



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:33 AM EDT

PDB ID : 3GD5  
Title : Crystal structure of ornithine carbamoyltransferase from *Gloeobacter violaceus*  
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Deposited on : 2009-02-23  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

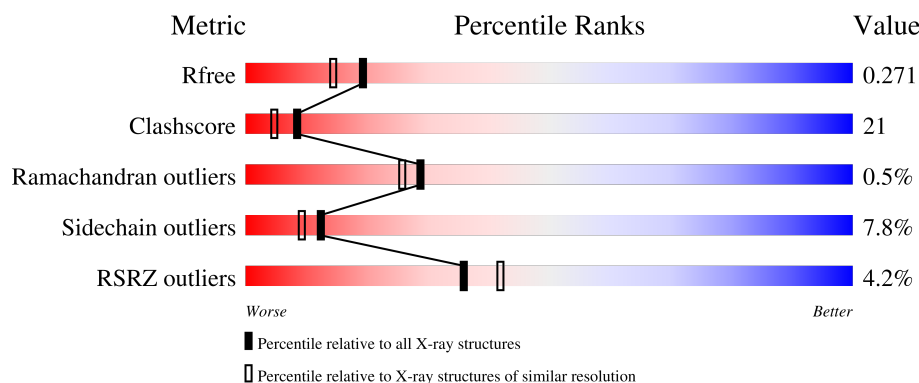
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	323	
1	B	323	
1	C	323	
1	D	323	
1	E	323	

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Mol	Chain	Length	Quality of chain
1	F	323	<div><div></div><div>4%</div><div>58%</div><div>25%</div><div>12%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13303 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 Ornithine carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2195	1383	399	405	8			
1	B	285	Total	C	N	O	S	0	0	0
			2195	1383	399	405	8			
1	C	285	Total	C	N	O	S	0	0	0
			2195	1383	399	405	8			
1	D	285	Total	C	N	O	S	0	0	0
			2195	1383	399	405	8			
1	E	285	Total	C	N	O	S	0	0	0
			2195	1383	399	405	8			
1	F	285	Total	C	N	O	S	0	0	0
			2195	1383	399	405	8			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q7NGR7
A	2	SER	-	expression tag	UNP Q7NGR7
A	3	LEU	-	expression tag	UNP Q7NGR7
A	316	GLU	-	expression tag	UNP Q7NGR7
A	317	GLY	-	expression tag	UNP Q7NGR7
A	318	HIS	-	expression tag	UNP Q7NGR7
A	319	HIS	-	expression tag	UNP Q7NGR7
A	320	HIS	-	expression tag	UNP Q7NGR7
A	321	HIS	-	expression tag	UNP Q7NGR7
A	322	HIS	-	expression tag	UNP Q7NGR7
A	323	HIS	-	expression tag	UNP Q7NGR7
B	1	MET	-	expression tag	UNP Q7NGR7
B	2	SER	-	expression tag	UNP Q7NGR7
B	3	LEU	-	expression tag	UNP Q7NGR7
B	316	GLU	-	expression tag	UNP Q7NGR7
B	317	GLY	-	expression tag	UNP Q7NGR7
B	318	HIS	-	expression tag	UNP Q7NGR7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	319	HIS	-	expression tag	UNP Q7NGR7
B	320	HIS	-	expression tag	UNP Q7NGR7
B	321	HIS	-	expression tag	UNP Q7NGR7
B	322	HIS	-	expression tag	UNP Q7NGR7
B	323	HIS	-	expression tag	UNP Q7NGR7
C	1	MET	-	expression tag	UNP Q7NGR7
C	2	SER	-	expression tag	UNP Q7NGR7
C	3	LEU	-	expression tag	UNP Q7NGR7
C	316	GLU	-	expression tag	UNP Q7NGR7
C	317	GLY	-	expression tag	UNP Q7NGR7
C	318	HIS	-	expression tag	UNP Q7NGR7
C	319	HIS	-	expression tag	UNP Q7NGR7
C	320	HIS	-	expression tag	UNP Q7NGR7
C	321	HIS	-	expression tag	UNP Q7NGR7
C	322	HIS	-	expression tag	UNP Q7NGR7
C	323	HIS	-	expression tag	UNP Q7NGR7
D	1	MET	-	expression tag	UNP Q7NGR7
D	2	SER	-	expression tag	UNP Q7NGR7
D	3	LEU	-	expression tag	UNP Q7NGR7
D	316	GLU	-	expression tag	UNP Q7NGR7
D	317	GLY	-	expression tag	UNP Q7NGR7
D	318	HIS	-	expression tag	UNP Q7NGR7
D	319	HIS	-	expression tag	UNP Q7NGR7
D	320	HIS	-	expression tag	UNP Q7NGR7
D	321	HIS	-	expression tag	UNP Q7NGR7
D	322	HIS	-	expression tag	UNP Q7NGR7
D	323	HIS	-	expression tag	UNP Q7NGR7
E	1	MET	-	expression tag	UNP Q7NGR7
E	2	SER	-	expression tag	UNP Q7NGR7
E	3	LEU	-	expression tag	UNP Q7NGR7
E	316	GLU	-	expression tag	UNP Q7NGR7
E	317	GLY	-	expression tag	UNP Q7NGR7
E	318	HIS	-	expression tag	UNP Q7NGR7
E	319	HIS	-	expression tag	UNP Q7NGR7
E	320	HIS	-	expression tag	UNP Q7NGR7
E	321	HIS	-	expression tag	UNP Q7NGR7
E	322	HIS	-	expression tag	UNP Q7NGR7
E	323	HIS	-	expression tag	UNP Q7NGR7
F	1	MET	-	expression tag	UNP Q7NGR7
F	2	SER	-	expression tag	UNP Q7NGR7
F	3	LEU	-	expression tag	UNP Q7NGR7
F	316	GLU	-	expression tag	UNP Q7NGR7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	317	GLY	-	expression tag	UNP Q7NGR7
F	318	HIS	-	expression tag	UNP Q7NGR7
F	319	HIS	-	expression tag	UNP Q7NGR7
F	320	HIS	-	expression tag	UNP Q7NGR7
F	321	HIS	-	expression tag	UNP Q7NGR7
F	322	HIS	-	expression tag	UNP Q7NGR7
F	323	HIS	-	expression tag	UNP Q7NGR7

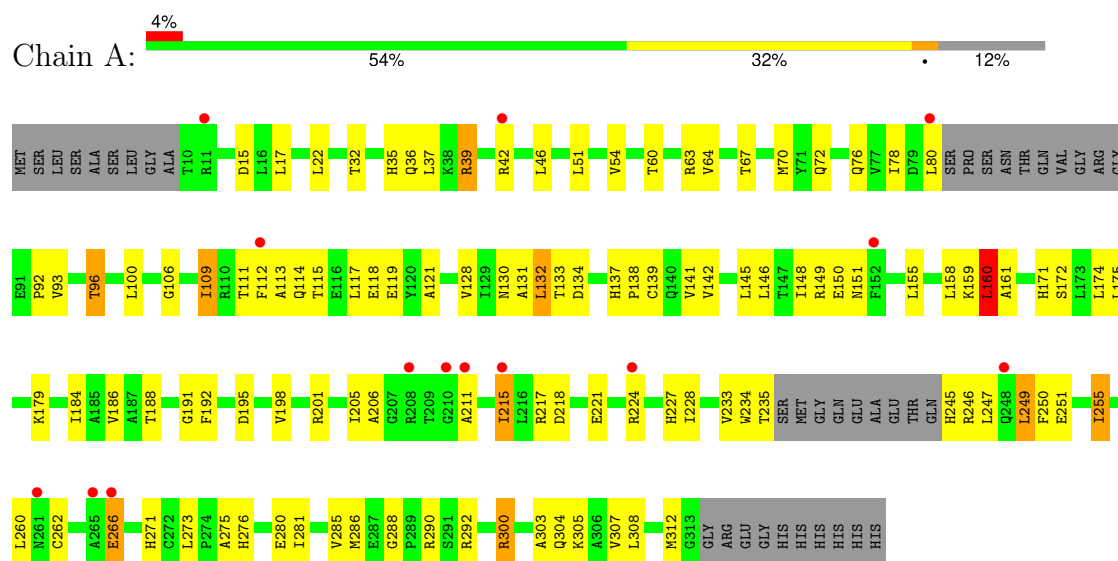
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	17	Total O 17 17	0	0
2	B	37	Total O 37 37	0	0
2	C	34	Total O 34 34	0	0
2	D	8	Total O 8 8	0	0
2	E	23	Total O 23 23	0	0
2	F	14	Total O 14 14	0	0

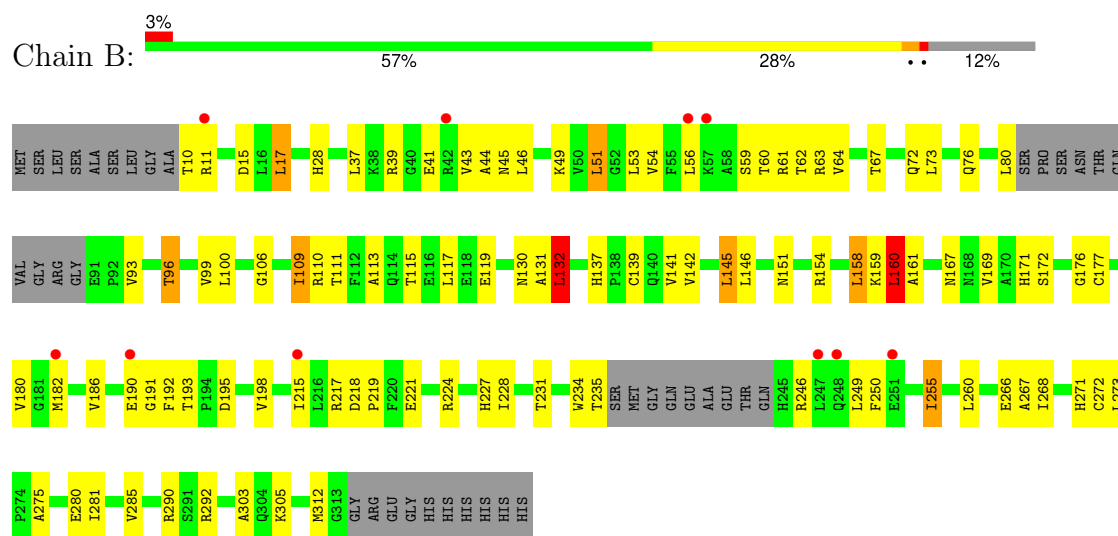
### 3 Residue-property plots [i](#)

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: Ornithine carbamoyltransferase



#### • Molecule 1: Ornithine carbamoyltransferase

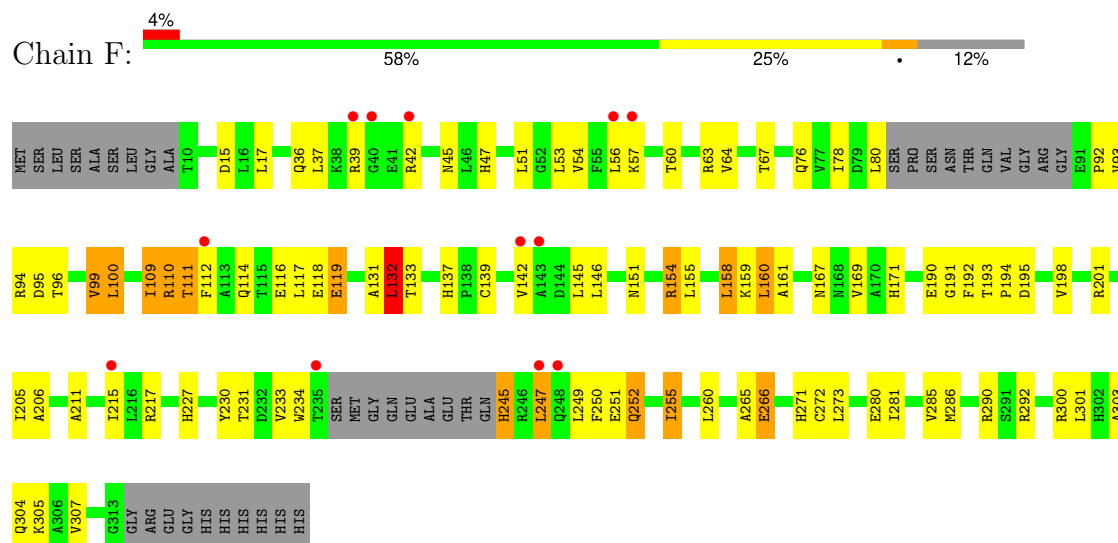


#### • Molecule 1: Ornithine carbamoyltransferase









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.56Å 142.42Å 149.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.94 – 2.10 39.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.94-2.10) 99.8 (39.77-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.271 0.239 , 0.271	Depositor DCC
$R_{free}$ test set	6195 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13303	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.34	0/2233	0.60	1/3031 (0.0%)
1	B	0.39	0/2233	0.64	1/3031 (0.0%)
1	C	0.38	0/2233	0.62	1/3031 (0.0%)
1	D	0.33	0/2233	0.59	0/3031
1	E	0.34	0/2233	0.59	0/3031
1	F	0.35	0/2233	0.61	0/3031
All	All	0.35	0/13398	0.61	3/18186 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	LEU	CA-CB-CG	5.65	128.30	115.30
1	A	160	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	160	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2195	0	2198	96	0
1	B	2195	0	2198	114	0
1	C	2195	0	2198	85	0
1	D	2195	0	2198	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2195	0	2198	87	0
1	F	2195	0	2198	85	0
2	A	17	0	0	3	0
2	B	37	0	0	4	0
2	C	34	0	0	1	0
2	D	8	0	0	3	0
2	E	23	0	0	1	0
2	F	14	0	0	1	0
All	All	13303	0	13188	548	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 21.

All (548) 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:D:54:VAL:HG13	1:D:109:ILE:HB	1.27	1.12
1:A:54:VAL:HG13	1:A:109:ILE:HB	1.30	1.10
1:C:54:VAL:HG13	1:C:109:ILE:HB	1.34	1.06
1:F:56:LEU:HD22	1:F:111:THR:HG23	1.40	1.03
1:B:145:LEU:HD11	1:B:182:MET:CE	1.93	0.97
1:B:54:VAL:HG13	1:B:109:ILE:HB	1.44	0.96
1:A:300:ARG:HH11	1:A:300:ARG:HB3	1.29	0.95
1:A:142:VAL:HG23	1:A:303:ALA:HB1	1.49	0.94
1:F:271:HIS:HD2	1:F:273:LEU:H	1.10	0.94
1:D:151:ASN:HD21	1:D:292:ARG:HE	1.03	0.93
1:D:271:HIS:HD2	1:D:273:LEU:H	1.16	0.93
1:E:271:HIS:HD2	1:E:273:LEU:H	1.07	0.92
1:A:271:HIS:HD2	1:A:273:LEU:H	1.14	0.91
1:B:271:HIS:HD2	1:B:273:LEU:H	1.18	0.91
1:D:142:VAL:HG23	1:D:303:ALA:HB1	1.51	0.91
1:B:151:ASN:HD21	1:B:292:ARG:HE	1.17	0.91
1:B:177:CYS:HA	1:B:182:MET:HE2	1.51	0.90
1:F:54:VAL:HG13	1:F:109:ILE:HB	1.52	0.89
1:B:142:VAL:HG23	1:B:303:ALA:HB1	1.51	0.89
1:C:142:VAL:HG23	1:C:303:ALA:HB1	1.55	0.89
1:D:255:ILE:HD11	1:D:285:VAL:HG11	1.55	0.89
1:C:271:HIS:HD2	1:C:273:LEU:H	1.16	0.89
1:F:252:GLN:H	1:F:252:GLN:NE2	1.73	0.86
1:E:54:VAL:HG13	1:E:109:ILE:HB	1.55	0.86
1:B:177:CYS:HA	1:B:182:MET:CE	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLY:HA3	1:F:249:LEU:HD13	1.58	0.85
1:B:63:ARG:O	1:B:67:THR:HG22	1.75	0.85
1:C:151:ASN:HD21	1:C:292:ARG:HE	1.17	0.85
1:E:255:ILE:HD11	1:E:285:VAL:HG11	1.57	0.85
1:D:151:ASN:HD21	1:D:292:ARG:NE	1.74	0.85
1:C:56:LEU:HD22	1:C:111:THR:HG22	1.59	0.85
1:E:159:LYS:H	1:E:227:HIS:HD2	1.24	0.84
1:C:255:ILE:HG23	1:C:281:ILE:HG22	1.59	0.83
1:C:216:LEU:HD11	1:C:222:ALA:HB2	1.60	0.83
1:D:151:ASN:ND2	1:D:292:ARG:HE	1.77	0.83
1:E:271:HIS:CD2	1:E:273:LEU:H	1.94	0.82
1:B:177:CYS:CA	1:B:182:MET:HG3	2.10	0.82
1:C:195:ASP:O	1:C:198:VAL:HG22	1.79	0.82
1:B:59:SER:HB2	1:B:110:ARG:HH11	1.45	0.81
1:B:177:CYS:HA	1:B:182:MET:HG3	1.62	0.81
1:A:54:VAL:CG1	1:A:109:ILE:HB	2.08	0.81
1:A:63:ARG:O	1:A:67:THR:HG22	1.82	0.80
1:F:142:VAL:HG23	1:F:303:ALA:HB1	1.63	0.80
1:B:177:CYS:HA	1:B:182:MET:CG	2.12	0.80
1:C:63:ARG:O	1:C:67:THR:HG22	1.82	0.80
1:A:201:ARG:CZ	1:A:205:ILE:HD11	2.11	0.79
1:B:145:LEU:HD11	1:B:182:MET:HE3	1.64	0.79
1:A:280:GLU:HG2	1:A:281:ILE:HG13	1.62	0.79
1:A:159:LYS:H	1:A:227:HIS:HD2	1.28	0.79
1:C:151:ASN:ND2	1:C:292:ARG:HE	1.81	0.79
1:E:160:LEU:HD12	1:E:161:ALA:N	1.98	0.79
1:B:180:VAL:HG23	1:B:182:MET:HG2	1.64	0.78
1:B:131:ALA:O	1:B:132:LEU:HB2	1.82	0.78
1:C:131:ALA:O	1:C:132:LEU:HB2	1.81	0.78
1:F:45:ASN:HD21	1:F:47:HIS:HB2	1.51	0.76
1:A:300:ARG:HB3	1:A:300:ARG:NH1	2.01	0.76
1:B:54:VAL:CG1	1:B:109:ILE:HB	2.14	0.76
1:B:159:LYS:H	1:B:227:HIS:HD2	1.34	0.76
1:B:106:GLY:HA3	1:B:312:MET:CE	2.16	0.75
1:F:151:ASN:HD21	1:F:292:ARG:HE	1.34	0.75
1:E:63:ARG:O	1:E:67:THR:HG22	1.85	0.75
1:E:160:LEU:HD13	1:E:228:ILE:HB	1.68	0.75
1:B:109:ILE:HD11	1:B:111:THR:HG23	1.68	0.75
1:B:151:ASN:ND2	1:B:292:ARG:HE	1.84	0.74
1:D:247:LEU:O	1:D:251:GLU:HG3	1.87	0.74
1:E:142:VAL:HG23	1:E:303:ALA:HB1	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:TRP:HB2	1:A:246:ARG:HH12	1.53	0.74
1:F:255:ILE:HD11	1:F:285:VAL:HG11	1.69	0.74
1:A:201:ARG:NH1	1:A:205:ILE:HD11	2.03	0.73
1:C:159:LYS:H	1:C:227:HIS:HD2	1.35	0.73
1:E:59:SER:HB2	1:E:110:ARG:NH1	2.04	0.73
1:D:159:LYS:H	1:D:227:HIS:HD2	1.36	0.73
1:F:95:ASP:O	1:F:99:VAL:HG12	1.88	0.73
1:F:60:THR:O	1:F:64:VAL:HG12	1.90	0.72
1:B:106:GLY:HA3	1:B:312:MET:HE1	1.71	0.72
1:B:177:CYS:CA	1:B:182:MET:HE2	2.18	0.72
1:B:109:ILE:HD11	1:B:111:THR:CG2	2.19	0.72
1:D:277:ARG:NH1	1:D:286:MET:SD	2.63	0.71
1:C:139:CYS:O	1:C:142:VAL:HG22	1.90	0.71
1:E:59:SER:HB2	1:E:110:ARG:HH11	1.55	0.71
1:F:195:ASP:O	1:F:198:VAL:HG22	1.90	0.71
1:D:304:GLN:HA	1:D:307:VAL:HG22	1.73	0.70
1:F:131:ALA:O	1:F:132:LEU:HB2	1.90	0.70
1:C:45:ASN:HD21	1:C:47:HIS:HB2	1.54	0.70
1:B:177:CYS:HA	1:B:182:MET:SD	2.31	0.70
1:F:271:HIS:CD2	1:F:273:LEU:H	2.02	0.70
1:D:142:VAL:CG2	1:D:303:ALA:HB1	2.20	0.69
1:E:60:THR:O	1:E:64:VAL:HG12	1.92	0.69
1:C:113:ALA:HB1	1:C:115:THR:HG22	1.73	0.69
1:C:271:HIS:CD2	1:C:273:LEU:H	2.06	0.69
1:D:154:ARG:HG3	1:D:158:LEU:HD11	1.75	0.69
1:B:151:ASN:HD21	1:B:292:ARG:NE	1.91	0.68
1:B:271:HIS:CD2	1:B:273:LEU:H	2.07	0.68
1:B:142:VAL:CG2	1:B:303:ALA:HB1	2.22	0.68
1:A:131:ALA:O	1:A:132:LEU:HB2	1.93	0.68
1:C:151:ASN:HD21	1:C:292:ARG:NE	1.89	0.68
1:F:36:GLN:HE22	1:F:42:ARG:HH11	1.41	0.68
1:E:151:ASN:ND2	1:E:292:ARG:HE	1.93	0.67
1:A:300:ARG:NH1	1:A:304:GLN:OE1	2.26	0.67
1:A:247:LEU:O	1:A:251:GLU:HB2	1.94	0.67
1:E:231:THR:HG21	1:E:281:ILE:HG23	1.76	0.67
1:D:201:ARG:CZ	1:D:205:ILE:HD11	2.23	0.67
1:A:255:ILE:HG23	1:A:281:ILE:HG23	1.77	0.67
1:A:142:VAL:CG2	1:A:303:ALA:HB1	2.24	0.67
1:B:192:PHE:CE1	1:B:249:LEU:HD21	2.30	0.66
1:B:180:VAL:CG2	1:B:182:MET:HG2	2.25	0.66
1:D:76:GLN:NE2	1:F:76:GLN:HE22	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:ILE:HG23	1:E:281:ILE:HG22	1.78	0.66
1:A:151:ASN:HD21	1:A:292:ARG:HE	1.42	0.66
1:D:160:LEU:HD12	1:D:161:ALA:N	2.11	0.66
1:F:160:LEU:HD12	1:F:161:ALA:N	2.10	0.66
1:F:231:THR:HG21	1:F:281:ILE:HG23	1.78	0.66
1:D:271:HIS:CD2	1:D:273:LEU:H	2.07	0.66
1:D:139:CYS:O	1:D:142:VAL:HG22	1.95	0.66
1:A:148:ILE:HD13	1:A:228:ILE:HD13	1.77	0.65
1:A:304:GLN:O	1:A:307:VAL:HG22	1.97	0.65
1:D:19:LEU:HD23	1:D:19:LEU:O	1.96	0.65
1:E:113:ALA:HB1	1:E:115:THR:HG22	1.78	0.65
1:E:151:ASN:HD21	1:E:292:ARG:HE	1.43	0.65
1:D:76:GLN:HE22	1:F:76:GLN:HE22	1.45	0.65
1:A:137:HIS:HD2	2:A:324:HOH:O	1.80	0.65
1:E:131:ALA:O	1:E:132:LEU:HB2	1.95	0.65
1:A:224:ARG:HA	1:A:262:CYS:O	1.97	0.64
1:B:139:CYS:O	1:B:142:VAL:HG22	1.98	0.64
1:C:255:ILE:HD11	1:C:285:VAL:HG11	1.78	0.64
1:B:142:VAL:HG23	1:B:303:ALA:CB	2.26	0.64
1:C:142:VAL:CG2	1:C:303:ALA:HB1	2.26	0.64
1:A:32:THR:O	1:A:36:GLN:HG3	1.97	0.64
1:A:174:LEU:HD23	1:A:184:ILE:HD13	1.80	0.64
1:A:271:HIS:CD2	1:A:273:LEU:H	2.06	0.64
1:E:93:VAL:HA	1:E:96:THR:HG23	1.80	0.64
1:A:93:VAL:HA	1:A:96:THR:HG23	1.78	0.64
1:A:22:LEU:O	1:A:179:LYS:HE2	1.99	0.63
1:A:234:TRP:HB2	1:A:246:ARG:NH1	2.12	0.63
1:B:160:LEU:HD22	1:B:228:ILE:HB	1.81	0.63
1:A:217:ARG:HA	1:A:217:ARG:HH21	1.65	0.62
1:B:176:GLY:O	1:B:182:MET:HE2	1.99	0.62
1:B:191:GLY:HA3	1:E:249:LEU:HD13	1.80	0.62
1:D:280:GLU:HG2	1:D:281:ILE:HG13	1.82	0.62
1:F:201:ARG:CZ	1:F:205:ILE:HD11	2.28	0.62
1:B:72:GLN:HE21	1:B:305:LYS:NZ	1.98	0.62
1:B:176:GLY:C	1:B:182:MET:HE2	2.19	0.62
1:A:146:LEU:O	1:A:150:GLU:HG3	1.99	0.62
1:F:56:LEU:HD22	1:F:111:THR:CG2	2.25	0.62
1:F:159:LYS:H	1:F:227:HIS:HD2	1.47	0.62
1:B:145:LEU:HD11	1:B:182:MET:HE1	1.81	0.61
1:E:35:HIS:O	1:E:39:ARG:HG2	1.99	0.61
1:D:255:ILE:HG13	1:D:281:ILE:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ILE:HD11	1:B:285:VAL:HG11	1.82	0.61
1:F:190:GLU:HA	1:F:217:ARG:NH1	2.15	0.61
1:A:106:GLY:HA3	1:A:312:MET:CE	2.31	0.61
1:D:234:TRP:CE2	1:D:250:PHE:HB3	2.36	0.61
1:D:301:LEU:O	1:D:305:LYS:HG3	2.00	0.61
1:D:304:GLN:O	1:D:307:VAL:HG22	2.00	0.61
1:B:39:ARG:HB2	1:B:41:GLU:HG3	1.83	0.60
1:D:63:ARG:O	1:D:67:THR:HG22	2.01	0.60
1:B:195:ASP:O	1:B:198:VAL:HG22	2.00	0.60
1:C:64:VAL:HA	1:C:67:THR:CG2	2.32	0.60
1:D:195:ASP:O	1:D:198:VAL:HG22	2.00	0.60
1:F:255:ILE:HG23	1:F:281:ILE:HG22	1.83	0.60
1:B:217:ARG:HH21	1:B:217:ARG:HA	1.66	0.60
1:D:255:ILE:HG13	1:D:255:ILE:O	2.00	0.60
1:E:195:ASP:O	1:E:198:VAL:HG22	2.02	0.60
1:A:139:CYS:O	1:A:142:VAL:HG22	2.02	0.60
1:D:159:LYS:H	1:D:227:HIS:CD2	2.17	0.60
1:F:304:GLN:O	1:F:307:VAL:HG22	2.01	0.60
1:C:186:VAL:HG13	1:C:215:ILE:HA	1.84	0.59
1:B:215:ILE:HG13	1:B:215:ILE:O	2.02	0.59
1:D:216:LEU:N	1:D:216:LEU:HD12	2.17	0.59
1:F:255:ILE:HG13	1:F:255:ILE:O	2.01	0.59
1:E:255:ILE:HG13	1:E:255:ILE:O	2.01	0.59
1:D:192:PHE:HE1	1:D:249:LEU:HD21	1.67	0.59
1:E:54:VAL:CG1	1:E:109:ILE:HB	2.28	0.59
1:F:57:LYS:HB3	1:F:110:ARG:HD2	1.84	0.59
1:C:142:VAL:HG23	1:C:303:ALA:CB	2.31	0.59
1:E:208:ARG:HB2	1:E:208:ARG:NH1	2.18	0.59
1:B:231:THR:HG21	1:B:281:ILE:HG23	1.84	0.59
1:D:277:ARG:HG3	2:D:330:HOH:O	2.01	0.59
1:C:111:THR:O	1:C:133:THR:HA	2.03	0.59
1:E:139:CYS:O	1:E:142:VAL:HG22	2.02	0.58
1:B:137:HIS:HD2	2:B:324:HOH:O	1.85	0.58
1:B:171:HIS:CD2	1:B:198:VAL:HG21	2.38	0.58
1:C:95:ASP:O	1:C:99:VAL:HG12	2.03	0.58
1:F:111:THR:HG22	1:F:112:PHE:H	1.68	0.58
1:D:91:GLU:OE1	1:D:96:THR:HG22	2.04	0.58
1:D:217:ARG:HA	1:D:217:ARG:HH21	1.69	0.58
1:E:109:ILE:HD11	1:E:111:THR:CG2	2.33	0.58
1:F:304:GLN:HA	1:F:307:VAL:HG22	1.85	0.58
1:E:159:LYS:N	1:E:227:HIS:HD2	1.99	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:HD11	1:A:285:VAL:HG11	1.86	0.58
1:D:64:VAL:HA	1:D:67:THR:HG22	1.86	0.57
1:F:151:ASN:ND2	1:F:292:ARG:HE	2.01	0.57
1:A:132:LEU:HD23	1:A:133:THR:N	2.20	0.57
1:F:201:ARG:O	1:F:205:ILE:HG12	2.05	0.57
1:A:60:THR:O	1:A:64:VAL:HG12	2.04	0.57
1:E:192:PHE:HE2	1:E:235:THR:HG21	1.70	0.57
1:F:167:ASN:OD1	1:F:169:VAL:HG22	2.05	0.57
1:F:151:ASN:HD21	1:F:292:ARG:NE	2.01	0.57
1:F:252:GLN:H	1:F:252:GLN:CD	2.09	0.57
1:F:93:VAL:HG21	1:F:119:GLU:HB3	1.87	0.56
1:D:67:THR:CG2	1:F:78:ILE:HD13	2.36	0.56
1:E:195:ASP:HB3	1:E:198:VAL:HG13	1.86	0.56
1:F:114:GLN:O	1:F:118:GLU:HG3	2.05	0.56
1:D:226:ALA:O	1:D:263:ALA:HB1	2.06	0.56
1:E:159:LYS:H	1:E:227:HIS:CD2	2.15	0.56
1:D:76:GLN:NE2	1:E:76:GLN:HE22	2.03	0.56
1:F:217:ARG:HA	1:F:217:ARG:HH21	1.69	0.56
1:C:234:TRP:CE2	1:C:250:PHE:HB3	2.41	0.56
1:F:63:ARG:O	1:F:67:THR:HG22	2.05	0.56
1:F:111:THR:O	1:F:133:THR:HA	2.05	0.56
1:D:189:PRO:HG3	1:D:253:TYR:CE2	2.39	0.56
1:C:72:GLN:HE21	1:C:305:LYS:NZ	2.04	0.56
1:D:146:LEU:O	1:D:150:GLU:HG3	2.05	0.55
1:B:76:GLN:NE2	1:C:76:GLN:HE22	2.04	0.55
1:A:245:HIS:HE1	1:F:193:THR:O	1.89	0.55
1:B:235:THR:HG22	1:B:250:PHE:CE2	2.41	0.55
1:C:106:GLY:HA3	1:C:312:MET:HE2	1.88	0.55
1:B:64:VAL:HA	1:B:67:THR:CG2	2.36	0.55
1:C:189:PRO:HG3	1:C:253:TYR:CE2	2.41	0.55
1:F:233:VAL:HG12	1:F:234:TRP:O	2.06	0.55
1:A:195:ASP:O	1:A:198:VAL:HG22	2.07	0.55
1:A:266:GLU:CD	1:A:266:GLU:H	2.10	0.55
1:C:106:GLY:HA3	1:C:312:MET:CE	2.37	0.55
1:C:109:ILE:HG13	1:C:110:ARG:N	2.21	0.55
1:D:64:VAL:HA	1:D:67:THR:CG2	2.37	0.55
1:E:234:TRP:CE2	1:E:250:PHE:HB3	2.42	0.55
1:C:233:VAL:HG12	1:C:234:TRP:O	2.07	0.54
1:F:139:CYS:O	1:F:142:VAL:HG22	2.07	0.54
1:B:106:GLY:HA3	1:B:312:MET:HE2	1.89	0.54
1:C:190:GLU:HA	1:C:217:ARG:CZ	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PHE:CE2	1:A:235:THR:HG21	2.42	0.54
1:A:171:HIS:CD2	1:A:198:VAL:HG21	2.43	0.54
1:D:93:VAL:HG21	1:D:119:GLU:HB3	1.89	0.54
1:E:17:LEU:HD12	1:E:117:LEU:HG	1.89	0.54
1:B:160:LEU:HD13	1:B:161:ALA:N	2.22	0.54
1:C:171:HIS:CD2	1:C:198:VAL:HG21	2.42	0.54
1:D:117:LEU:HD21	1:D:130:ASN:HB2	1.90	0.54
1:C:231:THR:HG21	1:C:281:ILE:HG23	1.90	0.54
1:C:249:LEU:HD13	1:D:191:GLY:HA3	1.90	0.54
1:D:160:LEU:HD23	1:D:177:CYS:SG	2.47	0.54
1:B:10:THR:OG1	1:B:11:ARG:N	2.40	0.54
1:A:307:VAL:HG23	1:A:308:LEU:N	2.23	0.54
1:A:76:GLN:NE2	1:B:76:GLN:HE22	2.05	0.54
1:A:300:ARG:HH11	1:A:300:ARG:CB	2.13	0.54
1:C:190:GLU:HA	1:C:217:ARG:NH1	2.23	0.54
1:B:224:ARG:HH11	1:B:224:ARG:HB2	1.74	0.53
1:C:64:VAL:HA	1:C:67:THR:HG22	1.88	0.53
1:F:190:GLU:HA	1:F:217:ARG:CZ	2.38	0.53
1:B:113:ALA:HB1	1:B:115:THR:HG22	1.90	0.53
1:E:160:LEU:HD13	1:E:228:ILE:CB	2.37	0.53
1:A:121:ALA:HA	1:A:128:VAL:HG21	1.90	0.53
1:D:217:ARG:NH2	1:D:217:ARG:HB2	2.24	0.53
1:E:160:LEU:HD12	1:E:161:ALA:H	1.70	0.53
1:C:267:ALA:O	1:C:290:ARG:HD3	2.08	0.53
1:D:76:GLN:HE22	1:E:76:GLN:HE22	1.56	0.53
1:E:266:GLU:CD	1:E:266:GLU:H	2.12	0.53
1:A:206:ALA:HB1	1:A:211:ALA:O	2.08	0.53
1:E:56:LEU:HD21	1:E:116:GLU:OE1	2.08	0.52
1:E:80:LEU:HD12	1:F:60:THR:HG23	1.90	0.52
1:E:174:LEU:HD23	1:E:184:ILE:HD13	1.91	0.52
1:A:234:TRP:CE2	1:A:250:PHE:HB3	2.44	0.52
1:B:267:ALA:N	1:B:290:ARG:HH21	2.06	0.52
1:E:137:HIS:HD2	2:E:324:HOH:O	1.93	0.52
1:A:149:ARG:HB2	1:A:155:LEU:HD21	1.90	0.52
1:C:56:LEU:HD13	1:C:111:THR:HG22	1.92	0.52
1:E:35:HIS:CE1	1:E:39:ARG:HE	2.27	0.52
1:E:114:GLN:O	1:E:118:GLU:HG3	2.10	0.52
1:F:271:HIS:HD2	1:F:273:LEU:N	1.93	0.52
1:A:249:LEU:HD13	1:F:191:GLY:HA3	1.91	0.52
1:B:72:GLN:NE2	1:B:305:LYS:HZ2	2.08	0.52
1:A:151:ASN:HD21	1:A:292:ARG:NE	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLN:NE2	1:B:305:LYS:NZ	2.57	0.52
1:D:137:HIS:HD2	2:D:324:HOH:O	1.92	0.52
1:A:109:ILE:HD11	1:A:111:THR:HG23	1.91	0.52
1:D:80:LEU:N	1:D:80:LEU:HD22	2.25	0.52
1:F:206:ALA:HB1	1:F:211:ALA:O	2.10	0.52
1:B:141:VAL:HG21	1:B:172:SER:HB3	1.92	0.52
1:D:109:ILE:HD11	1:D:111:THR:CG2	2.40	0.51
1:A:64:VAL:HA	1:A:67:THR:CG2	2.40	0.51
1:E:271:HIS:HE1	1:E:280:GLU:OE2	1.93	0.51
1:F:110:ARG:HG2	1:F:132:LEU:HB3	1.91	0.51
1:B:177:CYS:N	1:B:182:MET:HE2	2.25	0.51
1:C:56:LEU:CD2	1:C:111:THR:HG22	2.38	0.51
1:F:142:VAL:CG2	1:F:303:ALA:HB1	2.37	0.51
1:F:171:HIS:CD2	1:F:198:VAL:HG21	2.45	0.51
1:A:142:VAL:HG23	1:A:303:ALA:CB	2.32	0.51
1:D:159:LYS:N	1:D:227:HIS:HD2	2.07	0.51
1:E:64:VAL:HA	1:E:67:THR:CG2	2.41	0.51
1:B:109:ILE:CD1	1:B:111:THR:HG23	2.39	0.51
1:E:192:PHE:CE2	1:E:235:THR:HG21	2.46	0.51
1:B:64:VAL:HA	1:B:67:THR:HG22	1.92	0.51
1:D:201:ARG:NH1	1:D:205:ILE:HD11	2.25	0.51
1:D:266:GLU:H	1:D:266:GLU:CD	2.13	0.51
1:A:151:ASN:ND2	1:A:292:ARG:HE	2.09	0.50
1:D:142:VAL:HG23	1:D:303:ALA:CB	2.32	0.50
1:D:254:GLN:HG3	1:D:279:GLU:O	2.12	0.50
1:D:281:ILE:HD12	1:D:281:ILE:O	2.11	0.50
1:A:64:VAL:HA	1:A:67:THR:HG22	1.93	0.50
1:D:131:ALA:O	1:D:132:LEU:HB2	2.11	0.50
1:E:255:ILE:HG23	1:E:281:ILE:CG2	2.41	0.50
1:F:110:ARG:HD3	1:F:110:ARG:C	2.31	0.50
1:A:109:ILE:HD11	1:A:111:THR:CG2	2.41	0.50
1:C:255:ILE:O	1:C:255:ILE:HG13	2.10	0.50
1:E:79:ASP:O	1:E:80:LEU:HD13	2.12	0.50
1:F:247:LEU:O	1:F:251:GLU:HB2	2.10	0.50
1:C:139:CYS:HA	1:C:142:VAL:HG22	1.94	0.50
1:F:194:PRO:HD2	1:F:215:ILE:CD1	2.42	0.50
1:C:80:LEU:N	1:C:80:LEU:HD22	2.27	0.50
1:D:72:GLN:HE21	1:D:305:LYS:NZ	2.10	0.50
1:F:281:ILE:O	1:F:281:ILE:HD12	2.12	0.50
1:A:218:ASP:OD2	1:A:221:GLU:HB2	2.12	0.49
1:B:59:SER:HB2	1:B:110:ARG:NH1	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:TRP:CE2	1:B:250:PHE:HB3	2.46	0.49
1:D:272:CYS:O	1:D:273:LEU:HB2	2.12	0.49
1:E:121:ALA:HA	1:E:128:VAL:HG21	1.94	0.49
1:B:221:GLU:HA	1:B:224:ARG:HH12	1.77	0.49
1:B:255:ILE:HG23	1:B:281:ILE:CG2	2.42	0.49
1:F:111:THR:HG21	1:F:116:GLU:CD	2.32	0.49
1:B:145:LEU:CD1	1:B:182:MET:CE	2.81	0.49
1:F:192:PHE:CE1	1:F:249:LEU:HD21	2.47	0.49
1:A:93:VAL:HA	1:A:96:THR:CG2	2.41	0.49
1:D:214:GLN:HB3	1:D:216:LEU:HD11	1.93	0.49
1:D:233:VAL:HG13	1:D:276:HIS:CD2	2.47	0.49
1:A:106:GLY:HA3	1:A:312:MET:HE1	1.94	0.49
1:C:114:GLN:O	1:C:118:GLU:HG3	2.13	0.49
1:B:141:VAL:HG21	1:B:172:SER:CB	2.42	0.49
1:F:266:GLU:CD	1:F:266:GLU:H	2.15	0.49
1:B:15:ASP:HB3	1:B:17:LEU:HD13	1.94	0.49
1:E:155:LEU:O	1:E:158:LEU:HD23	2.13	0.49
1:B:96:THR:HA	1:B:99:VAL:HG12	1.95	0.49
1:C:304:GLN:O	1:C:307:VAL:HG22	2.13	0.49
1:E:146:LEU:O	1:E:150:GLU:HG3	2.13	0.49
1:A:175:LEU:O	1:A:179:LYS:HG3	2.13	0.48
1:D:109:ILE:HD11	1:D:111:THR:HG23	1.94	0.48
1:B:76:GLN:HE22	1:C:76:GLN:HE22	1.61	0.48
1:B:117:LEU:HD21	1:B:130:ASN:HB2	1.96	0.48
1:E:192:PHE:CE1	1:E:249:LEU:HD21	2.48	0.48
1:A:39:ARG:N	1:A:39:ARG:HD2	2.29	0.48
1:D:92:PRO:O	1:D:96:THR:HG23	2.14	0.48
1:F:56:LEU:CD2	1:F:111:THR:HG23	2.27	0.48
1:A:36:GLN:HB3	1:A:42:ARG:HB2	1.96	0.48
1:B:177:CYS:O	1:B:182:MET:HG3	2.14	0.48
1:C:109:ILE:HD11	1:C:111:THR:CG2	2.43	0.48
1:D:67:THR:HG21	1:F:78:ILE:HD13	1.95	0.48
1:E:267:ALA:O	1:E:290:ARG:HD3	2.13	0.48
1:C:159:LYS:H	1:C:227:HIS:CD2	2.25	0.48
1:C:247:LEU:O	1:C:251:GLU:HB2	2.14	0.48
1:D:160:LEU:HD12	1:D:161:ALA:H	1.76	0.48
1:F:15:ASP:HB3	1:F:17:LEU:HD13	1.96	0.48
1:F:271:HIS:HE1	1:F:280:GLU:OE2	1.97	0.48
1:A:72:GLN:HE21	1:A:305:LYS:NZ	2.12	0.48
1:B:167:ASN:OD1	1:B:169:VAL:HG22	2.14	0.48
1:D:54:VAL:CG1	1:D:109:ILE:HB	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:CYS:C	1:B:182:MET:HG3	2.34	0.48
1:D:231:THR:HG21	1:D:281:ILE:HG23	1.95	0.48
1:F:234:TRP:CE2	1:F:250:PHE:HB3	2.49	0.48
1:F:301:LEU:O	1:F:305:LYS:HG3	2.14	0.48
1:A:186:VAL:HG13	1:A:215:ILE:HA	1.95	0.48
1:A:275:ALA:HB1	1:A:281:ILE:HD11	1.94	0.48
1:F:64:VAL:HA	1:F:67:THR:HG22	1.96	0.48
1:D:192:PHE:CE1	1:D:249:LEU:HD21	2.49	0.47
1:C:59:SER:HB2	1:C:110:ARG:NH1	2.29	0.47
1:D:114:GLN:O	1:D:118:GLU:HG3	2.13	0.47
1:F:272:CYS:O	1:F:273:LEU:HB2	2.14	0.47
1:C:137:HIS:HD2	2:C:327:HOH:O	1.96	0.47
1:B:45:ASN:HA	1:B:73:LEU:O	2.14	0.47
1:B:28:HIS:HE1	2:B:340:HOH:O	1.98	0.47
1:C:109:ILE:HD11	1:C:111:THR:HG23	1.96	0.47
1:E:51:LEU:HD13	1:E:53:LEU:HD21	1.96	0.47
1:E:194:PRO:HD2	1:E:215:ILE:HD13	1.96	0.47
1:C:56:LEU:HD22	1:C:111:THR:CG2	2.35	0.47
1:D:91:GLU:HG3	1:D:96:THR:HG22	1.97	0.47
1:D:234:TRP:CZ3	1:D:279:GLU:HB3	2.50	0.47
1:A:288:GLY:HA3	2:A:325:HOH:O	2.13	0.47
1:B:177:CYS:CA	1:B:182:MET:CE	2.82	0.47
1:B:280:GLU:HG2	1:B:281:ILE:HG13	1.97	0.47
1:E:142:VAL:CG2	1:E:303:ALA:HB1	2.42	0.47
1:E:208:ARG:HH11	1:E:208:ARG:CB	2.26	0.47
1:B:272:CYS:O	1:B:273:LEU:HB2	2.15	0.47
1:C:271:HIS:HE1	1:C:280:GLU:OE2	1.97	0.47
1:B:43:VAL:HG12	1:B:44:ALA:N	2.29	0.47
1:F:160:LEU:HD11	1:F:230:TYR:HB2	1.96	0.47
1:C:186:VAL:HG13	1:C:186:VAL:O	2.15	0.46
1:C:187:ALA:HA	1:C:216:LEU:O	2.14	0.46
1:F:100:LEU:HD12	1:F:100:LEU:HA	1.80	0.46
1:E:109:ILE:HD11	1:E:111:THR:HG21	1.97	0.46
1:A:192:PHE:HE2	1:A:235:THR:HG21	1.79	0.46
1:B:271:HIS:HE1	1:B:280:GLU:OE2	1.99	0.46
1:D:206:ALA:HB1	1:D:211:ALA:O	2.13	0.46
1:B:46:LEU:O	1:B:49:LYS:HB2	2.15	0.46
1:B:221:GLU:OE2	1:B:224:ARG:NH2	2.45	0.46
1:D:206:ALA:HB2	1:D:213:VAL:HG23	1.97	0.46
1:D:162:TYR:HD2	1:D:186:VAL:HG23	1.80	0.46
1:A:92:PRO:O	1:A:96:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLY:HA3	1:A:312:MET:HE2	1.97	0.46
1:B:145:LEU:CG	1:B:182:MET:HE1	2.46	0.46
1:C:186:VAL:CG1	1:C:215:ILE:HA	2.45	0.46
1:F:109:ILE:HG12	1:F:117:LEU:HD13	1.97	0.46
1:A:255:ILE:HG23	1:A:281:ILE:CG2	2.45	0.46
1:B:61:ARG:HH11	1:B:61:ARG:HB2	1.81	0.46
1:D:151:ASN:ND2	1:D:292:ARG:NE	2.50	0.46
1:B:60:THR:O	1:B:64:VAL:HG12	2.16	0.46
1:B:255:ILE:HG13	1:B:255:ILE:O	2.16	0.46
1:D:144:ASP:OD1	1:D:296:GLU:OE1	2.34	0.46
1:E:160:LEU:HD13	1:E:228:ILE:CG2	2.46	0.46
1:D:91:GLU:CD	1:D:96:THR:HG22	2.36	0.45
1:C:59:SER:HB2	1:C:110:ARG:HH11	1.81	0.45
1:C:186:VAL:HG12	1:C:214:GLN:O	2.16	0.45
1:D:67:THR:HG23	1:F:78:ILE:HD13	1.97	0.45
1:F:92:PRO:HB3	1:F:94:ARG:NH1	2.31	0.45
1:A:35:HIS:O	1:A:39:ARG:HD3	2.15	0.45
1:E:272:CYS:O	1:E:273:LEU:HB2	2.16	0.45
1:A:201:ARG:O	1:A:205:ILE:HG12	2.16	0.45
1:C:272:CYS:O	1:C:273:LEU:HB2	2.16	0.45
1:C:46:LEU:HD21	1:C:313:GLY:HA2	1.98	0.45
1:C:217:ARG:HA	1:C:217:ARG:HH21	1.82	0.45
1:C:154:ARG:NH1	1:C:156:ALA:O	2.50	0.45
1:B:145:LEU:CD1	1:B:182:MET:HE1	2.44	0.45
1:C:72:GLN:HE21	1:C:305:LYS:HZ1	1.65	0.45
1:E:136:GLU:HG2	1:E:172:SER:OG	2.17	0.45
1:E:56:LEU:HD13	1:E:111:THR:HG22	1.97	0.45
1:D:186:VAL:HG13	1:D:186:VAL:O	2.18	0.44
1:E:110:ARG:HG3	1:E:132:LEU:HB3	2.00	0.44
1:A:188:THR:O	1:A:217:ARG:HD3	2.16	0.44
1:C:51:LEU:HD13	1:C:53:LEU:HD21	2.00	0.44
1:E:32:THR:O	1:E:36:GLN:HG3	2.17	0.44
1:E:141:VAL:HG12	1:E:145:LEU:HD22	1.98	0.44
1:A:227:HIS:C	1:A:228:ILE:HG13	2.37	0.44
1:E:116:GLU:O	1:E:119:GLU:HB2	2.18	0.44
1:A:15:ASP:HB3	1:A:17:LEU:HD13	1.98	0.44
1:B:218:ASP:HA	1:B:219:PRO:HD2	1.87	0.44
1:A:113:ALA:HB1	1:A:115:THR:HG22	1.99	0.44
1:B:109:ILE:HD11	1:B:111:THR:HG21	1.99	0.44
1:C:30:LEU:HD21	1:C:307:VAL:HG12	2.00	0.44
1:F:15:ASP:CB	1:F:17:LEU:HD13	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ARG:CZ	1:B:158:LEU:HD13	2.47	0.44
1:D:131:ALA:O	1:D:132:LEU:CB	2.66	0.44
1:D:160:LEU:HD13	1:D:228:ILE:HB	1.99	0.44
1:D:233:VAL:HG13	1:D:276:HIS:HD2	1.83	0.44
1:E:167:ASN:OD1	1:E:169:VAL:HG22	2.17	0.44
1:A:307:VAL:CG2	1:A:308:LEU:N	2.80	0.44
1:B:255:ILE:HG23	1:B:281:ILE:HG22	1.99	0.44
1:A:141:VAL:HG21	1:A:172:SER:CB	2.47	0.44
1:B:61:ARG:HG3	1:B:62:THR:N	2.33	0.44
1:B:177:CYS:CB	1:B:182:MET:HG3	2.47	0.44
1:E:39:ARG:HB2	1:E:41:GLU:HG3	2.00	0.44
1:F:142:VAL:HG23	1:F:303:ALA:CB	2.41	0.44
1:B:72:GLN:HE21	1:B:305:LYS:HZ1	1.66	0.43
1:D:158:LEU:HA	1:D:227:HIS:CD2	2.53	0.43
1:B:93:VAL:HG22	2:B:327:HOH:O	2.16	0.43
1:B:99:VAL:HG13	1:B:100:LEU:N	2.33	0.43
1:A:115:THR:HA	1:A:118:GLU:OE1	2.17	0.43
1:D:109:ILE:HG13	1:D:110:ARG:N	2.32	0.43
1:D:155:LEU:C	1:D:158:LEU:HD13	2.38	0.43
1:E:141:VAL:HG21	1:E:172:SER:CB	2.48	0.43
1:B:190:GLU:HA	1:B:217:ARG:NH1	2.33	0.43
1:D:22:LEU:HD23	2:D:326:HOH:O	2.18	0.43
1:E:111:THR:O	1:E:133:THR:HA	2.17	0.43
1:A:114:GLN:O	1:A:118:GLU:HG3	2.19	0.43
1:F:36:GLN:NE2	1:F:42:ARG:HH11	2.12	0.43
1:D:56:LEU:HD22	1:D:111:THR:HG22	2.01	0.43
1:C:55:PHE:C	1:C:57:LYS:H	2.21	0.43
1:E:19:LEU:HD12	1:E:19:LEU:HA	1.77	0.43
1:E:231:THR:HG21	1:E:281:ILE:CG2	2.47	0.43
1:B:186:VAL:CG1	1:B:215:ILE:HG22	2.49	0.43
1:C:72:GLN:NE2	1:C:305:LYS:NZ	2.66	0.43
1:E:96:THR:HA	1:E:99:VAL:HG12	2.00	0.43
1:C:94:ARG:HB3	1:C:123:TYR:CE2	2.53	0.43
1:C:160:LEU:HD13	1:C:161:ALA:N	2.34	0.43
1:F:53:LEU:HD13	1:F:63:ARG:HG3	2.00	0.43
1:B:193:THR:HG22	2:B:331:HOH:O	2.19	0.42
1:E:194:PRO:HD2	1:E:215:ILE:CD1	2.49	0.42
1:C:227:HIS:O	1:C:267:ALA:HA	2.19	0.42
1:D:40:GLY:C	1:D:42:ARG:H	2.22	0.42
1:D:116:GLU:O	1:D:119:GLU:HB2	2.18	0.42
1:D:175:LEU:O	1:D:179:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:GLU:OE1	1:E:123:TYR:HE2	2.01	0.42
1:E:190:GLU:HA	1:E:217:ARG:NH1	2.34	0.42
1:B:159:LYS:H	1:B:227:HIS:CD2	2.24	0.42
1:E:190:GLU:HA	1:E:217:ARG:CZ	2.49	0.42
1:F:137:HIS:HD2	2:F:324:HOH:O	2.02	0.42
1:A:255:ILE:O	1:A:255:ILE:HG13	2.18	0.42
1:A:276:HIS:HD2	2:A:334:HOH:O	2.02	0.42
1:E:277:ARG:NH1	1:E:286:MET:SD	2.93	0.42
1:A:117:LEU:HD21	1:A:130:ASN:HB2	2.01	0.42
1:B:227:HIS:HB2	1:B:228:ILE:HD12	2.01	0.42
1:C:233:VAL:HG13	1:C:276:HIS:CD2	2.54	0.42
1:F:265:ALA:O	1:F:290:ARG:NH1	2.52	0.42
1:A:137:HIS:N	1:A:138:PRO:HD3	2.34	0.42
1:E:33:LEU:O	1:E:37:LEU:HD13	2.19	0.42
1:E:64:VAL:HA	1:E:67:THR:HG22	2.01	0.42
1:A:260:LEU:HD22	1:A:290:ARG:HD3	2.01	0.42
1:A:271:HIS:HE1	1:A:280:GLU:OE2	2.02	0.42
1:B:56:LEU:HD13	1:B:111:THR:HG22	2.01	0.42
1:C:15:ASP:HB3	1:C:17:LEU:HD13	2.01	0.42
1:D:53:LEU:HD23	1:D:108:ALA:HB3	2.02	0.42
1:D:268:ILE:HG12	1:D:292:ARG:HG3	2.02	0.42
1:F:194:PRO:HD2	1:F:215:ILE:HD11	2.00	0.42
1:C:13:ARG:HG3	1:C:13:ARG:HH11	1.84	0.42
1:C:281:ILE:C	1:C:281:ILE:HD12	2.40	0.42
1:A:215:ILE:HG23	1:A:215:ILE:O	2.20	0.42
1:F:255:ILE:HG23	1:F:281:ILE:CG2	2.48	0.42
1:A:15:ASP:CB	1:A:17:LEU:HD13	2.50	0.42
1:C:145:LEU:HD12	1:C:145:LEU:HA	1.93	0.41
1:E:139:CYS:HA	1:E:142:VAL:HG22	2.01	0.41
1:B:131:ALA:O	1:B:132:LEU:CB	2.57	0.41
1:E:78:ILE:HD13	1:F:67:THR:CG2	2.50	0.41
1:E:189:PRO:HG3	1:E:253:TYR:CE2	2.55	0.41
1:F:154:ARG:CG	1:F:155:LEU:N	2.83	0.41
1:A:78:ILE:HD13	1:B:67:THR:HG23	2.01	0.41
1:B:43:VAL:CG1	1:B:44:ALA:N	2.83	0.41
1:B:177:CYS:O	1:B:182:MET:CG	2.68	0.41
1:C:19:LEU:HD12	1:C:19:LEU:HA	1.89	0.41
1:B:186:VAL:HG13	1:B:186:VAL:O	2.19	0.41
1:D:64:VAL:CA	1:D:67:THR:HG22	2.50	0.41
1:D:198:VAL:HG23	1:D:199:SER:N	2.34	0.41
1:D:277:ARG:HD3	1:D:283:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:VAL:HG23	1:E:308:LEU:N	2.34	0.41
1:F:281:ILE:HD13	1:F:286:MET:HB2	2.01	0.41
1:A:46:LEU:HD12	1:A:70:MET:SD	2.60	0.41
1:A:111:THR:O	1:A:133:THR:HA	2.21	0.41
1:B:275:ALA:HB1	1:B:281:ILE:HD11	2.01	0.41
1:D:72:GLN:NE2	1:D:305:LYS:NZ	2.68	0.41
1:F:96:THR:O	1:F:99:VAL:HG13	2.20	0.41
1:B:51:LEU:HD13	1:B:53:LEU:HD21	2.02	0.41
1:C:160:LEU:CD1	1:C:160:LEU:C	2.89	0.41
1:A:80:LEU:HD22	1:A:80:LEU:N	2.35	0.41
1:B:145:LEU:HD11	1:B:182:MET:SD	2.60	0.41
1:C:32:THR:O	1:C:36:GLN:HG3	2.20	0.41
1:D:121:ALA:HA	1:D:128:VAL:HG21	2.03	0.41
1:A:78:ILE:HD13	1:B:67:THR:CG2	2.51	0.41
1:B:193:THR:O	1:E:245:HIS:HE1	2.03	0.41
1:C:231:THR:HG21	1:C:281:ILE:CG2	2.51	0.41
1:D:217:ARG:HH21	1:D:217:ARG:CA	2.31	0.41
1:C:111:THR:HG21	1:C:116:GLU:OE2	2.20	0.41
1:C:309:ALA:O	1:C:313:GLY:HA3	2.20	0.41
1:D:218:ASP:OD2	1:D:221:GLU:HB2	2.20	0.41
1:E:15:ASP:HB2	1:E:17:LEU:CD2	2.51	0.41
1:F:155:LEU:O	1:F:158:LEU:HB2	2.21	0.41
1:A:112:PHE:O	1:A:134:ASP:HB2	2.21	0.40
1:A:160:LEU:HD13	1:A:161:ALA:N	2.35	0.40
1:C:138:PRO:O	1:C:142:VAL:HG13	2.21	0.40
1:D:275:ALA:HB1	1:D:281:ILE:HD11	2.02	0.40
1:D:174:LEU:HD23	1:D:184:ILE:HD13	2.03	0.40
1:C:186:VAL:HG13	1:C:215:ILE:CD1	2.51	0.40
1:F:245:HIS:O	1:F:249:LEU:HB2	2.22	0.40
1:B:190:GLU:HA	1:B:217:ARG:CZ	2.52	0.40
1:A:233:VAL:HG12	1:A:234:TRP:O	2.21	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	279/323 (86%)	266 (95%)	11 (4%)	2 (1%)	22	18
1	B	279/323 (86%)	267 (96%)	11 (4%)	1 (0%)	34	32
1	C	279/323 (86%)	268 (96%)	10 (4%)	1 (0%)	34	32
1	D	279/323 (86%)	259 (93%)	18 (6%)	2 (1%)	22	18
1	E	279/323 (86%)	266 (95%)	11 (4%)	2 (1%)	22	18
1	F	279/323 (86%)	268 (96%)	10 (4%)	1 (0%)	34	32
All	All	1674/1938 (86%)	1594 (95%)	71 (4%)	9 (0%)	29	26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	LEU
1	C	132	LEU
1	D	132	LEU
1	E	132	LEU
1	F	132	LEU
1	A	132	LEU
1	A	249	LEU
1	E	249	LEU
1	D	190	GLU

### 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	225/254 (89%)	210 (93%)	15 (7%)	16	13
1	B	225/254 (89%)	208 (92%)	17 (8%)	13	10
1	C	225/254 (89%)	209 (93%)	16 (7%)	14	11
1	D	225/254 (89%)	205 (91%)	20 (9%)	9	6
1	E	225/254 (89%)	211 (94%)	14 (6%)	18	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	225/254 (89%)	202 (90%)	23 (10%)	7	4
All	All	1350/1524 (89%)	1245 (92%)	105 (8%)	12	9

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	39	ARG
1	A	51	LEU
1	A	96	THR
1	A	100	LEU
1	A	109	ILE
1	A	119	GLU
1	A	145	LEU
1	A	158	LEU
1	A	160	LEU
1	A	215	ILE
1	A	255	ILE
1	A	266	GLU
1	A	286	MET
1	A	300	ARG
1	B	17	LEU
1	B	37	LEU
1	B	51	LEU
1	B	80	LEU
1	B	96	THR
1	B	109	ILE
1	B	119	GLU
1	B	132	LEU
1	B	145	LEU
1	B	146	LEU
1	B	158	LEU
1	B	160	LEU
1	B	246	ARG
1	B	255	ILE
1	B	260	LEU
1	B	266	GLU
1	B	268	ILE
1	C	17	LEU
1	C	37	LEU
1	C	39	ARG
1	C	51	LEU

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Mol	Chain	Res	Type
1	C	96	THR
1	C	100	LEU
1	C	109	ILE
1	C	132	LEU
1	C	145	LEU
1	C	146	LEU
1	C	158	LEU
1	C	160	LEU
1	C	217	ARG
1	C	246	ARG
1	C	255	ILE
1	C	266	GLU
1	D	17	LEU
1	D	37	LEU
1	D	39	ARG
1	D	51	LEU
1	D	54	VAL
1	D	96	THR
1	D	100	LEU
1	D	109	ILE
1	D	119	GLU
1	D	132	LEU
1	D	145	LEU
1	D	146	LEU
1	D	216	LEU
1	D	217	ARG
1	D	246	ARG
1	D	255	ILE
1	D	266	GLU
1	D	268	ILE
1	D	290	ARG
1	D	300	ARG
1	E	51	LEU
1	E	96	THR
1	E	100	LEU
1	E	109	ILE
1	E	119	GLU
1	E	132	LEU
1	E	145	LEU
1	E	146	LEU
1	E	215	ILE
1	E	217	ARG

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Mol	Chain	Res	Type
1	E	247	LEU
1	E	255	ILE
1	E	260	LEU
1	E	266	GLU
1	F	37	LEU
1	F	39	ARG
1	F	51	LEU
1	F	80	LEU
1	F	99	VAL
1	F	100	LEU
1	F	109	ILE
1	F	110	ARG
1	F	111	THR
1	F	119	GLU
1	F	132	LEU
1	F	145	LEU
1	F	146	LEU
1	F	154	ARG
1	F	158	LEU
1	F	160	LEU
1	F	245	HIS
1	F	247	LEU
1	F	252	GLN
1	F	255	ILE
1	F	260	LEU
1	F	266	GLU
1	F	300	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	76	GLN
1	A	137	HIS
1	A	151	ASN
1	A	227	HIS
1	A	245	HIS
1	A	271	HIS
1	A	276	HIS
1	B	28	HIS
1	B	45	ASN
1	B	72	GLN

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Mol	Chain	Res	Type
1	B	137	HIS
1	B	151	ASN
1	B	227	HIS
1	B	271	HIS
1	B	276	HIS
1	C	72	GLN
1	C	76	GLN
1	C	137	HIS
1	C	151	ASN
1	C	227	HIS
1	C	271	HIS
1	C	276	HIS
1	D	72	GLN
1	D	76	GLN
1	D	137	HIS
1	D	151	ASN
1	D	227	HIS
1	D	271	HIS
1	D	276	HIS
1	E	35	HIS
1	E	72	GLN
1	E	137	HIS
1	E	151	ASN
1	E	227	HIS
1	E	245	HIS
1	E	271	HIS
1	F	36	GLN
1	F	72	GLN
1	F	122	HIS
1	F	137	HIS
1	F	151	ASN
1	F	227	HIS
1	F	252	GLN
1	F	271	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	285/323 (88%)	0.28	14 (4%)	29 35	33, 45, 63, 77	0
1	B	285/323 (88%)	0.02	10 (3%)	44 50	26, 36, 54, 67	0
1	C	285/323 (88%)	-0.11	1 (0%)	92 93	26, 36, 51, 63	0
1	D	285/323 (88%)	0.57	20 (7%)	16 20	32, 50, 67, 73	0
1	E	285/323 (88%)	0.41	15 (5%)	26 32	30, 41, 63, 82	0
1	F	285/323 (88%)	0.17	12 (4%)	36 42	29, 41, 61, 74	0
All	All	1710/1938 (88%)	0.23	72 (4%)	36 42	26, 41, 62, 82	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	248	GLN	5.0
1	D	11	ARG	4.8
1	B	182	MET	4.5
1	B	248	GLN	4.2
1	D	122	HIS	4.2
1	E	11	ARG	4.0
1	D	313	GLY	4.0
1	A	224	ARG	3.9
1	A	210	GLY	3.8
1	E	141	VAL	3.5
1	D	248	GLN	3.3
1	E	10	THR	3.3
1	E	224	ARG	3.3
1	E	143	ALA	3.3
1	F	248	GLN	3.2
1	A	11	ARG	3.2
1	C	11	ARG	3.2
1	A	248	GLN	3.1
1	E	220	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	207	GLY	3.0
1	A	208	ARG	3.0
1	D	200	ALA	3.0
1	F	112	PHE	3.0
1	A	266	GLU	3.0
1	B	11	ARG	2.9
1	F	142	VAL	2.9
1	A	265	ALA	2.8
1	D	270	LEU	2.8
1	F	56	LEU	2.8
1	F	247	LEU	2.8
1	B	57	LYS	2.8
1	D	143	ALA	2.7
1	E	145	LEU	2.7
1	D	224	ARG	2.7
1	D	113	ALA	2.7
1	E	142	VAL	2.7
1	E	146	LEU	2.7
1	E	252	GLN	2.7
1	F	42	ARG	2.7
1	D	57	LYS	2.6
1	D	208	ARG	2.6
1	A	42	ARG	2.5
1	D	115	THR	2.5
1	D	265	ALA	2.5
1	A	112	PHE	2.5
1	F	57	LYS	2.5
1	D	261	ASN	2.4
1	B	251	GLU	2.4
1	F	39	ARG	2.4
1	D	123	TYR	2.4
1	A	80	LEU	2.4
1	D	220	PHE	2.4
1	F	215	ILE	2.4
1	A	261	ASN	2.3
1	E	43	VAL	2.3
1	A	211	ALA	2.3
1	F	40	GLY	2.3
1	B	42	ARG	2.3
1	F	235	THR	2.3
1	D	125	GLY	2.2
1	E	109	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	62	THR	2.1
1	B	190	GLU	2.1
1	B	56	LEU	2.1
1	B	247	LEU	2.1
1	D	221	GLU	2.1
1	F	143	ALA	2.1
1	A	152	PHE	2.1
1	A	215	ILE	2.0
1	D	140	GLN	2.0
1	B	215	ILE	2.0
1	E	139	CYS	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.