



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:23 PM GMT

PDB ID : 4GWH  
Title : Crystal structure of acyl-CoA thioesterase tesB from Yersinia pestis  
Authors : Swarbrick, C.M.D.; Forwood, J.K.  
Deposited on : 2012-09-03  
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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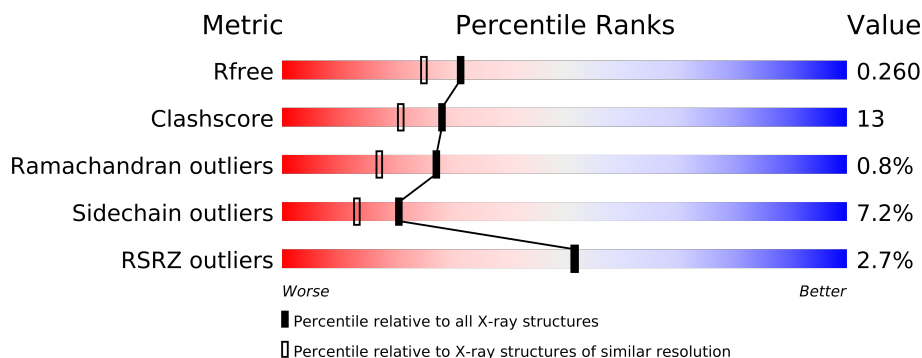
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	288	
1	B	288	
1	C	288	
1	D	288	
1	E	288	
1	F	288	
1	G	288	
1	H	288	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17725 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Acyl-CoA thioesterase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	28	0	0
			2097	1334	367	389	7			
1	B	275	Total	C	N	O	S	11	0	0
			2199	1398	387	407	7			
1	C	269	Total	C	N	O	S	15	0	0
			2154	1371	377	399	7			
1	D	268	Total	C	N	O	S	30	0	0
			2139	1358	376	398	7			
1	E	270	Total	C	N	O	S	11	0	0
			2150	1367	377	399	7			
1	F	265	Total	C	N	O	S	24	0	0
			2112	1342	370	393	7			
1	G	268	Total	C	N	O	S	26	0	0
			2138	1359	375	397	7			
1	H	269	Total	C	N	O	S	13	0	0
			2147	1364	377	399	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	SER	-	EXPRESSION TAG	UNP Q0WCE2
A	288	ASN	-	EXPRESSION TAG	UNP Q0WCE2
B	287	SER	-	EXPRESSION TAG	UNP Q0WCE2
B	288	ASN	-	EXPRESSION TAG	UNP Q0WCE2
C	287	SER	-	EXPRESSION TAG	UNP Q0WCE2
C	288	ASN	-	EXPRESSION TAG	UNP Q0WCE2
D	287	SER	-	EXPRESSION TAG	UNP Q0WCE2
D	288	ASN	-	EXPRESSION TAG	UNP Q0WCE2
E	287	SER	-	EXPRESSION TAG	UNP Q0WCE2
E	288	ASN	-	EXPRESSION TAG	UNP Q0WCE2
F	287	SER	-	EXPRESSION TAG	UNP Q0WCE2
F	288	ASN	-	EXPRESSION TAG	UNP Q0WCE2
G	287	SER	-	EXPRESSION TAG	UNP Q0WCE2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	288	ASN	-	EXPRESSION TAG	UNP Q0WCE2
H	287	SER	-	EXPRESSION TAG	UNP Q0WCE2
H	288	ASN	-	EXPRESSION TAG	UNP Q0WCE2

- Molecule 2 is water.

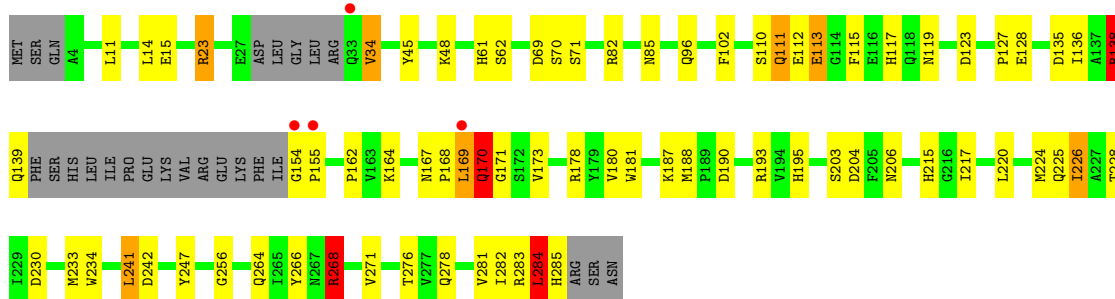
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	68	Total O 68 68	0	0
2	B	82	Total O 82 82	0	0
2	C	67	Total O 67 67	0	0
2	D	89	Total O 89 89	0	0
2	E	74	Total O 74 74	0	0
2	F	59	Total O 59 59	0	0
2	G	80	Total O 80 80	0	0
2	H	70	Total O 70 70	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

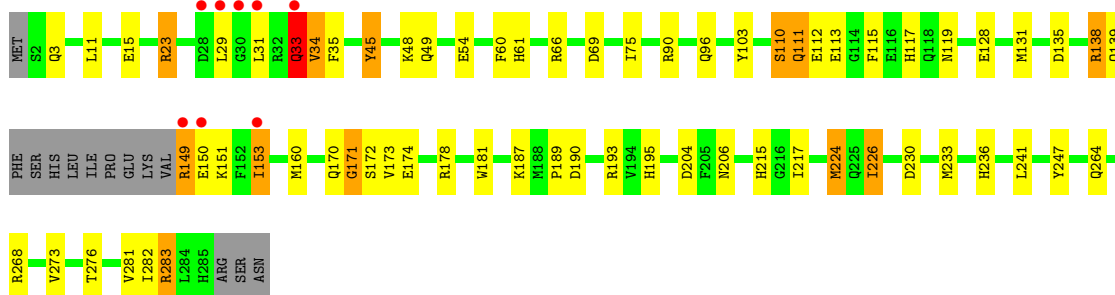
#### • Molecule 1: Acyl-CoA thioesterase II

Chain A: 



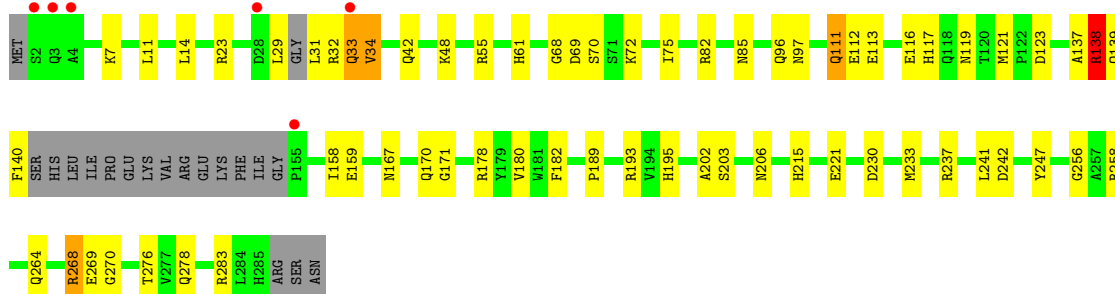
#### • Molecule 1: Acyl-CoA thioesterase II

Chain B: 



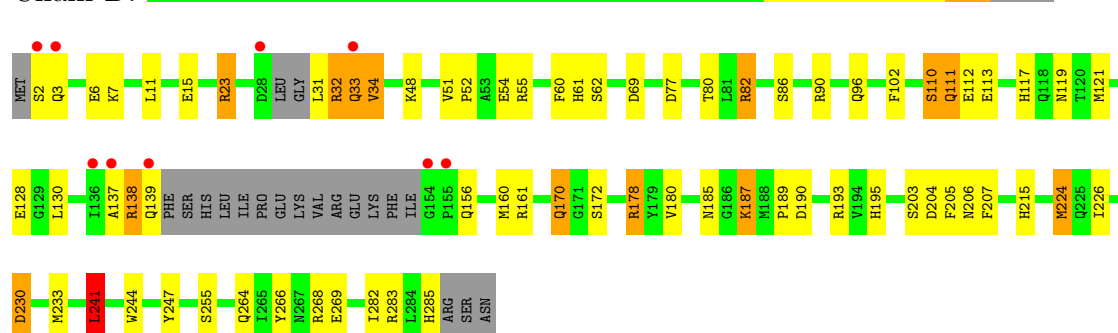
#### • Molecule 1: Acyl-CoA thioesterase II

Chain C: 



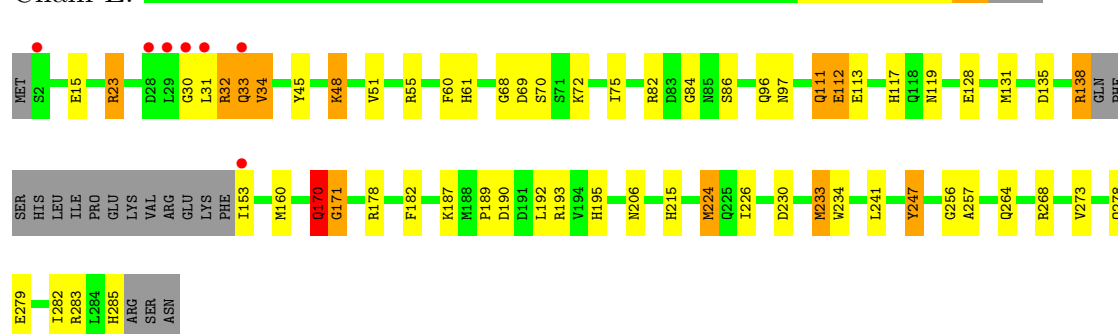
- Molecule 1: Acyl-CoA thioesterase II

Chain D:



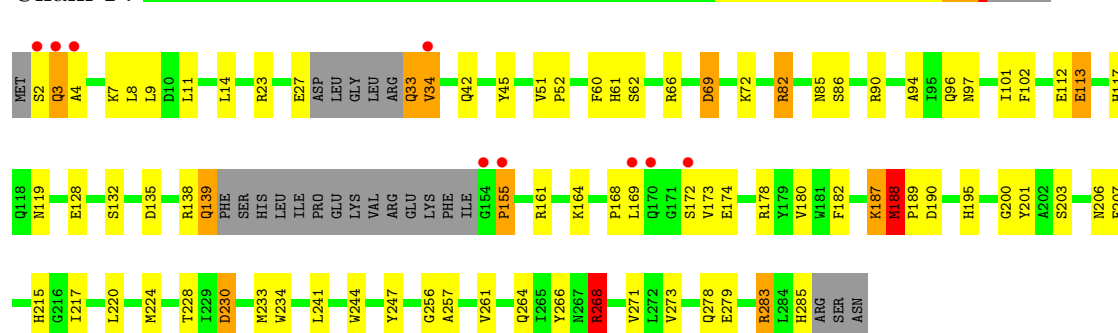
- Molecule 1: Acyl-CoA thioesterase II

Chain E:



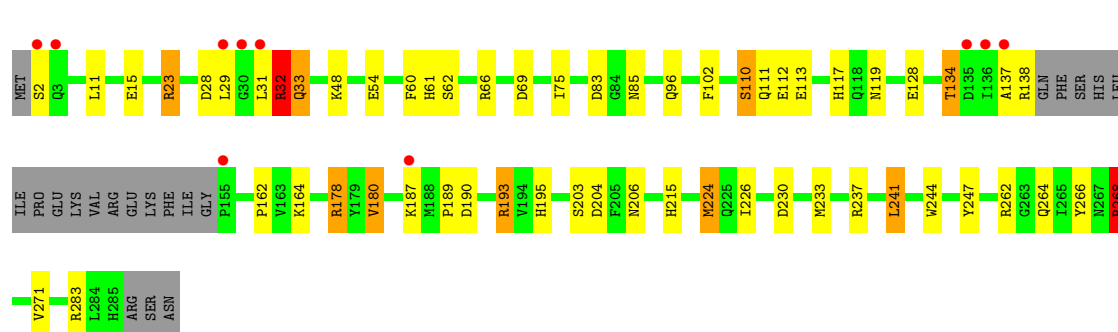
- Molecule 1: Acyl-CoA thioesterase II

Chain F:



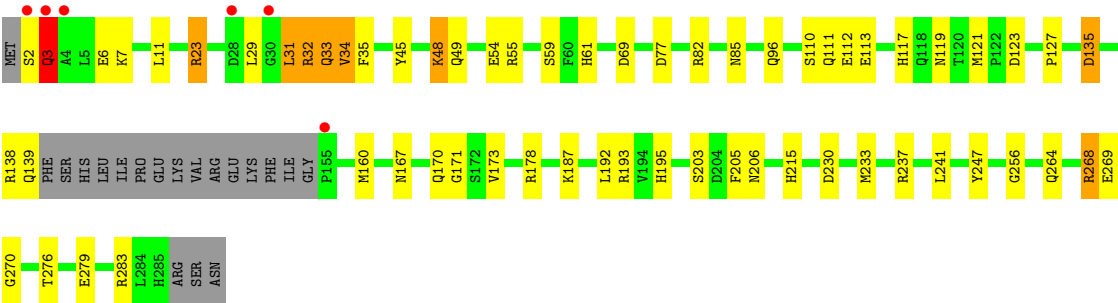
- Molecule 1: Acyl-CoA thioesterase II

Chain G:



● Molecule 1: Acyl-CoA thioesterase II

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.55Å 170.82Å 101.98Å 90.00° 109.44° 90.00°	Depositor
Resolution (Å)	49.04 – 2.00 49.04 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.8 (49.04-2.00) 89.7 (49.04-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.16 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.210 , 0.261 0.210 , 0.260	Depositor DCC
$R_{free}$ test set	7216 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 35.0	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 143004 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17725	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 85.51 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2323e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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



## 5 Model quality i

### 5.1 Standard geometry i

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	8/2152 (0.4%)	1.18	16/2915 (0.5%)
1	B	1.16	5/2256 (0.2%)	1.19	12/3054 (0.4%)
1	C	1.18	4/2210 (0.2%)	1.16	18/2992 (0.6%)
1	D	1.21	8/2194 (0.4%)	1.27	22/2971 (0.7%)
1	E	1.26	5/2206 (0.2%)	1.24	12/2989 (0.4%)
1	F	1.22	9/2167 (0.4%)	1.22	15/2935 (0.5%)
1	G	1.33	5/2194 (0.2%)	1.16	16/2972 (0.5%)
1	H	1.13	3/2203 (0.1%)	1.16	15/2984 (0.5%)
All	All	1.23	47/17582 (0.3%)	1.20	126/23812 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	2
All	All	0	4

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	PRO	CA-CB	-24.92	1.03	1.53
1	G	31	LEU	CA-CB	-22.53	1.01	1.53
1	G	138	ARG	CA-CB	-20.76	1.08	1.53
1	F	33	GLN	CA-CB	-20.55	1.08	1.53
1	A	155	PRO	N-CD	-19.27	1.20	1.47
1	C	29	LEU	CA-CB	-17.89	1.12	1.53
1	E	31	LEU	CA-CB	-16.98	1.14	1.53
1	G	29	LEU	CA-CB	-15.94	1.17	1.53
1	G	28	ASP	CA-CB	15.60	1.88	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	29	LEU	CB-CG	-14.58	1.10	1.52
1	A	284	LEU	CA-CB	-13.99	1.21	1.53
1	D	137	ALA	CA-CB	-13.74	1.23	1.52
1	C	31	LEU	CA-CB	-12.33	1.25	1.53
1	A	111	GLN	CA-CB	-10.15	1.31	1.53
1	E	32	ARG	CA-CB	-9.99	1.31	1.53
1	D	138	ARG	CA-CB	-9.72	1.32	1.53
1	D	31	LEU	CA-CB	-8.78	1.33	1.53
1	F	187	LYS	CA-CB	8.51	1.72	1.53
1	F	285	HIS	CA-CB	-8.51	1.35	1.53
1	D	32	ARG	C-N	8.22	1.52	1.34
1	D	139	GLN	CB-CG	-7.36	1.32	1.52
1	B	103	TYR	CG-CD2	7.28	1.48	1.39
1	D	32	ARG	CA-CB	-7.18	1.38	1.53
1	A	285	HIS	CA-CB	-7.16	1.38	1.53
1	D	32	ARG	CA-C	6.81	1.70	1.52
1	F	45	TYR	CE1-CZ	6.41	1.46	1.38
1	F	234	TRP	CD2-CE2	6.22	1.48	1.41
1	G	244	TRP	CD2-CE2	5.97	1.48	1.41
1	F	3	GLN	CA-CB	-5.93	1.41	1.53
1	A	181	TRP	CD2-CE2	5.92	1.48	1.41
1	F	155	PRO	N-CD	-5.90	1.39	1.47
1	H	31	LEU	CB-CG	5.89	1.69	1.52
1	A	234	TRP	CD2-CE2	5.71	1.48	1.41
1	F	244	TRP	CD2-CE2	5.66	1.48	1.41
1	A	170	GLN	CB-CG	-5.63	1.37	1.52
1	B	45	TYR	CB-CG	5.56	1.59	1.51
1	B	45	TYR	CG-CD1	5.54	1.46	1.39
1	D	244	TRP	CD2-CE2	5.48	1.48	1.41
1	B	236	HIS	CG-CD2	5.48	1.45	1.35
1	H	32	ARG	CA-CB	-5.41	1.42	1.53
1	B	181	TRP	CD2-CE2	5.35	1.47	1.41
1	E	247	TYR	CB-CG	5.34	1.59	1.51
1	C	258	ARG	CZ-NH1	5.32	1.40	1.33
1	C	221	GLU	CD-OE2	5.29	1.31	1.25
1	F	283	ARG	CZ-NH1	5.17	1.39	1.33
1	E	234	TRP	CD2-CE2	5.09	1.47	1.41
1	E	45	TYR	CD2-CE2	5.04	1.47	1.39

All (126) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	33	GLN	N-CA-CB	15.28	138.10	110.60
1	E	23	ARG	NE-CZ-NH2	-14.30	113.15	120.30
1	E	23	ARG	NE-CZ-NH1	14.24	127.42	120.30
1	B	23	ARG	NE-CZ-NH1	14.20	127.40	120.30
1	B	23	ARG	NE-CZ-NH2	-13.14	113.73	120.30
1	F	23	ARG	NE-CZ-NH2	-12.62	113.99	120.30
1	D	31	LEU	N-CA-CB	-12.22	85.95	110.40
1	D	187	LYS	N-CA-CB	-11.93	89.13	110.60
1	A	23	ARG	NE-CZ-NH2	-11.68	114.46	120.30
1	F	187	LYS	CB-CA-C	-11.45	87.50	110.40
1	D	31	LEU	CB-CA-C	11.13	131.34	110.20
1	D	23	ARG	NE-CZ-NH2	-10.84	114.88	120.30
1	H	29	LEU	CB-CG-CD1	-10.54	93.08	111.00
1	H	23	ARG	NE-CZ-NH2	-10.49	115.06	120.30
1	D	137	ALA	N-CA-CB	9.94	124.01	110.10
1	G	28	ASP	N-CA-CB	-9.85	92.87	110.60
1	A	23	ARG	NE-CZ-NH1	9.83	125.22	120.30
1	G	29	LEU	N-CA-CB	-9.76	90.88	110.40
1	E	32	ARG	N-CA-CB	9.68	128.02	110.60
1	C	237	ARG	NE-CZ-NH2	9.68	125.14	120.30
1	G	23	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	D	32	ARG	N-CA-C	-9.27	85.98	111.00
1	C	23	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	D	23	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	C	23	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	F	268	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	E	160	MET	CG-SD-CE	-8.74	86.21	100.20
1	C	29	LEU	CB-CA-C	-8.73	93.60	110.20
1	A	285	HIS	CB-CA-C	-8.54	93.32	110.40
1	F	188	MET	CG-SD-CE	-8.38	86.80	100.20
1	H	29	LEU	CB-CG-CD2	8.30	125.11	111.00
1	H	31	LEU	CA-CB-CG	-8.22	96.39	115.30
1	B	138	ARG	NE-CZ-NH2	8.14	124.37	120.30
1	F	23	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	F	268	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	D	178	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	H	82	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	G	204	ASP	CB-CG-OD1	7.69	125.22	118.30
1	H	23	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	F	187	LYS	N-CA-CB	-7.58	96.95	110.60
1	D	31	LEU	CA-CB-CG	7.55	132.67	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	32	ARG	CB-CA-C	-7.50	95.40	110.40
1	A	204	ASP	CB-CG-OD1	7.49	125.04	118.30
1	C	55	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	B	226	ILE	CG1-CB-CG2	-7.39	95.14	111.40
1	D	230	ASP	CB-CG-OD2	7.34	124.90	118.30
1	B	224	MET	CG-SD-CE	-7.23	88.64	100.20
1	D	32	ARG	N-CA-CB	-7.15	97.72	110.60
1	E	55	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	B	31	LEU	N-CA-CB	-6.89	96.62	110.40
1	E	224	MET	CG-SD-CE	-6.87	89.21	100.20
1	E	233	MET	CG-SD-CE	-6.83	89.27	100.20
1	D	204	ASP	CB-CG-OD1	6.60	124.24	118.30
1	F	285	HIS	CB-CA-C	-6.55	97.30	110.40
1	G	268	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	D	82	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	F	82	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	C	82	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	G	224	MET	CG-SD-CE	-6.35	90.04	100.20
1	C	32	ARG	N-CA-CB	-6.35	99.17	110.60
1	C	138	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	A	82	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	D	224	MET	CG-SD-CE	-6.26	90.19	100.20
1	C	258	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	268	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	B	131	MET	CG-SD-CE	6.09	109.95	100.20
1	A	170	GLN	CA-CB-CG	6.04	126.70	113.40
1	H	77	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	111	GLN	N-CA-CB	5.99	121.38	110.60
1	C	82	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	D	32	ARG	CA-C-O	-5.88	107.75	120.10
1	D	32	ARG	C-N-CA	-5.85	107.07	121.70
1	B	11	LEU	CB-CG-CD2	-5.83	101.09	111.00
1	E	131	MET	CG-SD-CE	5.81	109.49	100.20
1	B	66	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	G	23	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	111	GLN	CB-CA-C	5.77	121.93	110.40
1	G	178	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	B	160	MET	CG-SD-CE	-5.74	91.01	100.20
1	H	77	ASP	CB-CG-OD1	-5.71	113.17	118.30
1	C	55	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	E	48	LYS	CD-CE-NZ	-5.66	98.68	111.70
1	F	69	ASP	CB-CG-OD2	5.65	123.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	31	LEU	N-CA-CB	-5.63	99.14	110.40
1	A	285	HIS	N-CA-CB	5.58	120.65	110.60
1	D	241	LEU	CB-CG-CD1	5.56	120.45	111.00
1	H	237	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	D	55	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	242	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	77	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	82	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	G	66	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	E	31	LEU	CB-CA-C	-5.41	99.92	110.20
1	H	31	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	C	237	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	G	83	ASP	CB-CG-OD2	5.39	123.16	118.30
1	E	192	LEU	CB-CG-CD1	5.38	120.14	111.00
1	B	90	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	H	55	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	D	241	LEU	CB-CG-CD2	5.34	120.08	111.00
1	G	11	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	204	ASP	CB-CG-OD1	5.30	123.08	118.30
1	F	283	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	155	PRO	N-CA-CB	5.29	109.65	103.30
1	A	154	GLY	C-N-CD	-5.29	108.95	120.60
1	F	90	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	H	55	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	33	GLN	N-CA-C	5.26	125.21	111.00
1	G	66	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	123	ASP	CB-CG-OD1	5.23	123.01	118.30
1	C	11	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	169	LEU	CB-CG-CD2	5.19	119.82	111.00
1	H	32	ARG	CB-CA-C	-5.19	100.03	110.40
1	D	82	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	F	230	ASP	CB-CG-OD2	5.17	122.95	118.30
1	G	138	ARG	CB-CA-C	-5.11	100.19	110.40
1	C	138	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	H	135	ASP	N-CA-CB	5.08	119.75	110.60
1	F	34	VAL	N-CA-C	5.08	124.72	111.00
1	G	237	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	242	ASP	CB-CG-OD1	5.06	122.85	118.30
1	D	11	LEU	CB-CG-CD2	-5.04	102.43	111.00
1	G	32	ARG	CB-CA-C	-5.03	100.34	110.40
1	G	262	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	H	192	LEU	CB-CG-CD2	5.01	119.52	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	170	GLN	C-N-CA	-5.01	111.79	122.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	ARG	Peptide
1	B	33	GLN	Peptide
1	D	32	ARG	Mainchain,Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2097	0	2024	64	1
1	B	2199	0	2132	71	0
1	C	2154	0	2083	60	0
1	D	2139	0	2065	71	0
1	E	2150	0	2083	48	0
1	F	2112	0	2037	62	0
1	G	2138	0	2070	45	0
1	H	2147	0	2078	55	1
2	A	68	0	0	2	0
2	B	82	0	0	3	0
2	C	67	0	0	0	0
2	D	89	0	0	0	0
2	E	74	0	0	0	0
2	F	59	0	0	1	0
2	G	80	0	0	0	0
2	H	70	0	0	0	0
All	All	17725	0	16572	418	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (418) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:149:ARG:CD	1:B:153:ILE:HD11	1.48	1.40
1:B:149:ARG:CD	1:B:153:ILE:CD1	2.17	1.21
1:B:149:ARG:HD2	1:B:153:ILE:CD1	1.70	1.20
1:E:112:GLU:OE2	1:F:283:ARG:NH2	1.80	1.14
1:H:138:ARG:O	1:H:139:GLN:HG3	1.49	1.12
1:A:128:GLU:OE2	1:A:268:ARG:NH2	1.86	1.08
1:H:268:ARG:HH11	1:H:268:ARG:CG	1.67	1.06
1:D:111:GLN:H	1:D:111:GLN:NE2	1.50	1.06
1:C:268:ARG:HH11	1:C:268:ARG:HG2	1.11	1.06
1:A:226:ILE:HG22	1:A:282:ILE:HG22	1.36	1.05
1:A:113:GLU:HG2	2:A:340:HOH:O	1.59	1.02
1:B:149:ARG:HD3	1:B:153:ILE:CD1	1.85	1.02
1:H:268:ARG:NH1	1:H:268:ARG:HG3	1.55	1.00
1:B:149:ARG:HD2	1:B:153:ILE:HD11	1.02	0.99
1:H:69:ASP:H	1:H:96:GLN:NE2	1.61	0.99
1:B:195:HIS:HD2	1:B:241:LEU:H	1.00	0.98
1:E:195:HIS:HD2	1:E:241:LEU:H	1.05	0.98
1:C:195:HIS:HD2	1:C:241:LEU:H	1.01	0.97
1:C:268:ARG:HH11	1:C:268:ARG:CG	1.77	0.96
1:B:149:ARG:HD3	1:B:153:ILE:HD11	1.43	0.95
1:A:203:SER:CB	1:A:233:MET:HE1	1.96	0.95
1:A:69:ASP:H	1:A:96:GLN:HE22	0.95	0.94
1:A:195:HIS:HD2	1:A:241:LEU:H	1.13	0.94
1:H:69:ASP:N	1:H:96:GLN:HE22	1.64	0.94
1:E:72:LYS:NZ	1:E:97:ASN:HD21	1.66	0.94
1:D:195:HIS:HD2	1:D:241:LEU:H	1.07	0.93
1:C:112:GLU:OE2	1:D:283:ARG:NH2	2.02	0.92
1:B:171:GLY:HA2	2:B:369:HOH:O	1.70	0.92
1:B:33:GLN:HG3	1:B:35:PHE:N	1.83	0.92
1:C:69:ASP:H	1:C:96:GLN:HE22	1.14	0.92
1:H:178:ARG:HH11	1:H:206:ASN:HD22	1.18	0.92
1:A:128:GLU:CD	1:A:268:ARG:HH22	1.73	0.91
1:A:195:HIS:CD2	1:A:241:LEU:H	1.89	0.90
1:H:195:HIS:HD2	1:H:241:LEU:H	1.14	0.89
1:D:111:GLN:N	1:D:111:GLN:NE2	2.19	0.89
1:F:195:HIS:HD2	1:F:241:LEU:H	1.18	0.89
1:F:69:ASP:H	1:F:96:GLN:HE22	1.11	0.88
1:G:195:HIS:HD2	1:G:241:LEU:H	1.21	0.88
1:F:128:GLU:OE2	1:F:268:ARG:NH2	2.07	0.87
1:H:268:ARG:HH11	1:H:268:ARG:HG3	0.75	0.87
1:D:33:GLN:HG3	1:D:34:VAL:N	1.90	0.87
1:F:168:PRO:HB2	1:F:220:LEU:HD12	1.58	0.86
1:H:138:ARG:C	1:H:139:GLN:HG3	1.96	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:128:GLU:OE1	1:F:268:ARG:NH2	2.08	0.86
1:B:33:GLN:NE2	1:B:151:LYS:NZ	2.24	0.86
1:B:195:HIS:CD2	1:B:241:LEU:H	1.92	0.85
1:F:128:GLU:CD	1:F:268:ARG:HH21	1.79	0.85
1:A:226:ILE:CG2	1:A:282:ILE:HG22	2.09	0.83
1:H:138:ARG:O	1:H:139:GLN:CG	2.27	0.83
1:C:195:HIS:CD2	1:C:241:LEU:H	1.93	0.82
1:B:33:GLN:NE2	1:B:151:LYS:HZ1	1.77	0.82
1:G:60:PHE:CZ	1:G:233:MET:HE3	2.14	0.82
1:A:283:ARG:NH2	1:B:112:GLU:OE1	2.10	0.82
1:C:137:ALA:O	1:C:139:GLN:O	1.95	0.82
1:C:69:ASP:H	1:C:96:GLN:NE2	1.78	0.82
1:A:69:ASP:H	1:A:96:GLN:NE2	1.77	0.82
1:B:138:ARG:O	1:B:139:GLN:HB2	1.78	0.82
1:C:170:GLN:HG3	1:C:171:GLY:H	1.45	0.81
1:F:268:ARG:HG2	1:F:268:ARG:HH11	1.43	0.81
1:C:138:ARG:HH21	1:C:138:ARG:HG2	1.43	0.81
1:D:119:ASN:HD21	1:D:264:GLN:HE22	1.30	0.80
1:C:48:LYS:HE3	1:C:193:ARG:HD2	1.62	0.80
1:B:33:GLN:HE21	1:B:151:LYS:NZ	1.80	0.80
1:F:128:GLU:CD	1:F:268:ARG:NH2	2.35	0.80
1:E:195:HIS:CD2	1:E:241:LEU:H	1.97	0.80
1:E:111:GLN:NE2	1:E:111:GLN:H	1.79	0.79
1:B:149:ARG:O	1:B:153:ILE:HG12	1.82	0.79
1:G:119:ASN:HD21	1:G:264:GLN:HE22	1.30	0.78
1:D:15:GLU:OE1	1:D:23:ARG:HD2	1.82	0.78
1:B:149:ARG:CD	1:B:153:ILE:HD12	2.13	0.78
1:H:69:ASP:H	1:H:96:GLN:HE22	0.83	0.78
1:B:69:ASP:H	1:B:96:GLN:HE22	1.31	0.78
1:E:283:ARG:NH2	1:F:112:GLU:OE2	2.17	0.77
1:E:33:GLN:O	1:E:34:VAL:HB	1.83	0.77
1:D:283:ARG:HD2	1:D:285:HIS:CE1	2.19	0.77
1:G:112:GLU:OE2	1:H:283:ARG:NH2	2.18	0.77
1:A:178:ARG:HH11	1:A:206:ASN:HD22	1.33	0.76
1:D:195:HIS:CD2	1:D:241:LEU:H	1.97	0.76
1:G:15:GLU:OE1	1:G:23:ARG:HD2	1.85	0.76
1:A:167:ASN:ND2	1:A:170:GLN:HB2	2.00	0.76
1:A:128:GLU:CD	1:A:268:ARG:NH2	2.33	0.76
1:A:69:ASP:N	1:A:96:GLN:HE22	1.80	0.76
1:C:268:ARG:NH1	1:C:268:ARG:HG2	1.94	0.75
1:D:111:GLN:H	1:D:111:GLN:CD	1.88	0.75
1:D:111:GLN:N	1:D:111:GLN:HE21	1.84	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:3:GLN:OE1	1:H:3:GLN:HA	1.87	0.75
1:G:54:GLU:OE1	1:G:110:SER:HB3	1.87	0.75
1:H:119:ASN:HD21	1:H:264:GLN:HE22	1.33	0.74
1:B:69:ASP:H	1:B:96:GLN:NE2	1.85	0.74
1:G:60:PHE:HZ	1:G:233:MET:HE3	1.52	0.74
1:C:119:ASN:HD21	1:C:264:GLN:HE22	1.33	0.74
1:D:178:ARG:HH11	1:D:206:ASN:HD22	1.34	0.74
1:G:69:ASP:H	1:G:96:GLN:HE22	1.36	0.74
1:G:69:ASP:H	1:G:96:GLN:NE2	1.86	0.73
1:B:226:ILE:HG22	1:B:282:ILE:HG22	1.71	0.73
1:B:54:GLU:OE1	1:B:110:SER:HB3	1.87	0.73
1:C:283:ARG:NH2	1:D:112:GLU:OE2	2.17	0.73
1:B:33:GLN:HG3	1:B:34:VAL:C	2.08	0.73
1:D:48:LYS:HE3	1:D:193:ARG:CD	2.19	0.73
1:D:48:LYS:HE3	1:D:193:ARG:HD2	1.72	0.72
1:D:60:PHE:CZ	1:D:233:MET:HE3	2.24	0.72
1:H:138:ARG:C	1:H:139:GLN:CG	2.55	0.72
1:F:119:ASN:HD21	1:F:264:GLN:HE22	1.37	0.72
1:G:128:GLU:OE1	1:G:268:ARG:NH2	2.23	0.72
1:E:72:LYS:HZ1	1:E:97:ASN:HD21	1.34	0.72
1:F:139:GLN:CG	1:F:139:GLN:O	2.38	0.71
1:B:178:ARG:HH11	1:B:206:ASN:HD22	1.37	0.71
1:C:69:ASP:N	1:C:96:GLN:HE22	1.88	0.71
1:G:224:MET:HG3	1:G:226:ILE:HG23	1.72	0.71
1:G:195:HIS:CD2	1:G:241:LEU:H	2.08	0.71
1:D:54:GLU:OE1	1:D:110:SER:HB3	1.91	0.71
1:D:128:GLU:OE2	1:D:268:ARG:NH2	2.24	0.70
1:F:72:LYS:HE3	1:F:97:ASN:OD1	1.92	0.70
1:B:119:ASN:HD21	1:B:264:GLN:HE22	1.37	0.70
1:D:15:GLU:OE1	1:D:23:ARG:CD	2.38	0.70
1:F:268:ARG:CG	1:F:268:ARG:HH11	2.03	0.70
1:H:195:HIS:CD2	1:H:241:LEU:H	2.04	0.70
1:D:69:ASP:H	1:D:96:GLN:NE2	1.88	0.70
1:C:33:GLN:HG3	1:C:34:VAL:N	2.07	0.70
1:F:139:GLN:HG3	1:F:139:GLN:O	1.90	0.69
1:F:69:ASP:N	1:F:96:GLN:HE22	1.89	0.69
1:E:178:ARG:HH11	1:E:206:ASN:HD22	1.37	0.69
1:E:119:ASN:HD21	1:E:264:GLN:HE22	1.37	0.69
1:A:230:ASP:HB2	1:B:61:HIS:HE1	1.58	0.69
1:G:283:ARG:NH2	1:H:112:GLU:OE1	2.26	0.69
1:D:69:ASP:H	1:D:96:GLN:HE22	1.41	0.68
1:F:60:PHE:CZ	1:F:233:MET:HE3	2.29	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:33:GLN:HE21	1:B:151:LYS:HZ1	1.35	0.67
1:H:119:ASN:HD21	1:H:264:GLN:NE2	1.93	0.67
1:E:69:ASP:H	1:E:96:GLN:HE22	1.43	0.67
1:A:138:ARG:HG2	1:A:138:ARG:HH21	1.61	0.66
1:F:69:ASP:H	1:F:96:GLN:NE2	1.91	0.66
1:E:48:LYS:HE3	1:E:193:ARG:HD2	1.76	0.66
1:B:149:ARG:O	1:B:153:ILE:CG1	2.43	0.66
1:A:117:HIS:ND1	1:B:215:HIS:HE1	1.95	0.65
1:C:119:ASN:HD21	1:C:264:GLN:NE2	1.95	0.65
1:A:15:GLU:OE1	1:A:23:ARG:HD2	1.97	0.65
1:D:60:PHE:HZ	1:D:233:MET:HE3	1.59	0.65
1:A:119:ASN:HD21	1:A:264:GLN:HE22	1.43	0.65
1:B:15:GLU:OE1	1:B:23:ARG:HD2	1.96	0.65
1:C:139:GLN:O	1:C:140:PHE:HD2	1.80	0.64
1:D:189:PRO:O	1:D:195:HIS:HE1	1.81	0.64
1:E:72:LYS:HZ2	1:E:97:ASN:HD21	1.45	0.64
1:E:69:ASP:H	1:E:96:GLN:NE2	1.96	0.64
1:E:135:ASP:O	1:E:138:ARG:HD2	1.98	0.64
1:B:60:PHE:CZ	1:B:233:MET:HE3	2.33	0.64
1:D:33:GLN:HG3	1:D:34:VAL:H	1.63	0.64
1:B:112:GLU:N	2:B:365:HOH:O	2.30	0.63
1:F:268:ARG:CG	1:F:268:ARG:NH1	2.60	0.63
1:C:178:ARG:HH11	1:C:206:ASN:HD22	1.47	0.63
1:F:178:ARG:HH11	1:F:206:ASN:HD22	1.47	0.63
1:A:203:SER:HB2	1:A:233:MET:HE1	1.82	0.62
1:E:226:ILE:HG22	1:E:282:ILE:HG22	1.81	0.62
1:H:33:GLN:HG2	1:H:35:PHE:H	1.63	0.62
1:F:203:SER:OG	1:F:233:MET:HE1	2.00	0.62
1:C:215:HIS:HE1	1:D:117:HIS:ND1	1.97	0.61
1:D:111:GLN:CA	1:D:111:GLN:HE21	2.13	0.61
1:D:130:LEU:O	1:D:161:ARG:HD3	2.00	0.61
1:C:195:HIS:HD2	1:C:241:LEU:N	1.86	0.61
1:B:149:ARG:HD3	1:B:153:ILE:HD12	1.72	0.60
1:E:15:GLU:OE1	1:E:23:ARG:HD2	2.01	0.60
1:H:160:MET:HE1	1:H:205:PHE:CD2	2.36	0.60
1:C:268:ARG:NH1	1:C:268:ARG:CG	2.45	0.60
1:G:15:GLU:OE1	1:G:23:ARG:CD	2.49	0.60
1:H:48:LYS:HE3	1:H:193:ARG:HD2	1.84	0.60
1:G:215:HIS:HE1	1:H:117:HIS:ND1	2.00	0.60
1:G:48:LYS:HE2	1:G:193:ARG:HD2	1.83	0.60
1:C:117:HIS:ND1	1:D:215:HIS:HE1	2.00	0.60
1:B:33:GLN:NE2	1:B:151:LYS:HZ2	1.98	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:128:GLU:OE2	1:B:268:ARG:NH2	2.31	0.59
1:G:283:ARG:NH2	1:H:112:GLU:OE2	2.32	0.59
1:A:193:ARG:HH11	1:A:193:ARG:HG3	1.66	0.59
1:B:135:ASP:O	1:B:138:ARG:HD3	2.03	0.59
1:D:33:GLN:O	1:D:34:VAL:HB	2.01	0.58
1:D:119:ASN:HD21	1:D:264:GLN:NE2	1.99	0.58
1:D:172:SER:HA	1:G:54:GLU:HG3	1.84	0.58
1:C:170:GLN:HG3	1:C:171:GLY:N	2.15	0.58
1:A:215:HIS:HE1	1:B:117:HIS:ND1	2.01	0.58
1:G:283:ARG:NH2	1:H:112:GLU:CD	2.56	0.58
1:C:112:GLU:CD	1:D:283:ARG:HH22	2.07	0.58
1:B:119:ASN:HD21	1:B:264:GLN:NE2	2.01	0.58
1:G:128:GLU:OE2	1:G:268:ARG:NH2	2.33	0.58
1:G:178:ARG:HH11	1:G:206:ASN:HD22	1.51	0.58
1:A:283:ARG:NH2	1:B:112:GLU:CD	2.55	0.58
1:H:34:VAL:O	1:H:35:PHE:HB3	2.04	0.58
1:G:189:PRO:O	1:G:195:HIS:HE1	1.86	0.58
1:F:60:PHE:HZ	1:F:233:MET:HE3	1.67	0.58
1:C:138:ARG:HG2	1:C:138:ARG:NH2	2.18	0.57
1:A:203:SER:OG	1:A:233:MET:CE	2.53	0.57
1:C:230:ASP:HB2	1:D:61:HIS:HE1	1.69	0.57
1:H:178:ARG:NH1	1:H:206:ASN:HD22	1.96	0.56
1:D:48:LYS:HE3	1:D:193:ARG:HD3	1.87	0.56
1:E:117:HIS:ND1	1:F:215:HIS:HE1	2.04	0.56
1:E:215:HIS:HE1	1:F:117:HIS:ND1	2.04	0.56
1:C:137:ALA:O	1:C:140:PHE:CD2	2.59	0.56
1:G:119:ASN:HD21	1:G:264:GLN:NE2	2.03	0.56
1:H:138:ARG:O	1:H:139:GLN:CB	2.53	0.56
1:G:117:HIS:ND1	1:H:215:HIS:HE1	2.04	0.56
1:C:61:HIS:HE1	1:D:230:ASP:HB2	1.71	0.56
1:A:203:SER:HB3	1:A:233:MET:HE1	1.84	0.55
1:A:230:ASP:HB2	1:B:61:HIS:CE1	2.38	0.55
1:F:119:ASN:HD21	1:F:264:GLN:NE2	2.04	0.55
1:A:48:LYS:HE3	1:A:193:ARG:CD	2.36	0.55
1:E:61:HIS:HE1	1:F:230:ASP:HB2	1.71	0.55
1:A:256:GLY:HA2	1:B:112:GLU:O	2.07	0.55
1:G:128:GLU:CD	1:G:268:ARG:NH2	2.60	0.55
1:H:48:LYS:HD2	1:H:48:LYS:O	2.06	0.55
1:B:217:ILE:HG21	1:B:224:MET:HE3	1.87	0.55
1:B:195:HIS:HD2	1:B:241:LEU:N	1.86	0.55
1:A:203:SER:OG	1:A:233:MET:HE1	2.05	0.54
1:H:203:SER:CB	1:H:233:MET:HE2	2.36	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:61:HIS:HE1	1:B:230:ASP:HB2	1.71	0.54
1:A:34:VAL:HG23	1:A:70:SER:HA	1.89	0.54
1:C:111:GLN:H	1:C:111:GLN:CD	2.11	0.54
1:E:33:GLN:O	1:E:68:GLY:O	2.25	0.54
1:F:168:PRO:CB	1:F:220:LEU:HD12	2.36	0.54
1:B:29:LEU:HD22	1:B:150:GLU:HB3	1.88	0.54
1:A:61:HIS:CE1	1:B:230:ASP:HB2	2.42	0.54
1:F:8:LEU:HD13	1:F:27:GLU:OE1	2.08	0.54
1:H:119:ASN:ND2	1:H:264:GLN:HE22	2.04	0.53
1:C:119:ASN:ND2	1:C:264:GLN:HE22	2.04	0.53
1:F:217:ILE:HG21	1:F:224:MET:HE3	1.90	0.53
1:D:226:ILE:HD12	1:D:226:ILE:O	2.09	0.53
1:C:167:ASN:ND2	1:C:170:GLN:HB3	2.24	0.53
1:E:195:HIS:HD2	1:E:241:LEU:N	1.89	0.53
1:A:15:GLU:OE1	1:A:23:ARG:CD	2.56	0.53
1:D:224:MET:HG3	1:D:226:ILE:HG23	1.91	0.53
1:F:4:ALA:HB2	1:F:155:PRO:O	2.08	0.53
1:C:283:ARG:NH2	1:D:112:GLU:CD	2.62	0.52
1:D:203:SER:OG	1:D:233:MET:HE1	2.08	0.52
1:A:233:MET:HE2	1:A:276:THR:HG22	1.90	0.52
1:A:283:ARG:NH2	1:B:112:GLU:OE2	2.43	0.52
1:D:203:SER:OG	1:D:233:MET:CE	2.58	0.52
1:D:128:GLU:CD	1:D:268:ARG:HH22	2.12	0.52
1:C:121:MET:SD	1:C:270:GLY:HA2	2.49	0.52
1:B:111:GLN:C	2:B:365:HOH:O	2.49	0.52
1:C:215:HIS:CE1	1:D:117:HIS:ND1	2.78	0.52
1:C:61:HIS:CE1	1:D:230:ASP:HB2	2.46	0.52
1:C:283:ARG:NH2	1:D:112:GLU:OE1	2.42	0.51
1:E:135:ASP:HA	1:E:138:ARG:HD2	1.93	0.51
1:H:3:GLN:OE1	1:H:3:GLN:CA	2.57	0.51
1:H:160:MET:HE1	1:H:205:PHE:CG	2.45	0.51
1:D:48:LYS:CE	1:D:193:ARG:HD2	2.40	0.51
1:D:33:GLN:CG	1:D:34:VAL:N	2.58	0.51
1:F:8:LEU:HD21	1:F:201:TYR:CE2	2.45	0.51
1:D:195:HIS:HD2	1:D:241:LEU:N	1.91	0.50
1:E:224:MET:HA	1:E:224:MET:HE2	1.92	0.50
1:H:268:ARG:NH1	1:H:268:ARG:CG	2.39	0.50
1:A:226:ILE:HG22	1:A:282:ILE:CG2	2.25	0.50
1:B:226:ILE:HA	1:B:281:VAL:O	2.11	0.50
1:G:128:GLU:CD	1:G:268:ARG:HH21	2.15	0.50
1:F:34:VAL:O	1:F:34:VAL:CG1	2.59	0.50
1:E:230:ASP:HB2	1:F:61:HIS:HE1	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:112:GLU:O	1:H:256:GLY:HA2	2.12	0.50
1:G:268:ARG:CG	1:G:268:ARG:HH11	2.25	0.50
1:D:33:GLN:CG	1:D:34:VAL:H	2.22	0.50
1:E:82:ARG:HH12	1:E:84:GLY:HA3	1.77	0.50
1:B:135:ASP:HA	1:B:138:ARG:CD	2.42	0.49
1:B:172:SER:O	1:B:174:GLU:HG2	2.12	0.49
1:C:33:GLN:HG3	1:C:34:VAL:H	1.77	0.49
1:A:48:LYS:HE3	1:A:193:ARG:HD2	1.94	0.49
1:C:230:ASP:HB2	1:D:61:HIS:CE1	2.47	0.49
1:E:182:PHE:CE1	1:E:241:LEU:HD21	2.48	0.49
1:C:283:ARG:HD3	1:D:112:GLU:OE2	2.12	0.49
1:D:119:ASN:ND2	1:D:264:GLN:HE22	2.05	0.49
1:A:138:ARG:HG2	1:A:138:ARG:NH2	2.26	0.49
1:B:119:ASN:ND2	1:B:264:GLN:HE22	2.08	0.49
1:G:62:SER:HB2	1:G:102:PHE:CE1	2.48	0.49
1:C:116:GLU:OE2	1:D:255:SER:HB2	2.13	0.49
1:D:48:LYS:CE	1:D:193:ARG:CD	2.90	0.49
1:G:215:HIS:CE1	1:H:117:HIS:ND1	2.80	0.49
1:G:69:ASP:N	1:G:96:GLN:HE22	2.08	0.49
1:E:230:ASP:O	1:E:278:GLN:HG3	2.12	0.49
1:H:203:SER:OG	1:H:233:MET:CE	2.61	0.48
1:E:282:ILE:HG13	1:E:282:ILE:O	2.13	0.48
1:B:48:LYS:HE3	1:B:193:ARG:HD2	1.95	0.48
1:C:33:GLN:O	1:C:34:VAL:HB	2.13	0.48
1:B:45:TYR:O	1:B:49:GLN:HG2	2.13	0.48
1:B:189:PRO:O	1:B:195:HIS:HE1	1.96	0.48
1:D:121:MET:HG3	1:D:266:TYR:CG	2.48	0.48
1:C:137:ALA:O	1:C:140:PHE:HD2	1.94	0.48
1:G:230:ASP:HB2	1:H:61:HIS:HE1	1.78	0.48
1:A:115:PHE:CZ	1:B:217:ILE:HD12	2.49	0.48
1:D:69:ASP:N	1:D:96:GLN:HE22	2.09	0.48
1:H:121:MET:SD	1:H:270:GLY:HA2	2.54	0.48
1:E:119:ASN:HD21	1:E:264:GLN:NE2	2.08	0.48
1:F:203:SER:OG	1:F:233:MET:CE	2.61	0.48
1:H:34:VAL:O	1:H:35:PHE:CB	2.61	0.48
1:B:135:ASP:HA	1:B:138:ARG:HD2	1.96	0.47
1:A:112:GLU:OE1	1:B:283:ARG:NH2	2.48	0.47
1:C:159:GLU:O	1:C:182:PHE:HA	2.14	0.47
1:B:111:GLN:HB2	1:B:111:GLN:HE21	1.47	0.47
1:D:15:GLU:OE1	1:D:23:ARG:HD3	2.13	0.47
1:E:230:ASP:HB2	1:F:61:HIS:CE1	2.49	0.47
1:F:256:GLY:O	1:F:257:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:172:SER:O	1:F:174:GLU:HG2	2.14	0.47
1:G:119:ASN:ND2	1:G:264:GLN:HE22	2.07	0.47
1:A:48:LYS:HG2	1:A:193:ARG:HD2	1.96	0.47
1:C:72:LYS:HE3	1:C:97:ASN:OD1	2.14	0.47
1:E:128:GLU:OE2	1:E:268:ARG:NH2	2.34	0.47
1:F:230:ASP:OD1	1:F:279:GLU:HB3	2.15	0.47
1:F:188:MET:HG3	1:F:189:PRO:HD2	1.98	0.46
1:G:230:ASP:HB2	1:H:61:HIS:CE1	2.51	0.46
1:C:33:GLN:O	1:C:68:GLY:O	2.34	0.46
1:B:233:MET:HG3	1:B:276:THR:HG22	1.98	0.46
1:B:224:MET:HE3	1:B:224:MET:HB2	1.67	0.46
1:B:54:GLU:OE1	1:B:110:SER:CB	2.61	0.46
1:A:14:LEU:HB2	1:A:45:TYR:CE2	2.50	0.46
1:A:48:LYS:HE3	1:A:193:ARG:HD3	1.96	0.46
1:F:4:ALA:CB	1:F:155:PRO:O	2.64	0.46
1:H:203:SER:OG	1:H:233:MET:HE2	2.16	0.46
1:C:112:GLU:CD	1:D:283:ARG:NH2	2.66	0.45
1:E:117:HIS:ND1	1:F:215:HIS:CE1	2.84	0.45
1:E:256:GLY:O	1:E:257:ALA:HB3	2.16	0.45
1:D:54:GLU:CD	1:D:110:SER:HB3	2.35	0.45
1:F:66:ARG:HB2	1:F:101:ILE:HA	1.98	0.45
1:F:14:LEU:HD21	1:F:42:GLN:HG2	1.98	0.45
1:D:62:SER:HB2	1:D:102:PHE:CE1	2.51	0.45
1:A:127:PRO:HD2	1:A:268:ARG:HH12	1.82	0.45
1:A:233:MET:HE2	1:A:233:MET:HB2	1.71	0.45
1:E:224:MET:HB2	1:E:224:MET:HE3	1.63	0.45
1:D:156:GLN:O	1:D:185:ASN:ND2	2.50	0.45
1:F:228:THR:HG23	1:F:278:GLN:CD	2.37	0.45
1:E:170:GLN:O	1:E:171:GLY:O	2.35	0.45
1:A:164:LYS:HE2	1:C:138:ARG:HD2	1.99	0.45
1:G:266:TYR:HA	1:G:271:VAL:O	2.17	0.45
1:C:203:SER:HB2	1:C:276:THR:HG21	1.98	0.44
1:E:224:MET:HA	1:E:224:MET:CE	2.47	0.44
1:G:61:HIS:HE1	1:H:230:ASP:HB2	1.82	0.44
1:C:158:ILE:HD13	1:C:202:ALA:HB2	1.99	0.44
1:D:2:SER:O	1:D:6:GLU:HB2	2.18	0.44
1:C:256:GLY:HA2	1:D:112:GLU:O	2.17	0.44
1:F:62:SER:HB2	1:F:102:PHE:CE1	2.51	0.44
1:H:45:TYR:O	1:H:49:GLN:HG2	2.16	0.44
1:E:61:HIS:CE1	1:F:230:ASP:HB2	2.51	0.44
1:H:167:ASN:HD22	1:H:170:GLN:HB3	1.83	0.44
1:C:117:HIS:ND1	1:D:215:HIS:CE1	2.85	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:167:ASN:ND2	1:H:170:GLN:HB3	2.33	0.44
1:A:224:MET:HE1	1:A:284:LEU:CA	2.47	0.44
1:C:233:MET:HB2	1:C:233:MET:HE3	1.27	0.44
1:E:48:LYS:HE3	1:E:193:ARG:CD	2.45	0.44
1:E:224:MET:HG3	1:E:226:ILE:HG23	1.98	0.44
1:A:266:TYR:HA	1:A:271:VAL:O	2.18	0.44
1:A:128:GLU:OE1	1:A:268:ARG:NH2	2.28	0.44
1:D:111:GLN:CA	1:D:111:GLN:NE2	2.78	0.44
1:C:230:ASP:O	1:C:278:GLN:HG3	2.17	0.44
1:E:230:ASP:OD1	1:E:279:GLU:HB3	2.17	0.43
1:C:203:SER:OG	1:C:233:MET:CE	2.65	0.43
1:E:283:ARG:HD2	1:E:285:HIS:CE1	2.53	0.43
1:G:203:SER:OG	1:G:233:MET:CE	2.66	0.43
1:B:69:ASP:N	1:B:96:GLN:HE22	2.08	0.43
1:F:189:PRO:O	1:F:195:HIS:HE1	2.01	0.43
1:B:224:MET:HG3	1:B:226:ILE:HG23	1.99	0.43
1:F:94:ALA:HB3	1:F:102:PHE:HB3	2.00	0.43
1:H:2:SER:O	1:H:6:GLU:HB2	2.19	0.43
1:C:14:LEU:HD21	1:C:42:GLN:HB3	2.01	0.43
1:D:226:ILE:HG22	1:D:282:ILE:HG22	2.01	0.43
1:F:164:LYS:HE2	1:F:164:LYS:HB2	1.79	0.43
1:G:203:SER:OG	1:G:233:MET:HE1	2.19	0.43
1:B:226:ILE:O	1:B:226:ILE:HD12	2.19	0.43
1:G:224:MET:HA	1:G:224:MET:HE2	1.99	0.43
1:G:117:HIS:ND1	1:H:215:HIS:CE1	2.86	0.43
1:B:33:GLN:HE22	1:B:151:LYS:NZ	2.12	0.42
1:C:138:ARG:HH21	1:C:138:ARG:CG	2.24	0.42
1:H:203:SER:HB2	1:H:276:THR:HG21	2.01	0.42
1:A:112:GLU:CD	1:B:283:ARG:HH21	2.23	0.42
1:D:160:MET:HE1	1:D:205:PHE:CD2	2.54	0.42
1:A:226:ILE:HA	1:A:281:VAL:O	2.19	0.42
1:A:112:GLU:OE2	1:B:283:ARG:HD3	2.18	0.42
1:B:149:ARG:HD2	1:B:153:ILE:CG1	2.43	0.42
2:A:334:HOH:O	1:B:111:GLN:HA	2.17	0.42
1:G:134:THR:O	1:G:137:ALA:HB3	2.20	0.42
1:A:268:ARG:NH1	1:A:268:ARG:CG	2.82	0.42
1:A:136:ILE:O	1:A:139:GLN:HA	2.20	0.42
1:C:189:PRO:O	1:C:195:HIS:HE1	2.02	0.42
1:A:138:ARG:O	1:A:139:GLN:HB2	2.20	0.42
1:A:62:SER:HB2	1:A:102:PHE:CZ	2.55	0.42
1:F:195:HIS:CD2	1:F:241:LEU:H	2.11	0.42
1:F:268:ARG:HG2	1:F:268:ARG:NH1	2.21	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:111:GLN:CD	1:E:111:GLN:H	2.19	0.42
1:A:168:PRO:HB2	1:A:220:LEU:HD12	2.01	0.42
1:D:54:GLU:OE2	1:D:110:SER:HB3	2.20	0.42
1:E:283:ARG:NH2	1:F:112:GLU:CD	2.73	0.41
1:F:230:ASP:O	1:F:278:GLN:HG3	2.19	0.41
1:H:230:ASP:OD1	1:H:279:GLU:HB3	2.20	0.41
1:E:60:PHE:CZ	1:E:233:MET:HE3	2.55	0.41
1:D:170:GLN:HE21	1:D:170:GLN:HB2	1.54	0.41
1:F:200:GLY:HA2	1:F:233:MET:HE1	2.03	0.41
1:C:230:ASP:N	1:C:230:ASP:OD1	2.54	0.41
1:D:51:VAL:HG13	1:D:52:PRO:HD2	2.02	0.41
1:E:170:GLN:O	1:E:171:GLY:C	2.59	0.41
1:F:51:VAL:HG12	1:F:52:PRO:O	2.20	0.41
1:D:111:GLN:N	1:D:111:GLN:CD	2.64	0.41
1:F:60:PHE:C	1:F:60:PHE:CD1	2.93	0.41
1:G:61:HIS:CE1	1:H:230:ASP:HB2	2.55	0.41
1:D:80:THR:HA	1:D:90:ARG:HD3	2.02	0.41
1:A:224:MET:HE1	1:A:284:LEU:HA	2.02	0.41
1:B:170:GLN:HE21	1:B:170:GLN:HB2	1.55	0.41
1:G:162:PRO:HA	1:G:180:VAL:HB	2.03	0.41
1:F:182:PHE:CE1	1:F:241:LEU:HD21	2.56	0.41
1:G:268:ARG:HG3	1:G:268:ARG:HH11	1.86	0.41
1:F:8:LEU:O	1:F:9:LEU:C	2.56	0.41
1:G:61:HIS:HB3	1:H:61:HIS:ND1	2.36	0.41
1:A:162:PRO:HA	1:A:180:VAL:HB	2.02	0.41
1:F:113:GLU:HG2	2:F:351:HOH:O	2.20	0.41
1:H:127:PRO:HD2	1:H:268:ARG:NH2	2.36	0.41
1:C:178:ARG:NH1	1:C:206:ASN:HD22	2.17	0.41
1:A:268:ARG:HH11	1:A:268:ARG:CG	2.33	0.40
1:F:132:SER:HA	1:F:161:ARG:HG2	2.03	0.40
1:H:59:SER:HA	1:H:233:MET:O	2.21	0.40
1:E:82:ARG:NH1	1:E:84:GLY:HA3	2.36	0.40
1:A:217:ILE:HD13	1:B:115:PHE:CZ	2.56	0.40
1:A:228:THR:HG23	1:A:278:GLN:CD	2.42	0.40
1:F:207:PHE:CZ	1:F:261:VAL:HG23	2.56	0.40
1:F:266:TYR:HA	1:F:271:VAL:O	2.22	0.40
1:E:189:PRO:O	1:E:195:HIS:HE1	2.05	0.40
1:A:69:ASP:OD2	1:A:71:SER:OG	2.39	0.40
1:H:160:MET:HE1	1:H:205:PHE:CB	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:ASN:OD1	1:H:85:ASN:OD1[2_456]	1.91	0.29

## 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	257/288 (89%)	247 (96%)	8 (3%)	2 (1%)	27	17
1	B	271/288 (94%)	261 (96%)	7 (3%)	3 (1%)	21	10
1	C	263/288 (91%)	254 (97%)	8 (3%)	1 (0%)	43	36
1	D	262/288 (91%)	250 (95%)	9 (3%)	3 (1%)	21	10
1	E	266/288 (92%)	254 (96%)	9 (3%)	3 (1%)	21	10
1	F	259/288 (90%)	247 (95%)	12 (5%)	0	100	100
1	G	264/288 (92%)	252 (96%)	10 (4%)	2 (1%)	27	17
1	H	265/288 (92%)	254 (96%)	9 (3%)	2 (1%)	27	17
All	All	2107/2304 (91%)	2019 (96%)	72 (3%)	16 (1%)	27	17

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	VAL
1	G	33	GLN
1	B	33	GLN
1	B	171	GLY
1	D	33	GLN
1	D	138	ARG
1	H	3	GLN
1	H	171	GLY
1	A	171	GLY
1	A	34	VAL
1	C	34	VAL
1	G	32	ARG
1	D	34	VAL
1	E	34	VAL

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Mol	Chain	Res	Type
1	E	171	GLY
1	E	30	GLY

### 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	224/248 (90%)	206 (92%)	18 (8%)	17	10
1	B	235/248 (95%)	222 (94%)	13 (6%)	30	23
1	C	231/248 (93%)	219 (95%)	12 (5%)	32	25
1	D	229/248 (92%)	214 (93%)	15 (7%)	24	16
1	E	230/248 (93%)	214 (93%)	16 (7%)	21	14
1	F	226/248 (91%)	205 (91%)	21 (9%)	13	7
1	G	229/248 (92%)	212 (93%)	17 (7%)	20	12
1	H	230/248 (93%)	210 (91%)	20 (9%)	15	8
All	All	1834/1984 (92%)	1702 (93%)	132 (7%)	21	13

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	110	SER
1	A	111	GLN
1	A	113	GLU
1	A	135	ASP
1	A	138	ARG
1	A	169	LEU
1	A	170	GLN
1	A	173	VAL
1	A	187	LYS
1	A	188	MET
1	A	190	ASP
1	A	225	GLN
1	A	226	ILE
1	A	241	LEU

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Mol	Chain	Res	Type
1	A	247	TYR
1	A	268	ARG
1	A	284	LEU
1	B	3	GLN
1	B	75	ILE
1	B	110	SER
1	B	111	GLN
1	B	113	GLU
1	B	149	ARG
1	B	153	ILE
1	B	173	VAL
1	B	187	LYS
1	B	190	ASP
1	B	247	TYR
1	B	273	VAL
1	B	283	ARG
1	C	7	LYS
1	C	70	SER
1	C	75	ILE
1	C	85	ASN
1	C	111	GLN
1	C	113	GLU
1	C	123	ASP
1	C	138	ARG
1	C	180	VAL
1	C	247	TYR
1	C	268	ARG
1	C	269	GLU
1	D	3	GLN
1	D	7	LYS
1	D	82	ARG
1	D	86	SER
1	D	110	SER
1	D	111	GLN
1	D	113	GLU
1	D	170	GLN
1	D	180	VAL
1	D	187	LYS
1	D	190	ASP
1	D	207	PHE
1	D	241	LEU
1	D	247	TYR

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Mol	Chain	Res	Type
1	D	269	GLU
1	E	32	ARG
1	E	33	GLN
1	E	51	VAL
1	E	70	SER
1	E	75	ILE
1	E	86	SER
1	E	111	GLN
1	E	112	GLU
1	E	113	GLU
1	E	138	ARG
1	E	153	ILE
1	E	170	GLN
1	E	187	LYS
1	E	190	ASP
1	E	247	TYR
1	E	273	VAL
1	F	2	SER
1	F	3	GLN
1	F	7	LYS
1	F	11	LEU
1	F	33	GLN
1	F	82	ARG
1	F	85	ASN
1	F	86	SER
1	F	113	GLU
1	F	135	ASP
1	F	138	ARG
1	F	139	GLN
1	F	169	LEU
1	F	173	VAL
1	F	180	VAL
1	F	187	LYS
1	F	188	MET
1	F	190	ASP
1	F	247	TYR
1	F	268	ARG
1	F	273	VAL
1	G	2	SER
1	G	32	ARG
1	G	33	GLN
1	G	75	ILE

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Mol	Chain	Res	Type
1	G	85	ASN
1	G	110	SER
1	G	111	GLN
1	G	113	GLU
1	G	134	THR
1	G	164	LYS
1	G	180	VAL
1	G	187	LYS
1	G	190	ASP
1	G	193	ARG
1	G	241	LEU
1	G	247	TYR
1	G	268	ARG
1	H	3	GLN
1	H	7	LYS
1	H	11	LEU
1	H	23	ARG
1	H	31	LEU
1	H	32	ARG
1	H	33	GLN
1	H	34	VAL
1	H	48	LYS
1	H	54	GLU
1	H	110	SER
1	H	111	GLN
1	H	113	GLU
1	H	123	ASP
1	H	135	ASP
1	H	173	VAL
1	H	187	LYS
1	H	247	TYR
1	H	268	ARG
1	H	269	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	97	ASN
1	A	195	HIS
1	A	206	ASN
1	A	215	HIS

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Mol	Chain	Res	Type
1	A	264	GLN
1	B	33	GLN
1	B	96	GLN
1	B	111	GLN
1	B	170	GLN
1	B	195	HIS
1	B	206	ASN
1	B	215	HIS
1	B	264	GLN
1	C	33	GLN
1	C	96	GLN
1	C	195	HIS
1	C	206	ASN
1	C	215	HIS
1	C	264	GLN
1	C	285	HIS
1	D	96	GLN
1	D	111	GLN
1	D	170	GLN
1	D	195	HIS
1	D	206	ASN
1	D	215	HIS
1	D	264	GLN
1	D	285	HIS
1	E	49	GLN
1	E	96	GLN
1	E	97	ASN
1	E	111	GLN
1	E	177	ASN
1	E	195	HIS
1	E	206	ASN
1	E	215	HIS
1	E	264	GLN
1	F	96	GLN
1	F	195	HIS
1	F	206	ASN
1	F	215	HIS
1	F	264	GLN
1	G	96	GLN
1	G	170	GLN
1	G	195	HIS
1	G	206	ASN

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Mol	Chain	Res	Type
1	G	215	HIS
1	G	264	GLN
1	H	96	GLN
1	H	111	GLN
1	H	195	HIS
1	H	206	ASN
1	H	215	HIS
1	H	264	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	263/288 (91%)	-0.20	4 (1%)	70	70	12, 23, 48, 62	6 (2%)
1	B	275/288 (95%)	-0.32	8 (2%)	49	49	9, 17, 39, 76	2 (0%)
1	C	269/288 (93%)	-0.22	6 (2%)	59	59	10, 23, 49, 62	3 (1%)
1	D	268/288 (93%)	-0.21	9 (3%)	43	43	10, 20, 49, 71	6 (2%)
1	E	270/288 (93%)	-0.36	7 (2%)	53	53	9, 18, 39, 62	2 (0%)
1	F	265/288 (92%)	-0.08	9 (3%)	43	43	12, 24, 50, 64	5 (1%)
1	G	268/288 (93%)	-0.18	10 (3%)	39	39	9, 20, 50, 75	5 (1%)
1	H	269/288 (93%)	-0.20	6 (2%)	59	59	11, 22, 49, 60	3 (1%)
All	All	2147/2304 (93%)	-0.22	59 (2%)	52	52	9, 21, 49, 76	32 (1%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	31	LEU	6.9
1	D	154	GLY	6.5
1	E	153	ILE	5.3
1	B	153	ILE	4.8
1	D	137	ALA	4.5
1	G	30	GLY	4.3
1	F	155	PRO	3.9
1	E	28	ASP	3.8
1	G	137	ALA	3.6
1	E	30	GLY	3.5
1	G	136	ILE	3.4
1	D	2	SER	3.3
1	D	136	ILE	3.3
1	B	150	GLU	3.3
1	A	169	LEU	3.3
1	B	149	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	28	ASP	3.1
1	G	2	SER	3.1
1	F	154	GLY	3.0
1	H	30	GLY	3.0
1	F	2	SER	3.0
1	H	155	PRO	2.9
1	B	30	GLY	2.9
1	C	3	GLN	2.9
1	B	28	ASP	2.8
1	H	3	GLN	2.8
1	D	28	ASP	2.8
1	G	31	LEU	2.8
1	H	28	ASP	2.7
1	B	33	GLN	2.7
1	G	135	ASP	2.6
1	A	154	GLY	2.6
1	C	2	SER	2.6
1	C	33	GLN	2.5
1	G	3	GLN	2.5
1	G	187	LYS	2.5
1	E	31	LEU	2.5
1	G	29	LEU	2.5
1	F	172	SER	2.5
1	H	4	ALA	2.5
1	C	155	PRO	2.4
1	D	139	GLN	2.4
1	D	33	GLN	2.4
1	C	4	ALA	2.4
1	A	155	PRO	2.3
1	D	155	PRO	2.3
1	E	33	GLN	2.2
1	G	155	PRO	2.2
1	F	169	LEU	2.2
1	D	3	GLN	2.2
1	H	2	SER	2.2
1	A	33	GLN	2.1
1	F	34	VAL	2.1
1	F	3	GLN	2.1
1	E	29	LEU	2.1
1	F	4	ALA	2.0
1	F	170	GLN	2.0
1	B	29	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	2	SER	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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.