG2	1.67	0.60
1:E:374:TYR:CD2	1:E:375:GLU:HG3	2.36	0.60
1:F:74:GLN:NE2	1:F:76:GLY:H	1.99	0.60
1:G:169:GLU:HG3	1:G:172:ARG:NH2	2.16	0.60
1:F:123:GLU:HB3	1:F:346:MET:HE2	1.83	0.59
1:F:340:LEU:HD11	1:F:347:VAL:HG13	1.85	0.59
1:A:106:LYS:HE3	4:A:473:HOH:O	2.03	0.59
1:D:29:LYS:HD3	1:D:295:TYR:OH	2.03	0.59
1:H:29:LYS:HG2	4:H:565:HOH:O	2.02	0.59
1:F:74:GLN:HE21	1:F:76:GLY:HA3	1.68	0.59
1:D:119:ARG:HG3	1:D:119:ARG:HH11	1.69	0.58
1:E:39:ILE:HD12	1:E:99:ALA:HB3	1.86	0.58
1:C:204:GLU:OE2	1:C:236:SER:OG	2.21	0.58
1:F:4:VAL:HG12	1:F:41:THR:HB	1.85	0.57
1:H:4:VAL:HG13	1:H:42:GLU:HB3	1.84	0.57
1:C:373:ALA:C	1:C:374:TYR:O	2.40	0.57
1:D:52:VAL:CB	4:D:1978:HOH:O	2.52	0.57
1:F:11:THR:HG22	1:F:37:ILE:HG22	1.86	0.57
1:D:35:TYR:OH	1:D:59:HIS:HD2	1.88	0.57
1:B:35:TYR:OH	1:B:59:HIS:HD2	1.87	0.57
1:C:70:LEU:HD21	1:C:85:ILE:HD11	1.86	0.57
1:D:89:HIS:CD2	1:D:91:ARG:HB2	2.39	0.57
1:G:153:LYS:HE2	4:G:1993:HOH:O	2.04	0.57
1:E:90:GLN:HE22	1:E:246:LYS:CG	2.18	0.57
1:F:292:ALA:HB3	1:F:325:ILE:HD12	1.86	0.56
1:D:86:GLN:NE2	1:D:271:ASN:O	2.39	0.55
1:B:248:PRO:HD3	1:B:275:GLU:CG	2.36	0.55
1:F:366:ARG:NH1	1:F:367:TYR:OH	2.37	0.55
1:A:168:LYS:HG3	1:A:172:ARG:NH1	2.21	0.55
1:C:138:GLN:O	1:C:142:ARG:HG2	2.06	0.55
1:F:373:ALA:O	1:F:375:GLU:HB2	2.07	0.54
1:H:65:ARG:NH2	1:H:88:TRP:HB3	2.22	0.54
1:E:90:GLN:NE2	1:E:246:LYS:HG2	2.21	0.54
1:F:374:TYR:HA	1:F:375:GLU:CB	2.37	0.54
1:H:123:GLU:HB3	1:H:346:MET:HE2	1.90	0.54
1:A:348:HIS:N	1:A:348:HIS:CD2	2.76	0.54
1:E:136:SER:HB2	1:E:142:ARG:NH2	2.23	0.53
1:B:299:LEU:HD22	1:B:359:ILE:HD11	1.91	0.53
1:H:83:ARG:HB3	4:H:574:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:GLU:HB3	1:D:346:MET:HE2	1.90	0.52
1:D:205:ARG:NH1	4:D:2031:HOH:O	2.28	0.52
1:E:348:HIS:HB3	4:E:527:HOH:O	2.08	0.52
1:F:17:ARG:HE	1:F:374:TYR:HE1	1.57	0.52
1:C:142:ARG:HD3	4:C:506:HOH:O	2.10	0.52
1:H:191:ALA:HB3	1:H:219:PRO:HA	1.91	0.52
1:F:258:ARG:HD3	4:F:540:HOH:O	2.10	0.52
1:E:353:LYS:HD3	4:E:524:HOH:O	2.10	0.51
1:E:3:LEU:HD12	1:E:4:VAL:H	1.74	0.51
1:C:230:MET:CE	1:F:258:ARG:HD2	2.40	0.51
1:E:111:SER:HB3	1:E:352:GLY:O	2.10	0.51
1:B:248:PRO:CD	1:B:275:GLU:HG3	2.40	0.51
1:D:52:VAL:O	1:D:53:ASP:HB2	2.11	0.50
1:E:123:GLU:OE2	1:E:348:HIS:CE1	2.64	0.50
1:F:138:GLN:OE1	1:F:138:GLN:HA	2.11	0.50
1:E:252:VAL:N	1:E:253:PRO:HD2	2.27	0.49
1:B:248:PRO:HG3	1:B:279:CYS:SG	2.53	0.49
1:G:332:ASN:O	1:G:335:THR:HG22	2.12	0.49
1:B:214:GLY:O	1:B:238:PRO:HG2	2.12	0.49
1:E:136:SER:HB3	1:E:142:ARG:HH22	1.77	0.49
1:F:33:THR:O	1:F:34:CYS:HB2	2.13	0.49
1:H:23:GLY:HA2	1:H:131:GLN:HE21	1.78	0.49
1:G:169:GLU:HG3	1:G:172:ARG:HH21	1.77	0.49
1:A:354:GLY:HA3	4:A:473:HOH:O	2.12	0.48
4:A:474:HOH:O	1:D:205:ARG:HD2	2.12	0.48
1:B:80:SER:O	1:B:84:THR:HG23	2.13	0.48
1:C:114:GLU:OE2	1:D:2:ALA:HB3	2.12	0.48
1:F:5:LYS:HD3	1:F:72:GLY:O	2.14	0.48
1:A:60:VAL:HG22	1:A:64:LYS:CG	2.44	0.48
1:A:374:TYR:O	1:A:375:GLU:CB	2.61	0.48
1:B:90:GLN:HE22	1:B:246:LYS:HB3	1.79	0.48
1:D:90:GLN:HG3	1:D:91:ARG:N	2.29	0.48
1:E:29:LYS:HE2	1:E:131:GLN:NE2	2.29	0.48
1:E:4:VAL:HG13	1:E:42:GLU:HB2	1.95	0.47
1:G:122:GLU:CG	4:G:1907:HOH:O	2.48	0.47
1:G:305:LEU:HB3	1:G:349:ILE:HD11	1.94	0.47
1:H:109:ASP:OD2	4:H:588:HOH:O	2.20	0.47
1:E:74:GLN:HB2	4:E:521:HOH:O	2.14	0.47
1:G:82:VAL:O	1:G:86:GLN:HG3	2.15	0.47
1:H:311:LEU:HD12	1:H:312:PRO:HD2	1.97	0.47
1:B:3:LEU:C	1:B:74:GLN:OE1	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:ARG:CZ	4:E:425:HOH:O	2.63	0.47
1:F:366:ARG:HD3	4:F:522:HOH:O	2.15	0.47
1:H:90:GLN:NE2	1:H:269:HIS:O	2.47	0.47
1:C:111:SER:OG	1:C:114:GLU:HG3	2.15	0.47
1:G:46:ASP:OD1	1:G:106:LYS:NZ	2.48	0.47
1:G:214:GLY:O	1:G:215:TRP:HB3	2.15	0.47
1:A:5:LYS:HB3	1:A:42:GLU:OE2	2.15	0.46
1:G:123:GLU:HB3	1:G:346:MET:CE	2.45	0.46
1:H:55:LEU:HB2	1:H:56:PRO:HD3	1.96	0.46
1:B:4:VAL:HG12	1:B:41:THR:HB	1.96	0.46
1:B:69:PHE:CE1	1:B:73:LYS:HE2	2.51	0.46
1:E:344:LYS:HB2	1:E:344:LYS:HE2	1.64	0.46
1:B:70:LEU:HD21	1:B:85:ILE:HD11	1.97	0.46
1:C:54:TRP:CZ2	1:C:56:PRO:HG2	2.50	0.46
1:D:168:LYS:HB3	1:D:168:LYS:HE2	1.76	0.46
1:G:168:LYS:HG3	1:G:172:ARG:NH1	2.31	0.46
1:A:168:LYS:CG	1:A:172:ARG:NH1	2.74	0.46
1:E:38:ARG:HG3	1:E:48:TRP:CE2	2.51	0.46
1:E:374:TYR:CD2	1:E:375:GLU:CG	2.93	0.46
1:B:331:GLU:OE1	4:B:625:HOH:O	2.20	0.46
1:C:82:VAL:O	1:C:86:GLN:HG3	2.16	0.46
1:E:82:VAL:HG12	1:E:86:GLN:HE21	1.81	0.46
1:A:373:ALA:C	1:A:374:TYR:O	2.45	0.45
1:B:318:LYS:HD2	1:B:318:LYS:HA	1.51	0.45
1:D:94:SER:HA	1:D:272:GLY:HA2	1.97	0.45
1:G:94:SER:HA	1:G:272:GLY:HA2	1.97	0.45
1:B:66:ILE:HD13	1:B:92:ALA:HB1	1.98	0.45
1:C:82:VAL:HG12	1:C:86:GLN:HE21	1.81	0.45
1:E:137:PRO:HB2	1:E:138:GLN:NE2	2.32	0.45
1:E:248:PRO:HG2	1:F:285:TYR:CZ	2.51	0.45
1:G:86:GLN:CD	1:G:271:ASN:HB3	2.37	0.45
1:H:5:LYS:HD3	1:H:72:GLY:O	2.16	0.45
1:H:161:LYS:NZ	1:H:190:ASP:OD2	2.49	0.45
1:B:258:ARG:HG2	4:G:2010:HOH:O	2.17	0.45
1:E:123:GLU:HB3	1:E:346:MET:HE2	1.98	0.45
1:G:123:GLU:HB3	1:G:346:MET:HE2	1.97	0.45
1:B:360:ASN:OD1	1:B:362:GLU:HB2	2.15	0.45
1:H:292:ALA:HB3	1:H:325:ILE:HG12	1.99	0.45
1:A:374:TYR:C	1:A:375:GLU:HG3	2.37	0.45
1:A:194:SER:HA	1:H:316:LYS:HG3	1.98	0.45
1:B:127:TYR:OH	1:B:326:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:VAL:HG21	1:B:276:PHE:HB2	2.00	0.44
1:C:50:GLU:HG2	1:C:268:MET:SD	2.57	0.44
1:E:374:TYR:C	1:E:375:GLU:HG3	2.38	0.44
1:H:139:TRP:HZ2	1:H:169:GLU:HG2	1.82	0.44
1:C:366:ARG:HD2	1:C:367:TYR:CE2	2.52	0.44
1:D:125:PRO:O	1:D:324:PRO:HA	2.18	0.44
1:F:327:TRP:CE2	1:F:342:PRO:HD3	2.52	0.44
1:A:224:GLN:HE22	1:G:252:VAL:HG12	1.81	0.44
1:D:161:LYS:NZ	1:D:190:ASP:OD2	2.48	0.44
1:F:125:PRO:O	1:F:324:PRO:HA	2.18	0.44
1:F:366:ARG:HD2	1:F:367:TYR:CZ	2.52	0.44
1:A:148:GLU:HG3	1:A:180:THR:HG21	1.98	0.44
1:E:224:GLN:NE2	4:E:548:HOH:O	2.44	0.44
1:D:90:GLN:HE22	1:D:270:VAL:C	2.21	0.44
1:E:305:LEU:HD13	1:E:347:VAL:HG11	1.99	0.44
1:F:327:TRP:CZ2	1:F:342:PRO:HD3	2.52	0.44
1:E:305:LEU:HB3	1:E:349:ILE:HD11	2.00	0.44
1:F:86:GLN:CD	1:F:271:ASN:HB3	2.38	0.44
1:E:4:VAL:HG12	1:E:41:THR:HB	1.99	0.44
1:A:50:GLU:HG2	1:A:268:MET:SD	2.58	0.44
1:A:108:ALA:CB	1:B:108:ALA:HB1	2.48	0.44
1:B:78:ARG:O	1:B:82:VAL:HG23	2.17	0.43
1:G:43:SER:OG	1:G:45:ILE:HG13	2.18	0.43
1:E:89:HIS:CE1	1:E:91:ARG:HB2	2.54	0.43
1:E:136:SER:HA	1:E:137:PRO:HD3	1.88	0.43
1:C:292:ALA:HB3	1:C:325:ILE:HG12	2.00	0.43
1:E:90:GLN:HE22	1:E:246:LYS:CD	2.31	0.43
1:A:109:ASP:O	1:A:353:LYS:HE2	2.18	0.43
1:D:4:VAL:HG22	4:D:1860:HOH:O	2.18	0.43
1:D:191:ALA:HB3	1:D:219:PRO:HA	2.01	0.43
1:H:248:PRO:CD	1:H:275:GLU:HG3	2.48	0.43
1:C:94:SER:HA	1:C:272:GLY:HA2	2.00	0.43
1:F:185:ILE:O	1:F:212:ASN:ND2	2.45	0.43
1:H:277:ARG:HD3	4:H:467:HOH:O	2.19	0.43
1:B:125:PRO:O	1:B:324:PRO:HA	2.19	0.43
1:E:91:ARG:HA	1:E:91:ARG:HD3	1.77	0.42
1:D:253:PRO:HG2	4:D:1921:HOH:O	2.19	0.42
1:H:243:GLU:HA	1:H:264:GLN:O	2.19	0.42
1:A:151:LEU:HA	1:A:151:LEU:HD23	1.71	0.42
1:B:224:GLN:HE22	1:D:252:VAL:HG12	1.84	0.42
1:B:257:GLN:O	1:B:258:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:337:LEU:HD23	1:F:337:LEU:HA	1.88	0.42
1:F:29:LYS:HD3	1:F:295:TYR:HH	1.82	0.42
1:B:84:THR:HA	1:B:87:LYS:HD2	2.01	0.42
1:B:160:VAL:HG11	1:B:177:LEU:HD13	2.01	0.42
1:E:123:GLU:HB3	1:E:346:MET:CE	2.49	0.42
1:H:119:ARG:CZ	1:H:122:GLU:HB3	2.50	0.42
1:C:86:GLN:CD	1:C:271:ASN:HB3	2.40	0.42
1:A:66:ILE:HD13	1:A:92:ALA:HB1	2.02	0.42
1:C:305:LEU:HD13	1:C:347:VAL:HG11	2.01	0.42
1:E:138:GLN:O	1:E:142:ARG:HG2	2.19	0.42
1:B:190:ASP:HA	1:B:217:GLU:HB3	2.01	0.42
1:G:136:SER:HA	1:G:137:PRO:HD2	1.78	0.42
1:H:51:CYS:O	1:H:52:VAL:HG23	2.19	0.42
1:C:24:ASP:HB3	1:C:161:LYS:HE3	2.02	0.42
1:C:374:TYR:CD2	1:C:375:GLU:N	2.88	0.42
1:D:367:TYR:O	1:D:368:LYS:C	2.58	0.42
1:H:344:LYS:HE3	1:H:344:LYS:HB2	1.58	0.42
1:A:127:TYR:HB3	1:A:157:GLN:HB2	2.02	0.41
1:C:11:THR:HG22	1:C:37:ILE:HG22	2.01	0.41
1:B:17:ARG:HE	1:B:17:ARG:HB2	1.50	0.41
1:B:140:ILE:O	1:B:144:VAL:HG23	2.20	0.41
1:F:3:LEU:O	1:F:74:GLN:OE1	2.37	0.41
1:G:252:VAL:N	1:G:253:PRO:HD2	2.34	0.41
1:H:168:LYS:HG2	1:H:172:ARG:HH12	1.85	0.41
1:A:124:ILE:HA	1:A:125:PRO:HD2	1.89	0.41
1:E:39:ILE:HD12	1:E:99:ALA:CB	2.50	0.41
1:E:367:TYR:O	1:E:368:LYS:C	2.58	0.41
1:C:227:ASP:HA	1:C:230:MET:HE3	2.01	0.41
1:E:337:LEU:HD23	1:E:363:ILE:HB	2.03	0.41
1:A:5:LYS:HB2	1:A:5:LYS:HE3	1.39	0.41
1:A:90:GLN:OE1	1:A:246:LYS:HG2	2.21	0.41
1:G:148:GLU:OE2	1:G:180:THR:HG21	2.20	0.41
1:B:62:PHE:HA	1:B:66:ILE:HB	2.03	0.41
1:E:144:VAL:HG13	1:E:180:THR:HG21	2.02	0.41
1:G:191:ALA:HB3	1:G:219:PRO:HA	2.03	0.41
1:C:46:ASP:OD1	1:C:46:ASP:N	2.53	0.41
1:A:252:VAL:N	1:A:253:PRO:HD2	2.36	0.41
1:E:30:ARG:NH2	4:E:582:HOH:O	2.42	0.41
1:F:3:LEU:C	1:F:74:GLN:OE1	2.58	0.41
1:F:305:LEU:HD13	1:F:347:VAL:HG11	2.02	0.41
1:H:86:GLN:CD	1:H:271:ASN:HB3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ILE:HD13	1:B:92:ALA:CB	2.50	0.41
1:B:349:ILE:HA	1:B:350:PRO:HD2	1.91	0.41
1:F:74:GLN:NE2	1:F:76:GLY:N	2.69	0.41
1:D:138:GLN:O	1:D:142:ARG:HG3	2.20	0.41
1:B:90:GLN:HE21	1:B:90:GLN:HB2	1.64	0.40
1:D:337:LEU:HD23	1:D:337:LEU:HA	1.90	0.40
1:G:215:TRP:CE3	1:G:262:ILE:HD13	2.56	0.40
1:B:157:GLN:HE22	1:B:324:PRO:HG3	1.86	0.40
1:B:191:ALA:HB3	1:B:219:PRO:HA	2.03	0.40
1:F:168:LYS:HE2	1:F:172:ARG:HH12	1.86	0.40
1:A:24:ASP:HB3	1:A:161:LYS:HE3	2.04	0.40
1:A:234:ARG:NH2	4:A:495:HOH:O	2.54	0.40
1:A:272:GLY:HA3	4:A:519:HOH:O	2.22	0.40
1:D:67:ILE:HB	1:D:68:PRO:HD3	2.03	0.40
1:E:136:SER:CB	1:E:142:ARG:HH22	2.28	0.40
1:H:94:SER:HA	1:H:272:GLY:HA2	2.03	0.40
1:H:240:ALA:HA	1:H:262:ILE:O	2.21	0.40
1:G:52:VAL:O	1:G:53:ASP:HB2	2.20	0.40
1:G:83:ARG:HD2	1:H:120:TYR:HE1	1.87	0.40

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	371/382 (97%)	359 (97%)	12 (3%)	0	100	100
1	B	373/382 (98%)	356 (95%)	17 (5%)	0	100	100
1	C	372/382 (97%)	357 (96%)	15 (4%)	0	100	100
1	D	375/382 (98%)	361 (96%)	14 (4%)	0	100	100
1	E	371/382 (97%)	352 (95%)	18 (5%)	1 (0%)	41	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	373/382 (98%)	353 (95%)	18 (5%)	2 (0%)	29	18
1	G	373/382 (98%)	359 (96%)	14 (4%)	0	100	100
1	H	373/382 (98%)	360 (96%)	13 (4%)	0	100	100
All	All	2981/3056 (98%)	2857 (96%)	121 (4%)	3 (0%)	51	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	74	GLN
1	F	181	ALA
1	F	166	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/323 (98%)	307 (97%)	9 (3%)	43	36
1	B	317/323 (98%)	309 (98%)	8 (2%)	47	41
1	C	316/323 (98%)	304 (96%)	12 (4%)	33	24
1	D	318/323 (98%)	312 (98%)	6 (2%)	57	53
1	E	316/323 (98%)	303 (96%)	13 (4%)	30	21
1	F	318/323 (98%)	312 (98%)	6 (2%)	57	53
1	G	317/323 (98%)	307 (97%)	10 (3%)	39	30
1	H	317/323 (98%)	307 (97%)	10 (3%)	39	30
All	All	2535/2584 (98%)	2461 (97%)	74 (3%)	42	35

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	65	ARG
1	A	138	GLN

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Mol	Chain	Res	Type
1	A	142	ARG
1	A	168	LYS
1	A	208	SER
1	A	209	GLU
1	A	362	GLU
1	A	375	GLU
1	B	42	GLU
1	B	90	GLN
1	B	136	SER
1	B	205	ARG
1	B	208	SER
1	B	275	GLU
1	B	318	LYS
1	B	359	ILE
1	C	3	LEU
1	C	17	ARG
1	C	52	VAL
1	C	65	ARG
1	C	88	TRP
1	C	136	SER
1	C	146	ASN
1	C	236	SER
1	C	318	LYS
1	C	338	VAL
1	C	344	LYS
1	C	375	GLU
1	D	80	SER
1	D	138	GLN
1	D	168	LYS
1	D	180	THR
1	D	318	LYS
1	D	349	ILE
1	E	3	LEU
1	E	19	GLU
1	E	65	ARG
1	E	74	GLN
1	E	94	SER
1	E	122	GLU
1	E	136	SER
1	E	142	ARG
1	E	168	LYS
1	E	358	GLU

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Mol	Chain	Res	Type
1	E	363	ILE
1	E	366	ARG
1	E	375	GLU
1	F	3	LEU
1	F	91	ARG
1	F	136	SER
1	F	179	HIS
1	F	288	VAL
1	F	375	GLU
1	G	3	LEU
1	G	4	VAL
1	G	60	VAL
1	G	65	ARG
1	G	80	SER
1	G	90	GLN
1	G	146	ASN
1	G	168	LYS
1	G	180	THR
1	G	225	PRO
1	H	19	GLU
1	H	29	LYS
1	H	74	GLN
1	H	88	TRP
1	H	132	SER
1	H	208	SER
1	H	275	GLU
1	H	349	ILE
1	H	353	LYS
1	H	372	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	146	ASN
1	A	224	GLN
1	A	341	GLN
1	B	59	HIS
1	B	89	HIS
1	B	90	GLN
1	B	157	GLN
1	B	192	ASN

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Mol	Chain	Res	Type
1	B	348	HIS
1	C	59	HIS
1	C	86	GLN
1	C	90	GLN
1	C	224	GLN
1	C	281	GLN
1	C	365	ASN
1	D	59	HIS
1	D	86	GLN
1	D	89	HIS
1	D	90	GLN
1	D	131	GLN
1	D	138	GLN
1	D	226	GLN
1	D	281	GLN
1	D	365	ASN
1	E	74	GLN
1	E	86	GLN
1	E	90	GLN
1	E	131	GLN
1	E	250	GLN
1	E	257	GLN
1	E	281	GLN
1	E	348	HIS
1	F	226	GLN
1	G	146	ASN
1	G	226	GLN
1	G	244	ASN
1	G	281	GLN
1	H	74	GLN
1	H	90	GLN
1	H	131	GLN
1	H	226	GLN
1	H	281	GLN
1	H	365	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 11 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	373/382 (97%)	-0.29	5 (1%)	77	79	10, 20, 35, 55	0
1	B	374/382 (97%)	-0.29	3 (0%)	86	87	13, 21, 34, 51	0
1	C	374/382 (97%)	-0.15	8 (2%)	63	66	14, 26, 42, 55	0
1	D	376/382 (98%)	-0.41	3 (0%)	86	87	10, 19, 32, 42	0
1	E	373/382 (97%)	-0.16	5 (1%)	77	79	12, 24, 41, 69	0
1	F	373/382 (97%)	0.04	14 (3%)	40	43	17, 32, 49, 69	0
1	G	374/382 (97%)	-0.22	7 (1%)	66	69	14, 23, 37, 64	0
1	H	374/382 (97%)	-0.20	7 (1%)	66	69	13, 24, 42, 62	0
All	All	2991/3056 (97%)	-0.21	52 (1%)	70	72	10, 23, 42, 69	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	374	TYR	5.3
1	A	3	LEU	5.3
1	E	374	TYR	5.3
1	C	88	TRP	4.9
1	A	374	TYR	4.7
1	E	375	GLU	4.6
1	F	375	GLU	4.6
1	H	375	GLU	4.4
1	F	88	TRP	4.3
1	A	4	VAL	4.1
1	G	3	LEU	4.0
1	H	88	TRP	4.0
1	B	3	LEU	3.8
1	G	373	ALA	3.7
1	G	2	ALA	3.4
1	A	88	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	179	HIS	3.1
1	B	375	GLU	3.1
1	F	362	GLU	3.0
1	G	375	GLU	2.9
1	E	88	TRP	2.9
1	D	2	ALA	2.9
1	G	374	TYR	2.9
1	C	2	ALA	2.8
1	E	373	ALA	2.8
1	F	372	SER	2.7
1	F	135	ASP	2.6
1	H	374	TYR	2.6
1	B	2	ALA	2.6
1	F	366	ARG	2.6
1	D	90	GLN	2.5
1	C	137	PRO	2.5
1	F	19	GLU	2.4
1	H	19	GLU	2.4
1	C	20	LYS	2.4
1	A	137	PRO	2.4
1	D	3	LEU	2.3
1	F	371	GLY	2.3
1	F	74	GLN	2.3
1	H	372	SER	2.3
1	F	373	ALA	2.2
1	F	138	GLN	2.2
1	E	372	SER	2.2
1	H	319	ASN	2.2
1	C	374	TYR	2.1
1	C	19	GLU	2.1
1	F	4	VAL	2.1
1	C	373	ALA	2.1
1	C	370	ASP	2.1
1	G	319	ASN	2.0
1	H	160	VAL	2.0
1	G	209	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	MG	H	400	1/1	0.96	0.10	23,23,23,23	0
2	MG	B	400	1/1	0.99	0.07	15,15,15,15	0
2	MG	C	400	1/1	0.99	0.04	23,23,23,23	0
2	MG	D	400	1/1	0.99	0.04	14,14,14,14	0
2	MG	E	400	1/1	0.99	0.10	20,20,20,20	0
2	MG	F	400	1/1	0.99	0.02	25,25,25,25	0
2	MG	G	400	1/1	0.99	0.10	20,20,20,20	0
2	MG	A	400	1/1	0.99	0.11	23,23,23,23	0
3	CL	D	1802	1/1	0.99	0.07	28,28,28,28	0
3	CL	G	1803	1/1	0.99	0.14	29,29,29,29	0
3	CL	D	1801	1/1	1.00	0.08	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.