



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:41 PM UTC

PDB ID : 2GGE / pdb_00002gge
Title : Crystal Structure of Mandelate Racemase/Muconate Lactonizing Enzyme from *Bacillus Subtilis* complexed with MG++ at 1.8 Å
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 ⓘ 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
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)

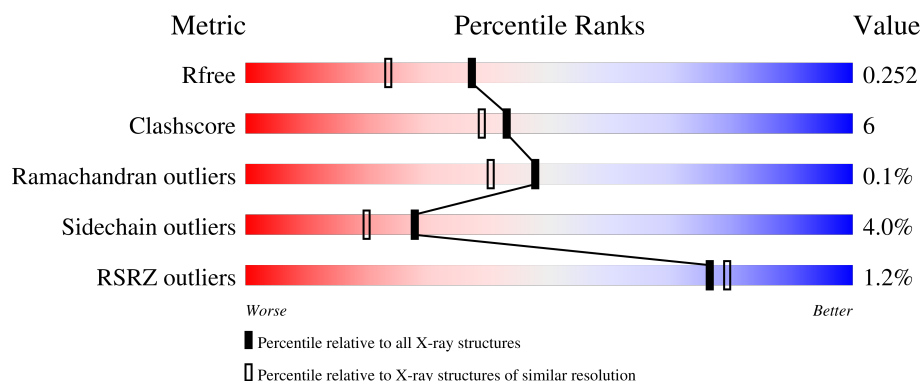
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 $\leq 5\%$. 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	382	% 80% 16% ..
1	B	382	79% 18% ..
1	C	382	% 81% 15% ..

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	382	83%13%
1	E	382	2% 79%17%
1	F	382	3% 81%14%
1	G	382	% 83%13%
1	H	382	% 80%16%

2 Entry composition

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

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 (CCD ID: 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 (CCD ID: 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

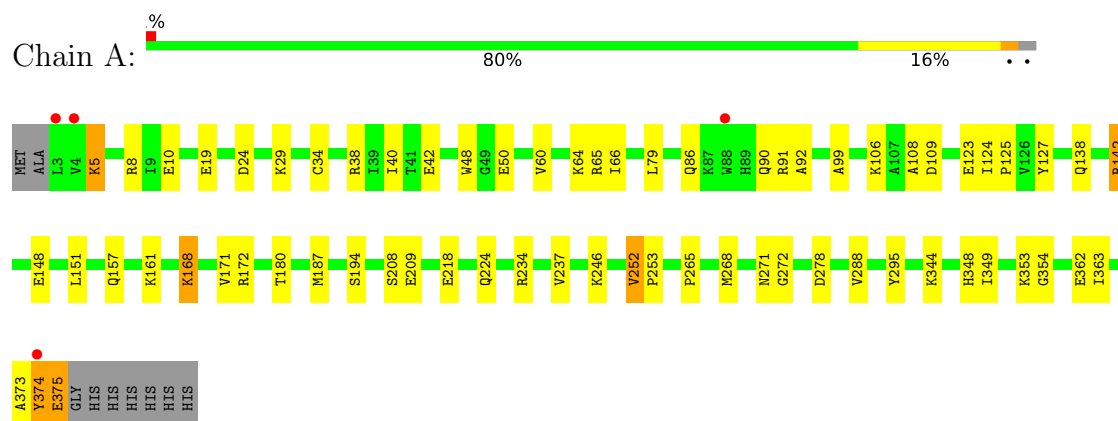
- Molecule 4 is water.

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

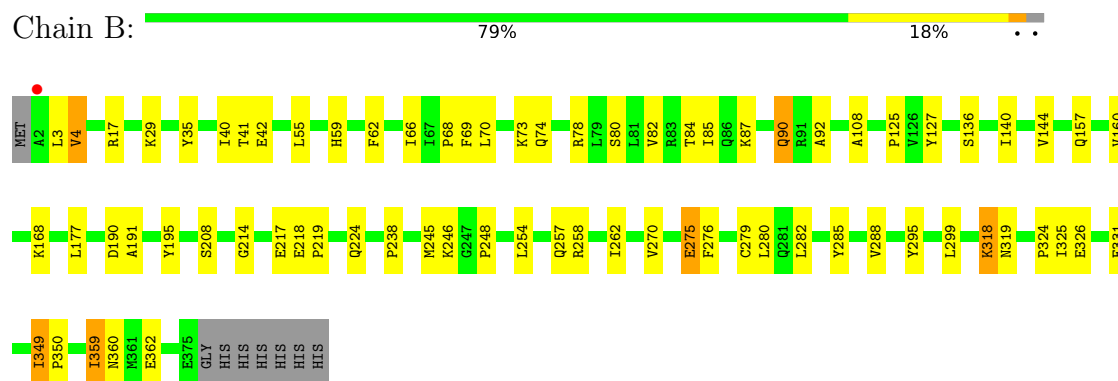
3 Residue-property plots [i](#)

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.

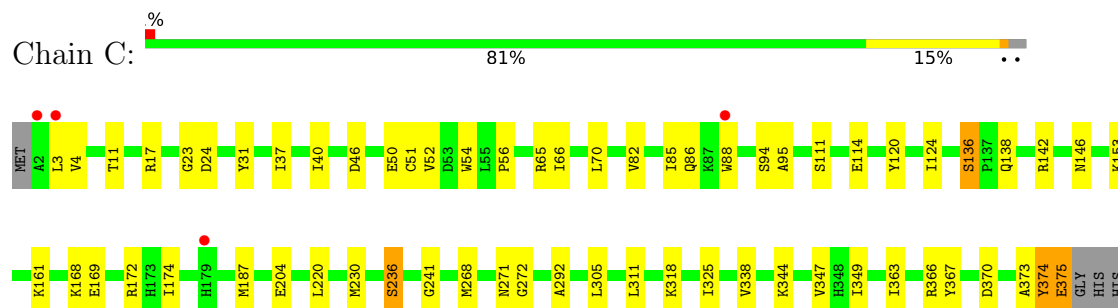
• Molecule 1: yitF



• Molecule 1: yitF



• Molecule 1: yitF



HIS
HIS
HIS
HIS

• Molecule 1: yitF

Chain D:  83% 13% ..

MET A2 L3 V4 K20 K29 Y35 E42 V52 D53 L58 H59 K64 I67 P68 S80 Q86 H89 Q90 R91 S94 A99 V112 R119 E123 I124 P125 A128 Q138 R142 K161 K168 T180 D190 A191 A200

R205 P219 F222 G241 G247 V251 V252 P253 V267 V270 N271 G272 V288 Y295 L305 K318 P324 L337 M346 T349 R366 Y367 K368 A373 H377 HIS HIS HIS HIS

• Molecule 1: yitF

Chain E:  79% 17% ...

MET ALA L3 V4 R8 E19 G23 K29 R30 R38 L39 T40 T41 E42 V48 G49 E50 K64 R65 Q74 V82 Q86 R87 R88 R89 Q90 R91 S94 N98 A99 A105 S111 E122 E123 F130 Q131 S136 P137 Q138 R142 S143 V144

S145 M146 V147 E148 K168 T180 M187 A197 R205 E218 Q224 A240 G241 K246 G247 P248 V252 P253 G272 Q281 L282 Y285 V288 L305 I325 L337 V338 K344 G345 M346 V347 H348 T349 G352 K353 E358 T363 R366

Y367 K368 A373 Y374 E375 GLY HIS HIS HIS HIS HIS HIS

• Molecule 1: yitF

Chain F:  81% 14% ..

MET ALA L3 V4 K5 T11 R17 G23 K29 T33 C34 I37 T41 L55 P56 G72 K73 Q74 G76 Q86 R87 R88 R89 Q90 E114 R119 E123 I124 P125 S136 P137 Q138 W139 I140 A149 I158 S166 F167 K168 R172

H179 T180 G181 G182 S183 S184 I185 T186 M187 N212 E218 F219 L220 V252 R258 C259 N271 R65 G272 Y285 V288 A292 Y295 L305 K318 P324 I325 E326 W327 L337 L340 Q341 P342 M346 V347 H348 T349 R366 Y367 K368 A373 Y374 E375 GLY

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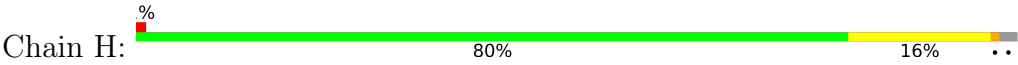
• Molecule 1: yitF

Chain G:  83% 13% ..

MET A2 L3 V4 I9 K20 P21 K29 S43 G44 I45 D46 V52 D53 V60 K64 R65 I66 I67 S80 L81 V82 R83 Q86 R87 W88 S94 N98 K106 E122 E123 I124 S136 P137 M146 V147 E148 K153 T165 K168 E169



● Molecule 1: yitF



4 Data and refinement statistics

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 – 1.89	Depositor EDS
% Data completeness (in resolution range)	85.7 (27.95-1.89) 86.0 (27.95-1.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.29%)	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)	0.37 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	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.*

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

5.1 Standard geometry

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

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	1.36	9/3058 (0.3%)	1.23	4/4145 (0.1%)
1	B	1.32	7/3069 (0.2%)	1.19	4/4160 (0.1%)
1	C	1.21	3/3063 (0.1%)	1.19	11/4152 (0.3%)
1	D	1.36	14/3084 (0.5%)	1.24	12/4180 (0.3%)
1	E	1.26	6/3058 (0.2%)	1.18	8/4145 (0.2%)
1	F	1.10	3/3070 (0.1%)	1.10	7/4161 (0.2%)
1	G	1.31	8/3074 (0.3%)	1.18	10/4167 (0.2%)
1	H	1.25	3/3069 (0.1%)	1.18	9/4160 (0.2%)
All	All	1.27	53/24545 (0.2%)	1.19	65/33270 (0.2%)

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 (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	252	VAL	CA-CB	10.08	1.59	1.54
1	G	252	VAL	CA-CB	9.42	1.59	1.54
1	D	200	ALA	CA-CB	-7.57	1.41	1.53
1	C	124	ILE	CA-CB	7.46	1.60	1.54
1	C	174	ILE	CA-CB	7.14	1.63	1.54
1	F	252	VAL	CA-CB	7.05	1.57	1.54
1	E	240	ALA	CA-CB	6.80	1.65	1.53
1	D	288	VAL	CA-CB	6.75	1.65	1.55
1	A	237	VAL	CA-CB	6.69	1.62	1.54
1	A	252	VAL	CA-CB	6.51	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	LEU	C-O	-6.35	1.16	1.24
1	G	218	GLU	CA-CB	6.25	1.58	1.52
1	B	349	ILE	CA-CB	6.19	1.64	1.54
1	E	23	GLY	N-CA	-6.06	1.38	1.45
1	E	105	ALA	CA-C	6.06	1.60	1.52
1	B	40	ILE	CA-CB	5.92	1.61	1.54
1	E	282	LEU	N-CA	5.87	1.53	1.46
1	D	67	ILE	CA-CB	-5.86	1.51	1.54
1	B	4	VAL	CA-C	5.78	1.59	1.52
1	D	128	ALA	CA-CB	5.76	1.61	1.53
1	B	218	GLU	C-O	-5.74	1.21	1.23
1	D	241	GLY	N-CA	5.73	1.51	1.45
1	E	218	GLU	N-CA	5.70	1.50	1.46
1	E	130	PHE	C-O	5.68	1.30	1.23
1	A	265	PRO	C-O	5.66	1.30	1.23
1	G	218	GLU	N-CA	5.58	1.50	1.46
1	D	267	VAL	CA-CB	-5.58	1.47	1.54
1	G	124	ILE	CA-CB	5.54	1.58	1.54
1	C	40	ILE	CA-CB	5.43	1.61	1.54
1	D	90	GLN	C-O	5.41	1.30	1.24
1	H	318	LYS	CA-C	5.39	1.60	1.52
1	B	262	ILE	CA-CB	5.38	1.61	1.54
1	B	55	LEU	C-O	-5.37	1.19	1.24
1	A	171	VAL	CA-CB	5.35	1.61	1.54
1	D	349	ILE	CA-CB	5.30	1.62	1.54
1	A	218	GLU	CA-CB	5.28	1.57	1.52
1	D	305	LEU	CA-C	5.27	1.59	1.52
1	A	99	ALA	N-CA	5.26	1.52	1.46
1	F	325	ILE	CA-CB	5.24	1.62	1.54
1	D	42	GLU	C-O	-5.22	1.18	1.24
1	F	140	ILE	CA-CB	5.22	1.60	1.54
1	D	99	ALA	C-O	5.21	1.30	1.24
1	D	124	ILE	CA-CB	5.19	1.58	1.54
1	H	189	LEU	N-CA	5.17	1.52	1.46
1	D	373	ALA	CA-CB	-5.16	1.44	1.53
1	G	263	ILE	CA-CB	5.13	1.61	1.54
1	G	94	SER	CA-C	5.10	1.59	1.52
1	A	288	VAL	C-O	5.06	1.29	1.23
1	G	252	VAL	C-O	-5.05	1.20	1.24
1	A	34	CYS	CB-SG	-5.04	1.64	1.81
1	D	20	LYS	CA-C	5.03	1.56	1.52
1	G	363	ILE	CA-CB	5.02	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	ILE	CA-CB	5.01	1.60	1.54

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	TYR	N-CA-C	-10.95	96.00	110.24
1	H	218	GLU	CA-C-N	-8.83	110.64	119.56
1	H	218	GLU	C-N-CA	-8.83	110.64	119.56
1	H	252	VAL	CA-C-N	-8.35	111.13	119.56
1	H	252	VAL	C-N-CA	-8.35	111.13	119.56
1	D	349	ILE	N-CA-CB	-8.25	101.01	110.17
1	D	349	ILE	CB-CA-C	8.15	120.05	110.68
1	A	363	ILE	N-CA-C	-7.88	103.17	110.82
1	B	4	VAL	N-CA-C	7.39	119.34	109.37
1	A	79	LEU	CA-C-N	7.31	129.95	120.44
1	A	79	LEU	C-N-CA	7.31	129.95	120.44
1	C	311	LEU	CA-C-N	-6.90	113.27	120.38
1	C	311	LEU	C-N-CA	-6.90	113.27	120.38
1	C	23	GLY	N-CA-C	6.78	121.23	111.12
1	C	349	ILE	CA-C-N	6.71	127.08	119.83
1	C	349	ILE	C-N-CA	6.71	127.08	119.83
1	C	120	TYR	N-CA-C	-6.54	105.12	113.23
1	D	58	LEU	N-CA-C	-6.52	104.25	111.36
1	F	272	GLY	N-CA-C	6.49	120.86	112.68
1	G	20	LYS	CA-C-N	6.42	126.44	119.89
1	G	20	LYS	C-N-CA	6.42	126.44	119.89
1	E	136	SER	CA-C-N	6.34	126.03	119.56
1	E	136	SER	C-N-CA	6.34	126.03	119.56
1	F	23	GLY	N-CA-C	6.34	121.85	111.27
1	G	9	ILE	N-CA-C	6.28	116.92	107.75
1	D	349	ILE	CA-CB-CG2	6.23	121.09	110.50
1	D	241	GLY	N-CA-C	6.15	118.87	110.69
1	C	4	VAL	N-CA-C	6.08	117.95	112.17
1	G	21	PRO	CB-CA-C	-6.08	103.61	111.39
1	H	323	GLU	CA-C-N	-6.05	114.53	120.52
1	H	323	GLU	C-N-CA	-6.05	114.53	120.52
1	B	319	ASN	N-CA-C	6.03	120.77	113.17
1	D	295	TYR	N-CA-C	-5.96	104.70	111.14
1	F	259	CYS	N-CA-C	5.95	118.72	111.82
1	E	148	GLU	N-CA-C	-5.93	104.90	111.36
1	D	247	GLY	CA-C-N	5.92	125.13	118.97
1	D	247	GLY	C-N-CA	5.92	125.13	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	222	PHE	N-CA-C	5.85	120.05	113.02
1	B	282	LEU	N-CA-C	-5.84	104.83	111.07
1	E	241	GLY	N-CA-C	5.81	119.00	110.80
1	H	191	ALA	N-CA-C	5.76	120.31	113.28
1	E	197	ALA	N-CA-C	5.61	117.84	111.11
1	E	252	VAL	N-CA-C	-5.59	105.64	112.35
1	C	374	TYR	N-CA-C	-5.59	98.89	110.80
1	D	67	ILE	CA-C-N	-5.56	113.17	119.28
1	D	67	ILE	C-N-CA	-5.56	113.17	119.28
1	C	241	GLY	N-CA-C	5.55	118.07	110.69
1	C	124	ILE	CB-CA-C	-5.48	104.81	110.13
1	G	136	SER	CA-C-N	5.38	125.05	119.56
1	G	136	SER	C-N-CA	5.38	125.05	119.56
1	H	247	GLY	CA-C-N	5.36	125.43	119.32
1	H	247	GLY	C-N-CA	5.36	125.43	119.32
1	F	218	GLU	O-C-N	5.33	123.98	121.53
1	F	4	VAL	N-CA-C	5.33	116.12	108.93
1	C	169	GLU	N-CA-C	5.28	117.11	111.36
1	G	366	ARG	N-CA-C	5.26	117.02	111.28
1	B	195	TYR	N-CA-C	5.24	118.53	110.42
1	E	285	TYR	N-CA-C	5.21	117.70	111.71
1	D	112	VAL	N-CA-C	5.19	115.81	110.36
1	G	67	ILE	N-CA-CB	5.13	114.45	110.45
1	F	183	SER	N-CA-C	5.10	119.26	113.19
1	F	179	HIS	N-CA-C	-5.04	106.44	112.59
1	G	4	VAL	N-CA-C	5.04	119.82	109.34
1	E	272	GLY	N-CA-C	5.00	117.89	112.29
1	G	64	LYS	N-CA-C	5.00	119.45	112.90

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 ⓘ

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	43	0
1	B	2990	0	2944	40	0
1	C	2984	0	2940	28	0
1	D	3004	0	2954	34	0
1	E	2979	0	2935	56	0
1	F	2991	0	2943	40	0
1	G	2994	0	2946	32	0
1	H	2990	0	2944	32	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	294	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 (294) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:146:ASN:CG	4:E:601:HOH:O	2.29	0.73
1:E:374:TYR:HD2	1:E:375:GLU:HG3	1.52	0.72
1:D:86:GLN:CD	1:D:271:ASN:HB3	2.15	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: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: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:HE2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:373:ALA:C	1:C:374:TYR:O	2.40	0.62
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:H:123:GLU:HB3	1:H:346:MET:HE2	1.84	0.59
1:F:340:LEU:HD11	1:F:347:VAL:HG13	1.85	0.59
1:G:98:MET:HE2	1:G:267:VAL:HG12	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:C:204:GLU:OE2	1:C:236:SER:OG	2.21	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: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: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:B:245:MET:HE3	1:B:254:LEU:HD11	1.88	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:G:98:MET:HE2	1:G:267:VAL:CG1	2.38	0.54
1:E:90:GLN:NE2	1:E:246:LYS:HG2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:374:TYR:HA	1:F:375:GLU:CB	2.37	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:D:123:GLU:HB3	1:D:346:MET:HE2	1.90	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
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:B:3:LEU:C	1:B:74:GLN:OE1	2.53	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:A:373:ALA:C	1:A:374:TYR:O	2.45	0.50
1:F:138:GLN:OE1	1:F:138:GLN:HA	2.11	0.50
1:G:86:GLN:CD	1:G:271:ASN:HB3	2.37	0.50
1:A:374:TYR:C	1:A:375:GLU:HG3	2.37	0.49
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:E:374:TYR:C	1:E:375:GLU:HG3	2.38	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:D:90:GLN:HE22	1:D:270:VAL:C	2.21	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:F:86:GLN:CD	1:F:271:ASN:HB3	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASP:OD2	1:B:285:TYR:OH	2.28	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:E:123:GLU:HB3	1:E:346:MET:HE2	1.96	0.47
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:86:GLN:CD	1:C:271:ASN:HB3	2.40	0.47
1:C:111:SER:OG	1:C:114:GLU:HG3	2.15	0.47
1:D:346:MET:HE3	1:D:346:MET:HB3	1.71	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:D:367:TYR:O	1:D:368:LYS:C	2.58	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:E:367:TYR:O	1:E:368:LYS:C	2.58	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:H:86:GLN:CD	1:H:271:ASN:HB3	2.40	0.46
1:D:161:LYS:NZ	1:D:190:ASP:OD2	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:LEU:C	1:F:74:GLN:OE1	2.58	0.46
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:F:158:ILE:HD11	1:F:187:MET:HE2	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: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:187:MET:HE3	1:E:187:MET:HB2	1.70	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: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
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:H:139:TRP:HZ2	1:H:169:GLU:HG2	1.82	0.44
1:C:136:SER:C	1:C:138:GLN:H	2.25	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: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: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: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:A:86:GLN:CD	1:A:271:ASN:HB3	2.43	0.43
1:C:136:SER:C	1:C:138:GLN:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:337:LEU:HD23	1:F:337:LEU:HA	1.88	0.42
1:C:31:TYR:CD2	1:C:31:TYR:C	2.97	0.42
1:E:50:GLU:O	1:E:98:MET:HE1	2.18	0.42
1:G:187:MET:HE3	1:G:187:MET:HB2	1.90	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: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:G:123:GLU:HB3	1:G:346:MET:HE2	2.01	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:C:370:ASP:OD1	1:C:370:ASP:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:187:MET:HE3	1:C:187:MET:HB2	1.95	0.41
1:E:39:ILE:HD12	1:E:99:ALA:CB	2.50	0.41
1:A:187:MET:HE3	1:A:187:MET:HB2	1.96	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:F:367:TYR:O	1:F:368:LYS:C	2.64	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:305:LEU:HD13	1:F:347:VAL:HG11	2.02	0.41
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:H:15:PHE:CD2	1:H:15:PHE:C	2.99	0.41
1:B:90:GLN:HE21	1:B:90:GLN:HB2	1.64	0.40
1:D:251:TYR:O	1:D:252:VAL:C	2.62	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:55:LEU:O	1:F:56:PRO:C	2.64	0.40
1:F:168:LYS:HE2	1:F:172:ARG:HH12	1.86	0.40
1:H:367:TYR:O	1:H:368:LYS:C	2.65	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

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	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%)	36	29
1	F	373/382 (98%)	353 (95%)	18 (5%)	2 (0%)	24	16
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%)	48	40

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

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%)	304 (96%)	12 (4%)	29	21
1	B	317/323 (98%)	306 (96%)	11 (4%)	32	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	316/323 (98%)	299 (95%)	17 (5%)	20	12
1	D	318/323 (98%)	308 (97%)	10 (3%)	35	29
1	E	316/323 (98%)	298 (94%)	18 (6%)	18	11
1	F	318/323 (98%)	308 (97%)	10 (3%)	35	29
1	G	317/323 (98%)	306 (96%)	11 (4%)	32	24
1	H	317/323 (98%)	305 (96%)	12 (4%)	29	21
All	All	2535/2584 (98%)	2434 (96%)	101 (4%)	28	20

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	19	GLU
1	A	65	ARG
1	A	138	GLN
1	A	142	ARG
1	A	168	LYS
1	A	208	SER
1	A	209	GLU
1	A	344	LYS
1	A	349	ILE
1	A	362	GLU
1	A	375	GLU
1	B	42	GLU
1	B	68	PRO
1	B	90	GLN
1	B	136	SER
1	B	168	LYS
1	B	208	SER
1	B	275	GLU
1	B	288	VAL
1	B	318	LYS
1	B	325	ILE
1	B	359	ILE
1	C	3	LEU
1	C	17	ARG
1	C	52	VAL
1	C	65	ARG
1	C	66	ILE
1	C	88	TRP

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Mol	Chain	Res	Type
1	C	136	SER
1	C	146	ASN
1	C	153	LYS
1	C	168	LYS
1	C	220	LEU
1	C	236	SER
1	C	318	LYS
1	C	338	VAL
1	C	344	LYS
1	C	363	ILE
1	C	375	GLU
1	D	4	VAL
1	D	52	VAL
1	D	64	LYS
1	D	80	SER
1	D	119	ARG
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	205	ARG
1	E	288	VAL
1	E	325	ILE
1	E	338	VAL
1	E	349	ILE
1	E	358	GLU
1	E	363	ILE
1	E	366	ARG
1	E	375	GLU
1	F	3	LEU
1	F	90	GLN
1	F	119	ARG

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Mol	Chain	Res	Type
1	F	136	SER
1	F	168	LYS
1	F	179	HIS
1	F	220	LEU
1	F	288	VAL
1	F	318	LYS
1	F	375	GLU
1	G	3	LEU
1	G	4	VAL
1	G	52	VAL
1	G	60	VAL
1	G	65	ARG
1	G	80	SER
1	G	146	ASN
1	G	168	LYS
1	G	180	THR
1	G	225	PRO
1	G	338	VAL
1	H	19	GLU
1	H	29	LYS
1	H	64	LYS
1	H	74	GLN
1	H	88	TRP
1	H	132	SER
1	H	148	GLU
1	H	168	LYS
1	H	325	ILE
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 (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	226	GLN
1	A	257	GLN
1	A	365	ASN
1	B	59	HIS
1	B	90	GLN
1	B	157	GLN
1	B	192	ASN

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Mol	Chain	Res	Type
1	B	244	ASN
1	B	348	HIS
1	C	86	GLN
1	C	150	GLN
1	C	192	ASN
1	C	281	GLN
1	C	365	ASN
1	D	16	HIS
1	D	59	HIS
1	D	90	GLN
1	D	138	GLN
1	D	150	GLN
1	D	192	ASN
1	D	224	GLN
1	D	226	GLN
1	D	250	GLN
1	D	281	GLN
1	D	341	GLN
1	D	365	ASN
1	E	86	GLN
1	E	89	HIS
1	E	90	GLN
1	E	131	GLN
1	E	138	GLN
1	E	150	GLN
1	E	192	ASN
1	E	250	GLN
1	E	281	GLN
1	E	348	HIS
1	E	365	ASN
1	F	157	GLN
1	F	224	GLN
1	F	281	GLN
1	F	360	ASN
1	G	74	GLN
1	G	89	HIS
1	G	146	ASN
1	G	192	ASN
1	G	244	ASN
1	H	74	GLN
1	H	90	GLN
1	H	131	GLN

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Mol	Chain	Res	Type
1	H	192	ASN
1	H	244	ASN
1	H	319	ASN
1	H	341	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 oligosaccharides 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 ⓘ

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	373/382 (97%)	-0.42	4 (1%) 78 80	10, 20, 35, 55	0
1	B	374/382 (97%)	-0.45	1 (0%) 90 91	9, 21, 34, 51	1 (0%)
1	C	374/382 (97%)	-0.20	4 (1%) 78 80	14, 26, 42, 55	0
1	D	376/382 (98%)	-0.53	1 (0%) 90 91	8, 19, 32, 42	1 (0%)
1	E	373/382 (97%)	-0.26	6 (1%) 70 74	12, 24, 41, 69	0
1	F	373/382 (97%)	0.09	12 (3%) 50 54	14, 32, 49, 69	2 (0%)
1	G	374/382 (97%)	-0.27	4 (1%) 78 80	13, 23, 37, 64	1 (0%)
1	H	374/382 (97%)	-0.30	4 (1%) 78 80	12, 24, 42, 62	1 (0%)
All	All	2991/3056 (97%)	-0.29	36 (1%) 76 79	8, 23, 42, 69	6 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	4.4
1	A	4	VAL	4.0
1	F	374	TYR	3.5
1	E	374	TYR	3.5
1	H	375	GLU	3.4
1	F	88	TRP	3.4
1	F	179	HIS	3.3
1	A	374	TYR	3.2
1	A	3	LEU	3.2
1	G	2	ALA	3.2
1	F	149	ALA	3.1
1	C	88	TRP	2.9
1	E	88	TRP	2.9
1	F	375	GLU	2.8
1	F	3	LEU	2.7
1	H	88	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	4	VAL	2.6
1	A	88	TRP	2.6
1	B	2	ALA	2.5
1	G	165	THR	2.5
1	C	179	HIS	2.5
1	E	3	LEU	2.4
1	E	375	GLU	2.3
1	F	180	THR	2.3
1	F	140	ILE	2.2
1	F	74	GLN	2.2
1	F	349	ILE	2.2
1	H	90	GLN	2.2
1	E	373	ALA	2.2
1	F	373	ALA	2.2
1	G	373	ALA	2.2
1	E	90	GLN	2.1
1	H	319	ASN	2.1
1	D	90	GLN	2.1
1	C	3	LEU	2.0
1	G	88	TRP	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($\text{\AA}^2$)	Q<0.9
2	MG	H	400	1/1	0.97	0.04	23,23,23,23	0
3	CL	D	1802	1/1	0.97	0.05	28,28,28,28	0
2	MG	D	400	1/1	0.98	0.02	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	G	400	1/1	0.98	0.06	20,20,20,20	0
2	MG	A	400	1/1	0.98	0.05	23,23,23,23	0
2	MG	B	400	1/1	0.98	0.02	15,15,15,15	0
3	CL	G	1803	1/1	0.98	0.11	29,29,29,29	0
2	MG	E	400	1/1	0.99	0.05	20,20,20,20	0
3	CL	D	1801	1/1	0.99	0.03	23,23,23,23	0
2	MG	F	400	1/1	0.99	0.02	25,25,25,25	0
2	MG	C	400	1/1	0.99	0.02	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.