



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:42 PM GMT

PDB ID : 1Q6W  
Title : X-Ray structure of Monoamine oxidase regulatory protein from Archaeoglobus fulgius  
Authors : Fedorov, A.A.; Fedorov, E.V.; Thirumuruhan, R.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2003-08-14  
Resolution : 2.81 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

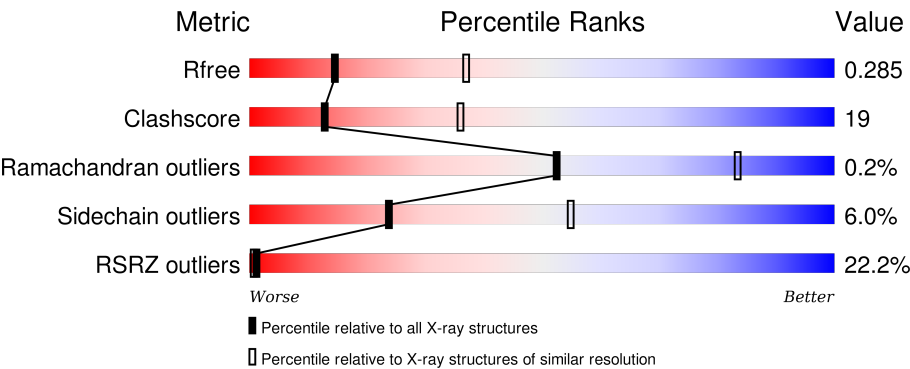
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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 <sub>free</sub>	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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. 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	161	<div><div>2%</div><div><div></div><div>60%</div><div>32%</div><div>• 6%</div></div></div>
1	B	161	<div><div>%</div><div><div></div><div>59%</div><div>32%</div><div>• 6%</div></div></div>
1	C	161	<div><div>%</div><div><div></div><div>61%</div><div>30%</div><div>• 5%</div></div></div>
1	D	161	<div><div>%</div><div><div></div><div>63%</div><div>29%</div><div>• 6%</div></div></div>
1	E	161	<div><div>%</div><div><div></div><div>63%</div><div>29%</div><div>• 6%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	161	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>60%31%6%</div></div>
1	G	161	<div><div><div></div><div></div><div></div><div></div></div><div>41%</div><div><div></div><div></div><div></div><div></div></div><div>57%33%7%</div></div>
1	H	161	<div><div><div></div><div></div><div></div><div></div></div><div>46%</div><div><div></div><div></div><div></div><div></div></div><div>53%37%7%</div></div>
1	I	161	<div><div><div></div><div></div><div></div><div></div></div><div>14%</div><div><div></div><div></div><div></div><div></div></div><div>52%37%7%</div></div>
1	J	161	<div><div><div></div><div></div><div></div><div></div></div><div>19%</div><div><div></div><div></div><div></div><div></div></div><div>55%35%7%</div></div>
1	K	161	<div><div><div></div><div></div><div></div><div></div></div><div>59%</div><div><div></div><div></div><div></div><div></div></div><div>57%34%7%</div></div>
1	L	161	<div><div><div></div><div></div><div></div><div></div></div><div>60%</div><div><div></div><div></div><div></div><div></div></div><div>60%30%7%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14224 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 monoamine oxidase regulatory protein, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	Se	0	0	0
			1192	779	190	221	2			
1	B	151	Total	C	N	O	Se	0	0	0
			1192	779	190	221	2			
1	C	153	Total	C	N	O	S	Se	0	0
			1208	790	192	223	1	2		
1	D	151	Total	C	N	O	Se	0	0	0
			1192	779	190	221	2			
1	E	151	Total	C	N	O	Se	0	0	0
			1192	779	190	221	2			
1	F	151	Total	C	N	O	Se	0	0	0
			1192	779	190	221	2			
1	G	149	Total	C	N	O	Se	0	0	0
			1176	770	185	219	2			
1	H	149	Total	C	N	O	Se	0	0	0
			1176	770	185	219	2			
1	I	149	Total	C	N	O	Se	0	0	0
			1176	770	185	219	2			
1	J	149	Total	C	N	O	Se	0	0	0
			1176	770	185	219	2			
1	K	149	Total	C	N	O	Se	0	0	0
			1176	770	185	219	2			
1	L	149	Total	C	N	O	Se	0	0	0
			1176	770	185	219	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	MSE	MET	MODIFIED RESIDUE	UNP O28346
A	78	MSE	MET	MODIFIED RESIDUE	UNP O28346
B	69	MSE	MET	MODIFIED RESIDUE	UNP O28346
B	78	MSE	MET	MODIFIED RESIDUE	UNP O28346
C	69	MSE	MET	MODIFIED RESIDUE	UNP O28346

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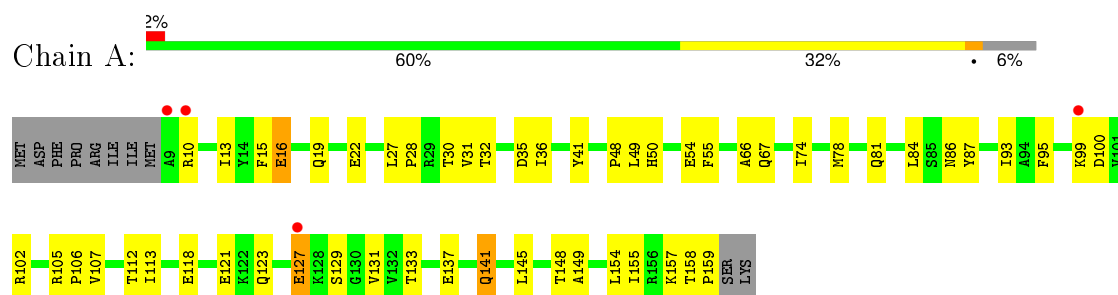
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Chain	Residue	Modelled	Actual	Comment	Reference
C	78	MSE	MET	MODIFIED RESIDUE	UNP O28346
D	69	MSE	MET	MODIFIED RESIDUE	UNP O28346
D	78	MSE	MET	MODIFIED RESIDUE	UNP O28346
E	69	MSE	MET	MODIFIED RESIDUE	UNP O28346
E	78	MSE	MET	MODIFIED RESIDUE	UNP O28346
F	69	MSE	MET	MODIFIED RESIDUE	UNP O28346
F	78	MSE	MET	MODIFIED RESIDUE	UNP O28346
G	69	MSE	MET	MODIFIED RESIDUE	UNP O28346
G	78	MSE	MET	MODIFIED RESIDUE	UNP O28346
H	69	MSE	MET	MODIFIED RESIDUE	UNP O28346
H	78	MSE	MET	MODIFIED RESIDUE	UNP O28346
I	69	MSE	MET	MODIFIED RESIDUE	UNP O28346
I	78	MSE	MET	MODIFIED RESIDUE	UNP O28346
J	69	MSE	MET	MODIFIED RESIDUE	UNP O28346
J	78	MSE	MET	MODIFIED RESIDUE	UNP O28346
K	69	MSE	MET	MODIFIED RESIDUE	UNP O28346
K	78	MSE	MET	MODIFIED RESIDUE	UNP O28346
L	69	MSE	MET	MODIFIED RESIDUE	UNP O28346
L	78	MSE	MET	MODIFIED RESIDUE	UNP O28346

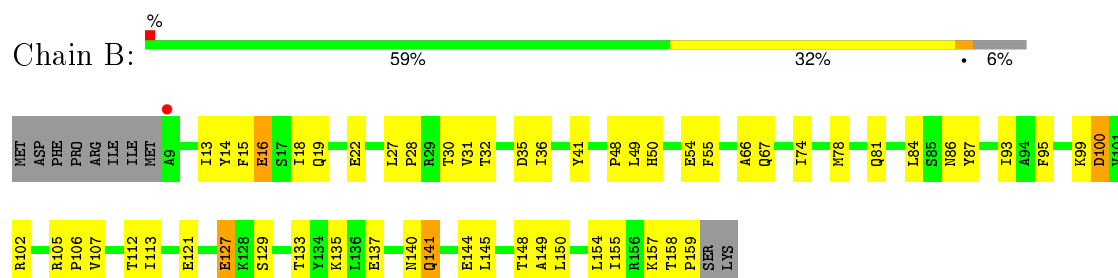
### 3 Residue-property plots [i](#)

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.

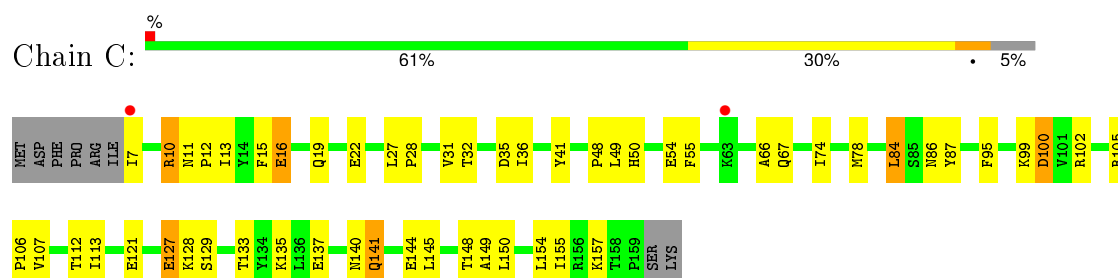
- Molecule 1: monoamine oxidase regulatory protein, putative



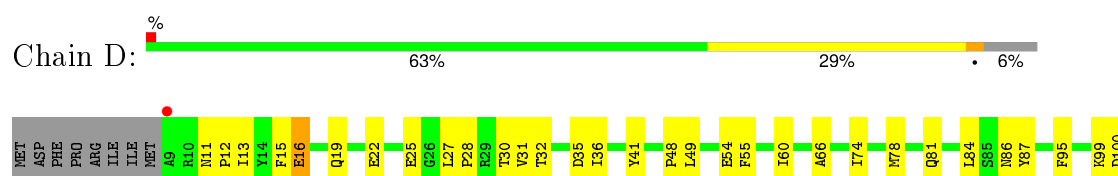
- Molecule 1: monoamine oxidase regulatory protein, putative



- Molecule 1: monoamine oxidase regulatory protein, putative

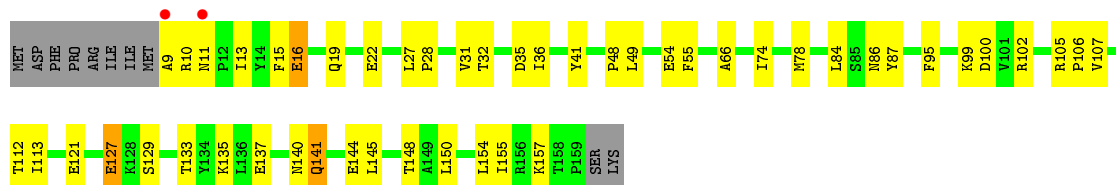


- Molecule 1: monoamine oxidase regulatory protein, putative

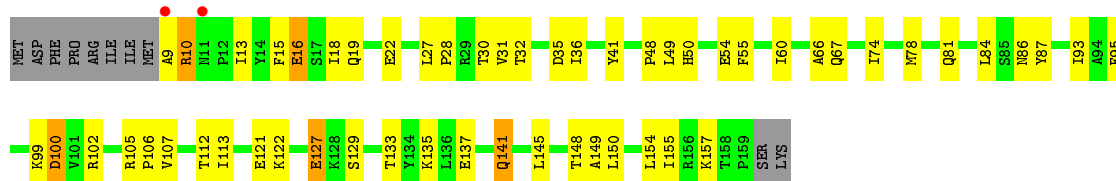




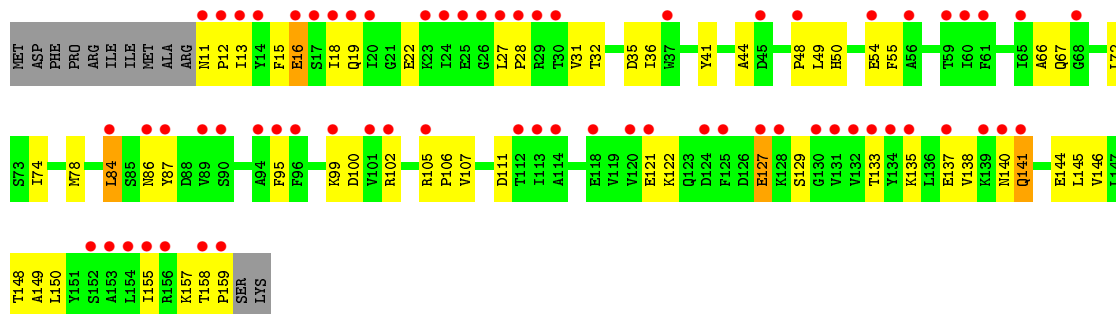
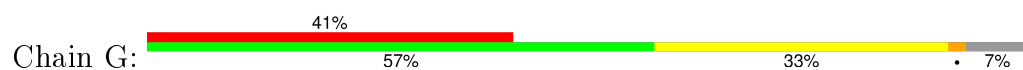
- Molecule 1: monoamine oxidase regulatory protein, putative



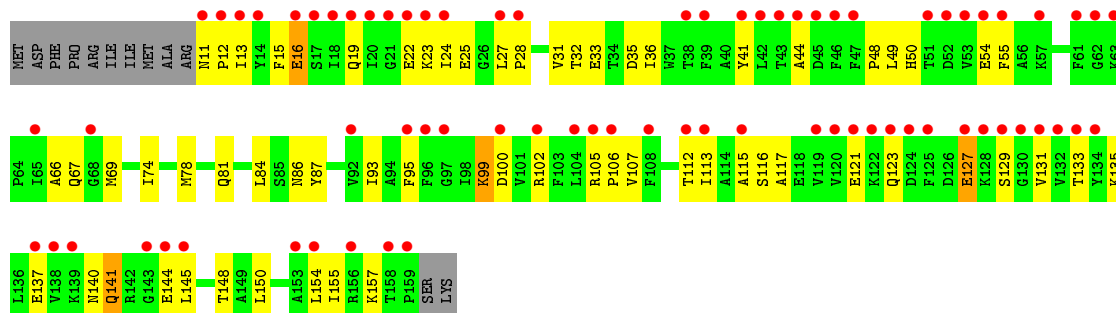
- Molecule 1: monoamine oxidase regulatory protein, putative



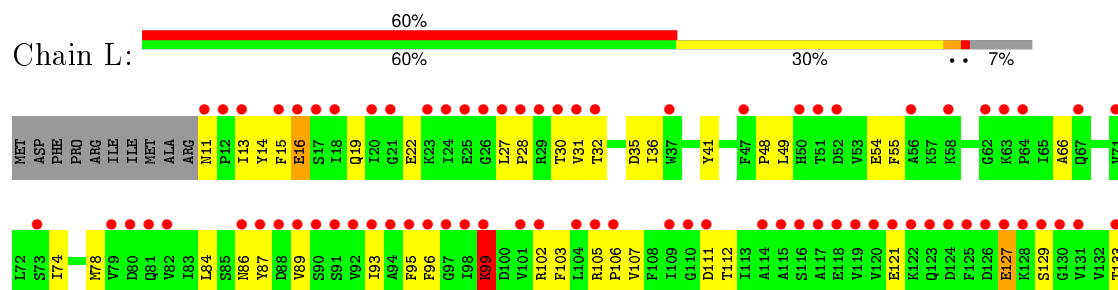
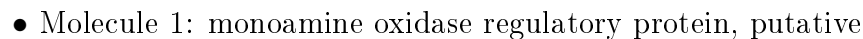
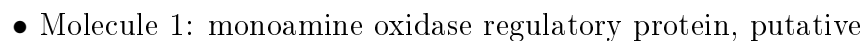
- Molecule 1: monoamine oxidase regulatory protein, putative

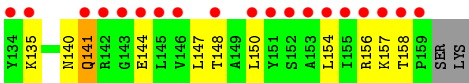


- Molecule 1: monoamine oxidase regulatory protein, putative



- Molecule 1: monoamine oxidase regulatory protein, putative





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.74Å 136.50Å 127.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.81 25.05 – 2.81	Depositor EDS
% Data completeness (in resolution range)	95.8 (20.00-2.81) 96.7 (25.05-2.81)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.242 , 0.276 0.257 , 0.285	Depositor DCC
$R_{free}$ test set	2688 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 78.6	EDS
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54645 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	14224	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.79% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.47	0/1214	0.65	0/1643
1	B	0.48	0/1214	0.67	0/1643
1	C	0.46	0/1230	0.65	0/1664
1	D	0.43	0/1214	0.65	0/1643
1	E	0.43	0/1214	0.64	0/1643
1	F	0.46	0/1214	0.66	0/1643
1	G	0.31	0/1198	0.61	0/1622
1	H	0.31	0/1198	0.60	0/1622
1	I	0.35	0/1198	0.62	0/1622
1	J	0.31	0/1198	0.61	0/1622
1	K	0.29	0/1198	0.60	0/1622
1	L	0.30	0/1198	0.60	0/1622
All	All	0.39	0/14488	0.63	0/19611

There are no bond length outliers.

There are no bond angle outliers.

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	1192	0	1218	46	1
1	B	1192	0	1218	51	0
1	C	1208	0	1238	43	1
1	D	1192	0	1218	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1192	0	1218	42	0
1	F	1192	0	1218	47	0
1	G	1176	0	1200	52	0
1	H	1176	0	1200	59	0
1	I	1176	0	1200	60	0
1	J	1176	0	1200	55	0
1	K	1176	0	1200	56	0
1	L	1176	0	1200	46	0
All	All	14224	0	14528	552	1

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 19.

All (552) 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:H:41:TYR:HB3	1:K:41:TYR:HB3	1.25	1.11
1:D:41:TYR:HB3	1:F:41:TYR:HB3	1.37	1.06
1:A:74:ILE:HG22	1:A:78:MSE:HE2	1.39	1.05
1:G:99:LYS:HB3	1:G:150:LEU:HB3	1.36	1.04
1:E:74:ILE:HG22	1:E:78:MSE:HE2	1.40	1.03
1:D:74:ILE:HG22	1:D:78:MSE:HE2	1.40	1.02
1:L:74:ILE:HG22	1:L:78:MSE:HE2	1.42	1.01
1:I:74:ILE:HG22	1:I:78:MSE:HE2	1.42	1.01
1:J:41:TYR:HB3	1:L:41:TYR:HB3	1.41	1.01
1:G:41:TYR:HB3	1:I:41:TYR:HB3	1.39	1.01
1:B:74:ILE:HG22	1:B:78:MSE:HE2	1.41	1.01
1:F:74:ILE:HG22	1:F:78:MSE:HE2	1.41	1.00
1:C:74:ILE:HG22	1:C:78:MSE:HE2	1.41	0.99
1:H:74:ILE:HG22	1:H:78:MSE:HE2	1.41	0.99
1:A:86:ASN:HD21	1:F:86:ASN:HD21	1.07	0.99
1:K:74:ILE:HG22	1:K:78:MSE:HE2	1.43	0.98
1:B:141:GLN:NE2	1:B:141:GLN:H	1.62	0.98
1:I:86:ASN:HD21	1:K:86:ASN:HD21	1.05	0.97
1:J:74:ILE:HG22	1:J:78:MSE:HE2	1.42	0.97
1:A:141:GLN:NE2	1:A:141:GLN:H	1.63	0.97
1:B:41:TYR:HB3	1:E:41:TYR:HB3	1.43	0.96
1:G:74:ILE:HG22	1:G:78:MSE:HE2	1.42	0.96
1:C:141:GLN:H	1:C:141:GLN:NE2	1.63	0.96
1:H:86:ASN:HD21	1:J:86:ASN:HD21	1.08	0.96
1:F:141:GLN:H	1:F:141:GLN:NE2	1.62	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:141:GLN:H	1:L:141:GLN:NE2	1.65	0.94
1:D:141:GLN:NE2	1:D:141:GLN:H	1.65	0.94
1:A:41:TYR:HB3	1:C:41:TYR:HB3	1.46	0.94
1:E:141:GLN:H	1:E:141:GLN:HE21	0.94	0.94
1:K:141:GLN:NE2	1:K:141:GLN:H	1.64	0.93
1:H:141:GLN:NE2	1:H:141:GLN:H	1.65	0.93
1:G:141:GLN:H	1:G:141:GLN:NE2	1.65	0.92
1:K:141:GLN:HE21	1:K:141:GLN:H	0.93	0.92
1:E:10:ARG:HG3	1:E:11:ASN:H	1.33	0.92
1:E:141:GLN:H	1:E:141:GLN:NE2	1.66	0.92
1:I:141:GLN:HE21	1:I:141:GLN:H	0.96	0.91
1:J:141:GLN:H	1:J:141:GLN:NE2	1.66	0.91
1:I:141:GLN:NE2	1:I:141:GLN:H	1.67	0.91
1:L:141:GLN:H	1:L:141:GLN:HE21	0.94	0.91
1:J:141:GLN:H	1:J:141:GLN:HE21	0.96	0.91
1:G:102:ARG:HB2	1:G:148:THR:HG22	1.52	0.90
1:D:141:GLN:HE21	1:D:141:GLN:H	0.93	0.89
1:H:141:GLN:HE21	1:H:141:GLN:H	0.93	0.88
1:G:141:GLN:H	1:G:141:GLN:HE21	0.94	0.88
1:B:141:GLN:HE21	1:B:141:GLN:H	0.88	0.88
1:A:141:GLN:HE21	1:A:141:GLN:N	1.73	0.87
1:F:105:ARG:HG3	1:F:106:PRO:HD2	1.56	0.87
1:C:141:GLN:H	1:C:141:GLN:HE21	0.91	0.87
1:B:141:GLN:HE21	1:B:141:GLN:N	1.70	0.86
1:L:99:LYS:HB3	1:L:150:LEU:HB3	1.57	0.86
1:A:105:ARG:HG3	1:A:106:PRO:HD2	1.58	0.86
1:A:141:GLN:HE21	1:A:141:GLN:H	0.91	0.86
1:C:141:GLN:HE21	1:C:141:GLN:N	1.73	0.85
1:D:141:GLN:HE21	1:D:141:GLN:N	1.75	0.85
1:F:141:GLN:HE21	1:F:141:GLN:H	0.91	0.85
1:E:105:ARG:HG3	1:E:106:PRO:HD2	1.58	0.85
1:H:105:ARG:HG3	1:H:106:PRO:HD2	1.59	0.85
1:C:105:ARG:HG3	1:C:106:PRO:HD2	1.59	0.85
1:F:141:GLN:HE21	1:F:141:GLN:N	1.73	0.84
1:K:141:GLN:HE21	1:K:141:GLN:N	1.75	0.84
1:K:105:ARG:HG3	1:K:106:PRO:HD2	1.58	0.84
1:I:105:ARG:HG3	1:I:106:PRO:HD2	1.60	0.84
1:B:86:ASN:HD21	1:D:86:ASN:HD21	1.26	0.84
1:J:105:ARG:HG3	1:J:106:PRO:HD2	1.61	0.83
1:J:141:GLN:HE21	1:J:141:GLN:N	1.77	0.83
1:L:105:ARG:HG3	1:L:106:PRO:HD2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:141:GLN:HE21	1:G:141:GLN:N	1.76	0.82
1:D:105:ARG:HG3	1:D:106:PRO:HD2	1.60	0.82
1:L:141:GLN:HE21	1:L:141:GLN:N	1.76	0.82
1:G:86:ASN:HD21	1:L:86:ASN:HD21	1.28	0.81
1:G:105:ARG:HG3	1:G:106:PRO:HD2	1.60	0.81
1:H:141:GLN:HE21	1:H:141:GLN:N	1.75	0.79
1:B:105:ARG:HG3	1:B:106:PRO:HD2	1.63	0.79
1:I:11:ASN:HD22	1:I:88:ASP:HB2	1.48	0.79
1:E:141:GLN:N	1:E:141:GLN:HE21	1.76	0.79
1:I:141:GLN:HE21	1:I:141:GLN:N	1.77	0.78
1:C:36:ILE:HD12	1:C:66:ALA:HA	1.68	0.76
1:L:36:ILE:HD12	1:L:66:ALA:HA	1.70	0.73
1:K:36:ILE:HD12	1:K:66:ALA:HA	1.70	0.73
1:J:129:SER:HA	1:J:157:LYS:HG3	1.71	0.73
1:H:36:ILE:HD12	1:H:66:ALA:HA	1.70	0.73
1:L:99:LYS:HE3	1:L:99:LYS:HA	1.71	0.73
1:H:123:GLN:HG3	1:H:131:VAL:CG2	2.18	0.73
1:K:112:THR:H	1:K:141:GLN:NE2	1.87	0.73
1:C:11:ASN:HB3	1:C:12:PRO:HD2	1.71	0.72
1:G:36:ILE:HD12	1:G:66:ALA:HA	1.70	0.72
1:I:36:ILE:HD12	1:I:66:ALA:HA	1.70	0.72
1:A:36:ILE:HD12	1:A:66:ALA:HA	1.72	0.72
1:A:102:ARG:HB2	1:A:148:THR:HG22	1.70	0.71
1:C:86:ASN:HD21	1:E:86:ASN:HD21	1.37	0.71
1:G:102:ARG:HB2	1:G:148:THR:CG2	2.20	0.70
1:E:36:ILE:HD12	1:E:66:ALA:HA	1.71	0.70
1:D:36:ILE:HD12	1:D:66:ALA:HA	1.74	0.70
1:J:36:ILE:HD12	1:J:66:ALA:HA	1.72	0.70
1:G:129:SER:HA	1:G:157:LYS:HG3	1.74	0.70
1:F:36:ILE:HD12	1:F:66:ALA:HA	1.72	0.70
1:I:112:THR:H	1:I:141:GLN:NE2	1.90	0.69
1:H:102:ARG:HB2	1:H:148:THR:HG22	1.75	0.68
1:C:99:LYS:O	1:D:99:LYS:O	2.12	0.68
1:H:11:ASN:N	1:H:12:PRO:HD2	2.08	0.68
1:F:129:SER:HA	1:F:157:LYS:HG3	1.76	0.68
1:B:36:ILE:HD12	1:B:66:ALA:HA	1.74	0.67
1:I:95:PHE:HZ	1:I:98:ILE:HD11	1.59	0.67
1:C:31:VAL:HG11	1:C:107:VAL:HG12	1.77	0.67
1:A:99:LYS:O	1:B:99:LYS:O	2.13	0.66
1:E:99:LYS:O	1:F:99:LYS:O	2.14	0.66
1:J:15:PHE:HA	1:J:155:ILE:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLU:HB3	1:A:133:THR:HB	1.78	0.66
1:C:11:ASN:CB	1:C:12:PRO:HD2	2.23	0.66
1:H:32:THR:HG23	1:H:35:ASP:H	1.61	0.65
1:H:112:THR:H	1:H:141:GLN:NE2	1.94	0.65
1:K:121:GLU:HB3	1:K:133:THR:HB	1.77	0.65
1:J:32:THR:HG23	1:J:35:ASP:H	1.62	0.65
1:K:32:THR:HG23	1:K:35:ASP:H	1.62	0.65
1:B:15:PHE:HA	1:B:155:ILE:HD11	1.79	0.65
1:J:112:THR:H	1:J:141:GLN:NE2	1.96	0.64
1:B:32:THR:HG23	1:B:35:ASP:H	1.60	0.64
1:E:31:VAL:HG11	1:E:107:VAL:HG12	1.78	0.64
1:E:32:THR:HG23	1:E:35:ASP:H	1.62	0.64
1:I:99:LYS:O	1:J:99:LYS:O	2.14	0.64
1:B:93:ILE:HD12	1:B:154:LEU:CD2	2.27	0.64
1:I:81:GLN:HG3	1:K:81:GLN:HE21	1.62	0.64
1:D:121:GLU:HB3	1:D:133:THR:HB	1.78	0.64
1:D:32:THR:HG23	1:D:35:ASP:H	1.62	0.64
1:C:32:THR:HG23	1:C:35:ASP:H	1.61	0.64
1:H:15:PHE:HA	1:H:155:ILE:HD11	1.80	0.63
1:F:121:GLU:HB3	1:F:133:THR:HB	1.80	0.63
1:G:32:THR:HG23	1:G:35:ASP:H	1.63	0.63
1:A:15:PHE:HA	1:A:155:ILE:HD11	1.81	0.63
1:I:81:GLN:HG3	1:K:81:GLN:NE2	2.12	0.63
1:I:81:GLN:NE2	1:K:81:GLN:HG3	2.12	0.63
1:C:102:ARG:HB2	1:C:148:THR:HG22	1.81	0.63
1:D:31:VAL:HG11	1:D:107:VAL:HG12	1.81	0.62
1:F:15:PHE:HA	1:F:155:ILE:HD11	1.81	0.62
1:L:32:THR:HG23	1:L:35:ASP:H	1.62	0.62
1:F:31:VAL:HG11	1:F:107:VAL:HG12	1.81	0.62
1:F:32:THR:HG23	1:F:35:ASP:H	1.63	0.62
1:A:32:THR:HG23	1:A:35:ASP:H	1.64	0.62
1:I:32:THR:HG23	1:I:35:ASP:H	1.64	0.62
1:I:102:ARG:HB2	1:I:148:THR:HG22	1.81	0.61
1:G:44:ALA:HB2	1:I:46:PHE:CE1	2.34	0.61
1:J:102:ARG:HB2	1:J:148:THR:HG22	1.82	0.61
1:J:31:VAL:HG11	1:J:107:VAL:HG12	1.82	0.61
1:F:93:ILE:HD12	1:F:154:LEU:CD2	2.31	0.61
1:B:102:ARG:HB2	1:B:148:THR:HG22	1.83	0.61
1:G:99:LYS:HG2	1:G:150:LEU:HD23	1.81	0.61
1:I:27:LEU:HD22	1:I:28:PRO:HD2	1.83	0.60
1:A:129:SER:HA	1:A:157:LYS:HG3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:ARG:HG3	1:E:11:ASN:N	2.10	0.60
1:J:121:GLU:HB3	1:J:133:THR:HB	1.82	0.60
1:A:158:THR:CG2	1:A:159:PRO:HD2	2.31	0.60
1:H:123:GLN:HG3	1:H:131:VAL:HG23	1.82	0.60
1:H:102:ARG:HB2	1:H:148:THR:CG2	2.31	0.60
1:L:102:ARG:HB2	1:L:148:THR:HG22	1.84	0.60
1:B:31:VAL:HG11	1:B:107:VAL:HG12	1.84	0.59
1:I:31:VAL:HG11	1:I:107:VAL:HG12	1.84	0.59
1:F:102:ARG:HB2	1:F:148:THR:HG22	1.83	0.59
1:K:31:VAL:HG11	1:K:107:VAL:HG12	1.84	0.59
1:F:27:LEU:HD22	1:F:28:PRO:HD2	1.84	0.59
1:I:121:GLU:HB3	1:I:133:THR:HB	1.85	0.59
1:I:95:PHE:CZ	1:I:98:ILE:HD11	2.38	0.58
1:H:27:LEU:HD22	1:H:28:PRO:HD2	1.84	0.58
1:D:102:ARG:HB2	1:D:148:THR:HG22	1.83	0.58
1:K:15:PHE:HA	1:K:155:ILE:HD11	1.85	0.58
1:I:100:ASP:O	1:I:149:ALA:HA	2.03	0.58
1:I:129:SER:HA	1:I:157:LYS:HG3	1.85	0.58
1:L:121:GLU:HB3	1:L:133:THR:HB	1.85	0.58
1:I:81:GLN:HE21	1:K:81:GLN:HG3	1.69	0.58
1:L:27:LEU:HD22	1:L:28:PRO:HD2	1.85	0.58
1:K:102:ARG:HB2	1:K:148:THR:HG22	1.86	0.58
1:G:11:ASN:N	1:G:12:PRO:HD2	2.19	0.58
1:G:27:LEU:HD22	1:G:28:PRO:HD2	1.85	0.58
1:B:27:LEU:HD22	1:B:28:PRO:HD2	1.85	0.58
1:J:27:LEU:HD22	1:J:28:PRO:HD2	1.85	0.58
1:C:100:ASP:O	1:C:149:ALA:HA	2.04	0.57
1:A:81:GLN:HG3	1:F:81:GLN:HE21	1.69	0.57
1:D:27:LEU:HD22	1:D:28:PRO:HD2	1.85	0.57
1:G:121:GLU:HB3	1:G:133:THR:HB	1.87	0.57
1:B:121:GLU:HB3	1:B:133:THR:HB	1.87	0.57
1:E:27:LEU:HD22	1:E:28:PRO:HD2	1.87	0.57
1:A:31:VAL:HG11	1:A:107:VAL:HG12	1.85	0.57
1:A:81:GLN:NE2	1:F:81:GLN:HG3	2.20	0.56
1:I:15:PHE:HA	1:I:155:ILE:HD11	1.86	0.56
1:H:31:VAL:HG11	1:H:107:VAL:HG12	1.87	0.56
1:A:81:GLN:HG3	1:F:81:GLN:NE2	2.20	0.56
1:D:127:GLU:H	1:D:127:GLU:CD	2.09	0.56
1:I:127:GLU:CD	1:I:127:GLU:H	2.09	0.56
1:A:102:ARG:HB2	1:A:148:THR:CG2	2.35	0.56
1:G:100:ASP:O	1:G:149:ALA:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:27:LEU:HD22	1:K:28:PRO:HD2	1.87	0.56
1:C:127:GLU:H	1:C:127:GLU:CD	2.10	0.56
1:J:116:SER:O	1:J:136:LEU:HD12	2.06	0.56
1:G:127:GLU:H	1:G:127:GLU:CD	2.09	0.56
1:F:127:GLU:CD	1:F:127:GLU:H	2.09	0.56
1:E:127:GLU:CD	1:E:127:GLU:H	2.10	0.56
1:B:15:PHE:HB3	1:B:157:LYS:HG2	1.87	0.55
1:A:27:LEU:HD22	1:A:28:PRO:HD2	1.87	0.55
1:D:100:ASP:O	1:D:149:ALA:HA	2.06	0.55
1:J:15:PHE:HB3	1:J:157:LYS:HG2	1.88	0.55
1:L:127:GLU:CD	1:L:127:GLU:H	2.09	0.55
1:L:96:PHE:CE1	1:L:154:LEU:HD12	2.41	0.55
1:D:15:PHE:HA	1:D:155:ILE:HD11	1.88	0.55
1:H:129:SER:HA	1:H:157:LYS:HG3	1.88	0.55
1:E:102:ARG:HB2	1:E:148:THR:HG22	1.89	0.55
1:J:127:GLU:H	1:J:127:GLU:CD	2.09	0.55
1:K:139:LYS:HA	1:K:144:GLU:O	2.06	0.55
1:H:127:GLU:CD	1:H:127:GLU:H	2.10	0.55
1:K:11:ASN:N	1:K:12:PRO:HD2	2.21	0.55
1:H:86:ASN:ND2	1:J:86:ASN:HD21	1.92	0.55
1:G:99:LYS:N	1:G:150:LEU:O	2.39	0.55
1:B:127:GLU:H	1:B:127:GLU:CD	2.10	0.55
1:C:112:THR:H	1:C:141:GLN:NE2	2.05	0.54
1:C:27:LEU:HD22	1:C:28:PRO:HD2	1.88	0.54
1:E:36:ILE:CD1	1:E:66:ALA:HA	2.37	0.54
1:I:16:GLU:OE1	1:I:16:GLU:N	2.40	0.54
1:C:36:ILE:CD1	1:C:66:ALA:HA	2.35	0.54
1:E:16:GLU:N	1:E:16:GLU:OE1	2.41	0.54
1:K:129:SER:HA	1:K:157:LYS:HG3	1.89	0.54
1:E:121:GLU:HB3	1:E:133:THR:HB	1.90	0.54
1:K:127:GLU:CD	1:K:127:GLU:H	2.11	0.54
1:I:98:ILE:HD13	1:I:151:TYR:CB	2.39	0.53
1:J:137:GLU:HG2	1:J:145:LEU:HD11	1.89	0.53
1:B:135:LYS:HA	1:B:150:LEU:HD12	1.90	0.53
1:H:16:GLU:OE1	1:H:16:GLU:N	2.41	0.53
1:G:36:ILE:CD1	1:G:66:ALA:HA	2.39	0.53
1:A:127:GLU:H	1:A:127:GLU:CD	2.11	0.53
1:A:81:GLN:HE21	1:F:81:GLN:HG3	1.73	0.53
1:H:86:ASN:HD21	1:J:86:ASN:ND2	1.92	0.53
1:F:16:GLU:OE1	1:F:16:GLU:N	2.40	0.53
1:I:98:ILE:HD13	1:I:151:TYR:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:123:GLN:HG3	1:H:131:VAL:HG22	1.89	0.53
1:G:15:PHE:HA	1:G:155:ILE:HD11	1.91	0.53
1:G:105:ARG:HB3	1:G:146:VAL:HG12	1.90	0.53
1:J:16:GLU:N	1:J:16:GLU:OE1	2.42	0.53
1:C:31:VAL:HG11	1:C:107:VAL:CG1	2.38	0.52
1:I:137:GLU:HG2	1:I:145:LEU:HD11	1.90	0.52
1:B:81:GLN:HG3	1:D:81:GLN:NE2	2.24	0.52
1:L:16:GLU:N	1:L:16:GLU:OE1	2.42	0.52
1:A:158:THR:HG23	1:A:159:PRO:HD2	1.91	0.52
1:B:81:GLN:NE2	1:D:81:GLN:HG3	2.24	0.52
1:E:112:THR:H	1:E:141:GLN:NE2	2.07	0.52
1:A:32:THR:HG22	1:A:35:ASP:OD1	2.09	0.52
1:D:16:GLU:OE1	1:D:16:GLU:N	2.42	0.52
1:K:99:LYS:HB3	1:K:150:LEU:HB3	1.91	0.52
1:C:10:ARG:HB3	1:C:10:ARG:HH11	1.74	0.52
1:I:102:ARG:HB2	1:I:148:THR:CG2	2.40	0.52
1:B:16:GLU:OE1	1:B:16:GLU:N	2.42	0.52
1:F:141:GLN:N	1:F:141:GLN:NE2	2.45	0.52
1:K:36:ILE:CD1	1:K:66:ALA:HA	2.39	0.52
1:G:16:GLU:N	1:G:16:GLU:OE1	2.43	0.52
1:G:158:THR:CG2	1:G:159:PRO:HD2	2.40	0.52
1:A:36:ILE:CD1	1:A:66:ALA:HA	2.40	0.51
1:L:141:GLN:NE2	1:L:141:GLN:N	2.47	0.51
1:I:36:ILE:CD1	1:I:66:ALA:HA	2.40	0.51
1:C:129:SER:OG	1:C:154:LEU:HD21	2.10	0.51
1:K:141:GLN:NE2	1:K:141:GLN:N	2.46	0.51
1:H:36:ILE:CD1	1:H:66:ALA:HA	2.39	0.51
1:F:48:PRO:HB2	1:F:55:PHE:CG	2.46	0.51
1:E:31:VAL:HG11	1:E:107:VAL:CG1	2.41	0.51
1:C:32:THR:HG22	1:C:35:ASP:OD1	2.10	0.51
1:L:129:SER:HA	1:L:157:LYS:HG3	1.92	0.51
1:C:10:ARG:HB3	1:C:10:ARG:NH1	2.26	0.51
1:J:33:GLU:CD	1:K:32:THR:OG1	2.49	0.51
1:D:112:THR:H	1:D:141:GLN:NE2	2.08	0.51
1:H:44:ALA:HB2	1:K:46:PHE:CE1	2.46	0.51
1:J:48:PRO:HB2	1:J:55:PHE:CG	2.45	0.51
1:H:11:ASN:N	1:H:12:PRO:CD	2.74	0.51
1:B:36:ILE:CD1	1:B:66:ALA:HA	2.41	0.51
1:D:32:THR:HG22	1:D:35:ASP:OD1	2.11	0.51
1:K:11:ASN:N	1:K:12:PRO:CD	2.74	0.51
1:B:81:GLN:HE21	1:D:81:GLN:HG3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:TYR:CE2	1:B:159:PRO:HD3	2.45	0.51
1:C:16:GLU:N	1:C:16:GLU:OE1	2.44	0.51
1:K:137:GLU:HG2	1:K:145:LEU:HD11	1.93	0.51
1:A:16:GLU:N	1:A:16:GLU:OE1	2.43	0.50
1:B:81:GLN:HG3	1:D:81:GLN:HE21	1.76	0.50
1:H:100:ASP:OD1	1:H:150:LEU:HB2	2.11	0.50
1:G:32:THR:HG22	1:G:35:ASP:OD1	2.11	0.50
1:F:31:VAL:HG11	1:F:107:VAL:CG1	2.41	0.50
1:L:48:PRO:HB2	1:L:55:PHE:CG	2.46	0.50
1:I:11:ASN:N	1:I:12:PRO:HD2	2.27	0.50
1:L:31:VAL:HG11	1:L:107:VAL:HG12	1.93	0.50
1:D:141:GLN:NE2	1:D:141:GLN:N	2.47	0.50
1:D:36:ILE:CD1	1:D:66:ALA:HA	2.40	0.50
1:J:119:VAL:HG22	1:J:134:TYR:CE2	2.46	0.50
1:G:48:PRO:HB2	1:G:55:PHE:CG	2.47	0.50
1:H:48:PRO:HB2	1:H:55:PHE:CG	2.46	0.50
1:K:16:GLU:OE1	1:K:16:GLU:N	2.41	0.50
1:L:135:LYS:HA	1:L:150:LEU:HD12	1.93	0.49
1:L:102:ARG:HB2	1:L:148:THR:CG2	2.42	0.49
1:E:48:PRO:HB2	1:E:55:PHE:CG	2.46	0.49
1:J:139:LYS:HA	1:J:144:GLU:O	2.12	0.49
1:K:48:PRO:HB2	1:K:55:PHE:CG	2.47	0.49
1:C:48:PRO:HB2	1:C:55:PHE:CG	2.47	0.49
1:A:93:ILE:HD12	1:A:154:LEU:CD2	2.42	0.49
1:E:78:MSE:HE1	1:E:113:ILE:HG13	1.92	0.49
1:F:137:GLU:HG2	1:F:145:LEU:HD11	1.93	0.49
1:I:48:PRO:HB2	1:I:55:PHE:CG	2.47	0.49
1:H:81:GLN:HG3	1:J:81:GLN:NE2	2.28	0.49
1:A:10:ARG:HH21	1:A:86:ASN:ND2	2.10	0.49
1:J:135:LYS:HA	1:J:150:LEU:HD12	1.94	0.49
1:F:10:ARG:HH11	1:F:10:ARG:HA	1.78	0.49
1:H:25:GLU:OE1	1:H:116:SER:HB3	2.13	0.49
1:A:31:VAL:HG11	1:A:107:VAL:CG1	2.41	0.49
1:H:81:GLN:NE2	1:J:81:GLN:HG3	2.28	0.49
1:F:15:PHE:HB3	1:F:157:LYS:HG2	1.94	0.49
1:K:31:VAL:HG11	1:K:107:VAL:CG1	2.43	0.49
1:L:99:LYS:HG2	1:L:150:LEU:HD23	1.95	0.49
1:L:36:ILE:CD1	1:L:66:ALA:HA	2.39	0.49
1:I:32:THR:HG22	1:I:35:ASP:OD1	2.12	0.49
1:G:18:ILE:O	1:G:122:LYS:NZ	2.31	0.49
1:C:121:GLU:HB3	1:C:133:THR:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:THR:HG22	1:H:35:ASP:OD1	2.13	0.48
1:B:78:MSE:HE1	1:B:113:ILE:HG13	1.93	0.48
1:E:10:ARG:HG3	1:E:10:ARG:HH11	1.77	0.48
1:E:32:THR:HG22	1:E:35:ASP:OD1	2.12	0.48
1:D:31:VAL:HG11	1:D:107:VAL:CG1	2.43	0.48
1:J:31:VAL:HG11	1:J:107:VAL:CG1	2.43	0.48
1:C:141:GLN:NE2	1:C:141:GLN:N	2.45	0.48
1:I:27:LEU:HD22	1:I:28:PRO:CD	2.43	0.48
1:D:19:GLN:O	1:D:22:GLU:HG3	2.13	0.48
1:I:30:THR:HA	1:I:112:THR:HA	1.96	0.48
1:F:13:ILE:HG23	1:F:87:TYR:CD1	2.48	0.48
1:K:32:THR:HG22	1:K:35:ASP:OD1	2.14	0.48
1:J:141:GLN:NE2	1:J:141:GLN:N	2.48	0.48
1:I:31:VAL:HG11	1:I:107:VAL:CG1	2.44	0.48
1:C:15:PHE:HA	1:C:155:ILE:HD11	1.96	0.48
1:G:19:GLN:O	1:G:22:GLU:HG3	2.12	0.48
1:C:137:GLU:HG2	1:C:145:LEU:HD11	1.94	0.48
1:K:19:GLN:O	1:K:22:GLU:HG3	2.13	0.48
1:J:19:GLN:O	1:J:22:GLU:HG3	2.13	0.48
1:L:19:GLN:O	1:L:22:GLU:HG3	2.14	0.48
1:B:112:THR:H	1:B:141:GLN:NE2	2.11	0.48
1:B:100:ASP:O	1:B:149:ALA:HA	2.13	0.48
1:J:36:ILE:CD1	1:J:66:ALA:HA	2.42	0.48
1:B:48:PRO:HB2	1:B:55:PHE:CG	2.49	0.47
1:K:32:THR:O	1:K:35:ASP:HB2	2.14	0.47
1:K:111:ASP:HB3	1:K:141:GLN:HE22	1.79	0.47
1:F:36:ILE:CD1	1:F:66:ALA:HA	2.42	0.47
1:C:102:ARG:HB2	1:C:148:THR:CG2	2.44	0.47
1:H:81:GLN:HG3	1:J:81:GLN:HE21	1.79	0.47
1:B:141:GLN:NE2	1:B:141:GLN:N	2.44	0.47
1:J:33:GLU:OE1	1:K:32:THR:OG1	2.33	0.47
1:B:32:THR:HG22	1:B:35:ASP:OD1	2.14	0.47
1:B:140:ASN:HD21	1:B:144:GLU:HB2	1.80	0.47
1:E:74:ILE:HG22	1:E:78:MSE:CE	2.29	0.47
1:L:112:THR:H	1:L:141:GLN:NE2	2.12	0.47
1:G:141:GLN:NE2	1:G:141:GLN:N	2.47	0.47
1:J:32:THR:HG22	1:J:35:ASP:OD1	2.15	0.47
1:K:129:SER:OG	1:K:154:LEU:HD21	2.15	0.47
1:D:129:SER:OG	1:D:154:LEU:HD21	2.15	0.47
1:F:19:GLN:O	1:F:22:GLU:HG3	2.15	0.47
1:E:129:SER:HA	1:E:157:LYS:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:ASN:HD21	1:G:144:GLU:HB2	1.80	0.47
1:I:19:GLN:O	1:I:22:GLU:HG3	2.14	0.47
1:J:32:THR:O	1:J:35:ASP:HB2	2.15	0.47
1:L:32:THR:HG22	1:L:35:ASP:OD1	2.15	0.47
1:L:14:TYR:CD2	1:L:158:THR:HA	2.50	0.47
1:H:141:GLN:NE2	1:H:141:GLN:N	2.47	0.47
1:G:32:THR:O	1:G:35:ASP:HB2	2.15	0.47
1:G:135:LYS:HA	1:G:150:LEU:HD12	1.97	0.46
1:A:112:THR:H	1:A:141:GLN:NE2	2.13	0.46
1:H:27:LEU:HD22	1:H:28:PRO:CD	2.45	0.46
1:L:140:ASN:HD21	1:L:144:GLU:HB2	1.80	0.46
1:H:78:MSE:HE1	1:H:113:ILE:HG13	1.96	0.46
1:E:15:PHE:HA	1:E:155:ILE:HD11	1.97	0.46
1:J:129:SER:CA	1:J:157:LYS:HG3	2.42	0.46
1:H:32:THR:OG1	1:I:33:GLU:CD	2.54	0.46
1:K:140:ASN:HD21	1:K:144:GLU:HB2	1.80	0.46
1:H:19:GLN:O	1:H:22:GLU:HG3	2.15	0.46
1:B:19:GLN:O	1:B:22:GLU:HG3	2.16	0.46
1:L:93:ILE:HD11	1:L:156:ARG:HD3	1.97	0.46
1:G:105:ARG:NH2	1:G:144:GLU:HB3	2.31	0.46
1:J:15:PHE:HA	1:J:155:ILE:CD1	2.44	0.46
1:I:140:ASN:HD21	1:I:144:GLU:HB2	1.80	0.46
1:B:129:SER:OG	1:B:154:LEU:HD21	2.15	0.46
1:K:120:VAL:HG11	1:K:135:LYS:HB2	1.98	0.46
1:B:31:VAL:HG11	1:B:107:VAL:CG1	2.45	0.46
1:G:137:GLU:HG2	1:G:145:LEU:HD11	1.97	0.46
1:B:13:ILE:HG23	1:B:87:TYR:CD1	2.50	0.46
1:H:32:THR:O	1:H:35:ASP:HB2	2.16	0.46
1:A:141:GLN:NE2	1:A:141:GLN:N	2.45	0.46
1:D:129:SER:HA	1:D:157:LYS:HG3	1.98	0.46
1:K:13:ILE:HG23	1:K:87:TYR:CD1	2.51	0.46
1:H:32:THR:OG1	1:I:33:GLU:OE1	2.33	0.45
1:B:129:SER:HA	1:B:157:LYS:HG3	1.98	0.45
1:K:95:PHE:O	1:L:103:PHE:CD1	2.69	0.45
1:F:32:THR:HG22	1:F:35:ASP:OD1	2.17	0.45
1:G:27:LEU:HD22	1:G:28:PRO:CD	2.46	0.45
1:J:27:LEU:HD22	1:J:28:PRO:CD	2.46	0.45
1:A:13:ILE:HG23	1:A:87:TYR:CD1	2.51	0.45
1:J:129:SER:OG	1:J:154:LEU:HD21	2.16	0.45
1:G:31:VAL:HG12	1:G:111:ASP:O	2.16	0.45
1:L:30:THR:HA	1:L:112:THR:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:99:LYS:HB3	1:I:150:LEU:HB3	1.98	0.45
1:K:139:LYS:HD2	1:K:143:GLY:O	2.16	0.45
1:D:13:ILE:HG23	1:D:87:TYR:CD1	2.52	0.45
1:C:78:MSE:HE1	1:C:113:ILE:HG13	1.97	0.45
1:C:32:THR:O	1:C:35:ASP:HB2	2.16	0.45
1:D:27:LEU:HD22	1:D:28:PRO:CD	2.46	0.45
1:A:19:GLN:O	1:A:22:GLU:HG3	2.16	0.45
1:G:72:LEU:HD23	1:H:69:MSE:HE1	1.99	0.45
1:F:18:ILE:O	1:F:122:LYS:NZ	2.37	0.45
1:G:129:SER:N	1:G:157:LYS:HE2	2.31	0.45
1:D:32:THR:O	1:D:35:ASP:HB2	2.17	0.45
1:A:48:PRO:HB2	1:A:55:PHE:CG	2.52	0.45
1:H:23:LYS:HA	1:H:117:ALA:O	2.16	0.45
1:F:10:ARG:HA	1:F:10:ARG:NH1	2.32	0.45
1:C:19:GLN:O	1:C:22:GLU:HG3	2.17	0.45
1:C:13:ILE:HG23	1:C:87:TYR:CD1	2.52	0.45
1:L:27:LEU:HD22	1:L:28:PRO:CD	2.45	0.44
1:J:13:ILE:HG23	1:J:87:TYR:CD1	2.52	0.44
1:B:27:LEU:HD22	1:B:28:PRO:CD	2.47	0.44
1:D:15:PHE:HB3	1:D:157:LYS:HG2	1.98	0.44
1:K:116:SER:O	1:K:136:LEU:HD12	2.17	0.44
1:L:32:THR:O	1:L:35:ASP:HB2	2.18	0.44
1:L:31:VAL:HG11	1:L:107:VAL:CG1	2.47	0.44
1:C:135:LYS:HA	1:C:150:LEU:HD12	1.99	0.44
1:I:32:THR:O	1:I:35:ASP:HB2	2.17	0.44
1:C:27:LEU:HD22	1:C:28:PRO:CD	2.47	0.44
1:J:111:ASP:HB3	1:J:141:GLN:HE22	1.82	0.44
1:K:135:LYS:HA	1:K:150:LEU:HD12	2.00	0.44
1:D:48:PRO:HB2	1:D:55:PHE:CG	2.51	0.44
1:A:74:ILE:HG22	1:A:78:MSE:CE	2.29	0.44
1:G:138:VAL:O	1:G:146:VAL:HG22	2.18	0.44
1:C:10:ARG:HG2	1:C:86:ASN:O	2.18	0.44
1:B:102:ARG:HB2	1:B:148:THR:CG2	2.46	0.44
1:D:102:ARG:HB2	1:D:148:THR:CG2	2.48	0.44
1:A:123:GLN:HB3	1:A:131:VAL:HG22	1.98	0.44
1:L:13:ILE:HG23	1:L:87:TYR:CD1	2.53	0.44
1:F:15:PHE:HB3	1:F:16:GLU:OE1	2.18	0.44
1:I:78:MSE:HE1	1:I:113:ILE:HG13	1.99	0.44
1:F:27:LEU:HD22	1:F:28:PRO:CD	2.47	0.44
1:I:15:PHE:HB3	1:I:16:GLU:OE1	2.18	0.44
1:H:81:GLN:HE21	1:J:81:GLN:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:ILE:HG23	1:G:87:TYR:CD1	2.53	0.44
1:F:100:ASP:O	1:F:149:ALA:HA	2.18	0.44
1:E:19:GLN:O	1:E:22:GLU:HG3	2.17	0.44
1:H:129:SER:OG	1:H:154:LEU:HD21	2.18	0.43
1:H:13:ILE:HG23	1:H:87:TYR:CD1	2.53	0.43
1:H:140:ASN:HD21	1:H:144:GLU:HB2	1.82	0.43
1:A:100:ASP:O	1:A:149:ALA:HA	2.18	0.43
1:E:140:ASN:HD21	1:E:144:GLU:HB2	1.84	0.43
1:F:9:ALA:HB1	1:F:87:TYR:O	2.18	0.43
1:F:112:THR:H	1:F:141:GLN:NE2	2.16	0.43
1:E:27:LEU:HD22	1:E:28:PRO:CD	2.48	0.43
1:G:84:LEU:HA	1:G:84:LEU:HD12	1.90	0.43
1:C:84:LEU:HA	1:C:84:LEU:HD12	1.88	0.43
1:E:141:GLN:N	1:E:141:GLN:NE2	2.48	0.43
1:J:60:ILE:HG12	1:J:60:ILE:O	2.18	0.43
1:A:137:GLU:HG2	1:A:145:LEU:HD11	2.00	0.43
1:F:78:MSE:HE1	1:F:113:ILE:HG13	1.99	0.43
1:K:47:PHE:CE1	1:L:89:VAL:HG21	2.54	0.43
1:A:32:THR:O	1:A:35:ASP:HB2	2.19	0.43
1:D:25:GLU:OE1	1:D:116:SER:HB3	2.19	0.43
1:A:15:PHE:HB3	1:A:16:GLU:OE1	2.19	0.43
1:L:15:PHE:HB3	1:L:16:GLU:OE1	2.19	0.43
1:J:30:THR:HA	1:J:112:THR:HA	2.01	0.43
1:K:15:PHE:HB3	1:K:157:LYS:HG2	2.00	0.43
1:E:129:SER:OG	1:E:154:LEU:HD21	2.18	0.43
1:D:78:MSE:HE1	1:D:113:ILE:HG13	2.01	0.42
1:I:129:SER:OG	1:I:154:LEU:HD21	2.18	0.42
1:I:139:LYS:HA	1:I:144:GLU:O	2.19	0.42
1:I:13:ILE:HG23	1:I:87:TYR:CD1	2.54	0.42
1:C:50:HIS:CD2	1:C:67:GLN:HG3	2.54	0.42
1:G:86:ASN:ND2	1:L:86:ASN:HD21	2.07	0.42
1:B:18:ILE:HG13	1:B:155:ILE:CD1	2.49	0.42
1:H:135:LYS:HA	1:H:150:LEU:HD12	2.00	0.42
1:A:27:LEU:HD22	1:A:28:PRO:CD	2.49	0.42
1:I:25:GLU:OE1	1:I:116:SER:HB3	2.19	0.42
1:L:140:ASN:ND2	1:L:144:GLU:HB2	2.35	0.42
1:D:30:THR:HA	1:D:112:THR:HA	2.02	0.42
1:A:15:PHE:HA	1:A:155:ILE:CD1	2.47	0.42
1:H:33:GLU:CD	1:L:32:THR:OG1	2.57	0.42
1:J:140:ASN:HD21	1:J:144:GLU:HB2	1.82	0.42
1:H:24:ILE:O	1:H:116:SER:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:93:ILE:HD12	1:J:154:LEU:CD2	2.50	0.42
1:I:101:VAL:HB	1:J:98:ILE:HB	2.00	0.42
1:K:15:PHE:HB3	1:K:16:GLU:OE1	2.20	0.42
1:K:27:LEU:HD22	1:K:28:PRO:CD	2.49	0.42
1:B:140:ASN:ND2	1:B:144:GLU:HB2	2.34	0.42
1:E:140:ASN:HB2	1:E:141:GLN:NE2	2.35	0.42
1:J:157:LYS:O	1:J:159:PRO:HD3	2.19	0.42
1:H:99:LYS:HB3	1:H:150:LEU:HB3	2.01	0.42
1:E:13:ILE:HG23	1:E:87:TYR:CD1	2.55	0.42
1:I:99:LYS:N	1:I:150:LEU:O	2.51	0.42
1:J:78:MSE:HE1	1:J:113:ILE:HG13	2.01	0.41
1:B:15:PHE:HA	1:B:155:ILE:CD1	2.49	0.41
1:E:27:LEU:HA	1:E:28:PRO:HD3	1.91	0.41
1:K:139:LYS:HB2	1:K:139:LYS:NZ	2.35	0.41
1:K:140:ASN:ND2	1:K:144:GLU:HB2	2.35	0.41
1:B:137:GLU:HG2	1:B:145:LEU:HD11	2.01	0.41
1:I:158:THR:HA	1:I:159:PRO:HD3	1.91	0.41
1:H:50:HIS:CD2	1:H:67:GLN:HG3	2.55	0.41
1:H:137:GLU:HG2	1:H:145:LEU:HD11	2.02	0.41
1:I:141:GLN:NE2	1:I:141:GLN:N	2.49	0.41
1:F:129:SER:CA	1:F:157:LYS:HG3	2.47	0.41
1:E:15:PHE:HB3	1:E:16:GLU:OE1	2.20	0.41
1:A:50:HIS:CD2	1:A:67:GLN:HG3	2.54	0.41
1:F:135:LYS:HA	1:F:150:LEU:HD12	2.02	0.41
1:B:74:ILE:HG22	1:B:78:MSE:CE	2.31	0.41
1:I:140:ASN:ND2	1:I:144:GLU:HB2	2.35	0.41
1:D:11:ASN:CG	1:D:12:PRO:HD2	2.40	0.41
1:H:121:GLU:HB3	1:H:133:THR:HB	2.02	0.41
1:A:30:THR:HA	1:A:112:THR:HA	2.02	0.41
1:B:15:PHE:HB3	1:B:16:GLU:OE1	2.21	0.41
1:G:27:LEU:HA	1:G:28:PRO:HD3	1.91	0.41
1:K:99:LYS:HD3	1:K:150:LEU:HD23	2.03	0.41
1:C:129:SER:HA	1:C:157:LYS:HG3	2.01	0.41
1:B:158:THR:HA	1:B:159:PRO:HD3	1.71	0.41
1:H:99:LYS:HD3	1:H:150:LEU:HD23	2.02	0.41
1:F:50:HIS:CD2	1:F:67:GLN:HG3	2.56	0.41
1:E:135:LYS:HA	1:E:150:LEU:HD12	2.02	0.41
1:G:50:HIS:CD2	1:G:67:GLN:HG3	2.55	0.41
1:E:9:ALA:HB1	1:E:87:TYR:O	2.21	0.41
1:H:115:ALA:HA	1:H:137:GLU:O	2.20	0.41
1:I:18:ILE:O	1:I:122:LYS:NZ	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:84:LEU:HD12	1:I:84:LEU:HA	1.88	0.41
1:F:30:THR:HA	1:F:112:THR:HA	2.02	0.41
1:H:93:ILE:HD12	1:H:154:LEU:CD2	2.50	0.41
1:L:15:PHE:HB3	1:L:157:LYS:HG2	2.02	0.41
1:G:31:VAL:HG11	1:G:107:VAL:HG12	2.01	0.41
1:G:158:THR:HG22	1:G:159:PRO:HD2	2.02	0.41
1:K:50:HIS:CD2	1:K:67:GLN:HG3	2.56	0.41
1:B:30:THR:HA	1:B:112:THR:HA	2.03	0.41
1:G:129:SER:CA	1:G:157:LYS:HG3	2.47	0.41
1:B:93:ILE:HD12	1:B:154:LEU:HD22	2.02	0.41
1:B:32:THR:O	1:B:35:ASP:HB2	2.21	0.41
1:E:32:THR:O	1:E:35:ASP:HB2	2.21	0.41
1:H:15:PHE:HB3	1:H:16:GLU:OE1	2.20	0.41
1:F:32:THR:O	1:F:35:ASP:HB2	2.21	0.41
1:L:96:PHE:HE1	1:L:154:LEU:HD12	1.86	0.41
1:D:15:PHE:HB3	1:D:16:GLU:OE1	2.21	0.41
1:L:31:VAL:HG12	1:L:111:ASP:O	2.20	0.41
1:D:137:GLU:HG2	1:D:145:LEU:HD11	2.01	0.41
1:I:50:HIS:CD2	1:I:67:GLN:HG3	2.56	0.41
1:F:60:ILE:O	1:F:60:ILE:HG12	2.21	0.41
1:A:78:MSE:HE1	1:A:113:ILE:HG13	2.02	0.41
1:G:140:ASN:ND2	1:G:144:GLU:HB2	2.36	0.41
1:J:15:PHE:HB3	1:J:16:GLU:OE1	2.20	0.41
1:I:81:GLN:CG	1:K:81:GLN:HE21	2.33	0.41
1:C:15:PHE:HB3	1:C:16:GLU:OE1	2.21	0.41
1:G:32:THR:OG1	1:K:33:GLU:CD	2.59	0.40
1:G:15:PHE:HB3	1:G:16:GLU:OE1	2.20	0.40
1:E:137:GLU:HG2	1:E:145:LEU:HD11	2.03	0.40
1:D:60:ILE:O	1:D:60:ILE:HG12	2.21	0.40
1:L:147:LEU:HD23	1:L:148:THR:N	2.36	0.40
1:C:140:ASN:HD21	1:C:144:GLU:HB2	1.85	0.40
1:E:102:ARG:HB2	1:E:148:THR:CG2	2.50	0.40
1:H:140:ASN:ND2	1:H:144:GLU:HB2	2.37	0.40
1:B:50:HIS:CD2	1:B:67:GLN:HG3	2.57	0.40
1:J:50:HIS:CD2	1:J:67:GLN:HG3	2.56	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:OE1	1:C:128:LYS:NZ[4_456]	2.16	0.04

## 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	149/161 (92%)	144 (97%)	5 (3%)	0	100	100
1	B	149/161 (92%)	143 (96%)	6 (4%)	0	100	100
1	C	151/161 (94%)	145 (96%)	6 (4%)	0	100	100
1	D	149/161 (92%)	145 (97%)	4 (3%)	0	100	100
1	E	149/161 (92%)	144 (97%)	5 (3%)	0	100	100
1	F	149/161 (92%)	144 (97%)	4 (3%)	1 (1%)	26	60
1	G	147/161 (91%)	143 (97%)	4 (3%)	0	100	100
1	H	147/161 (91%)	143 (97%)	3 (2%)	1 (1%)	26	60
1	I	147/161 (91%)	142 (97%)	5 (3%)	0	100	100
1	J	147/161 (91%)	144 (98%)	3 (2%)	0	100	100
1	K	147/161 (91%)	143 (97%)	4 (3%)	0	100	100
1	L	147/161 (91%)	142 (97%)	4 (3%)	1 (1%)	26	60
All	All	1778/1932 (92%)	1722 (97%)	53 (3%)	3 (0%)	52	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	99	LYS
1	F	10	ARG
1	H	99	LYS

### 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	130/138 (94%)	123 (95%)	7 (5%)	27	59
1	B	130/138 (94%)	122 (94%)	8 (6%)	23	53
1	C	132/138 (96%)	122 (92%)	10 (8%)	16	41
1	D	130/138 (94%)	123 (95%)	7 (5%)	27	59
1	E	130/138 (94%)	122 (94%)	8 (6%)	23	53
1	F	130/138 (94%)	122 (94%)	8 (6%)	23	53
1	G	129/138 (94%)	122 (95%)	7 (5%)	27	59
1	H	129/138 (94%)	122 (95%)	7 (5%)	27	59
1	I	129/138 (94%)	122 (95%)	7 (5%)	27	59
1	J	129/138 (94%)	120 (93%)	9 (7%)	19	46
1	K	129/138 (94%)	122 (95%)	7 (5%)	27	59
1	L	129/138 (94%)	120 (93%)	9 (7%)	19	46
All	All	1556/1656 (94%)	1462 (94%)	94 (6%)	24	55

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	49	LEU
1	A	54	GLU
1	A	84	LEU
1	A	95	PHE
1	A	127	GLU
1	A	141	GLN
1	B	16	GLU
1	B	49	LEU
1	B	54	GLU
1	B	84	LEU
1	B	95	PHE
1	B	100	ASP
1	B	127	GLU
1	B	141	GLN
1	C	7	ILE
1	C	10	ARG
1	C	16	GLU
1	C	49	LEU
1	C	54	GLU
1	C	84	LEU
1	C	95	PHE

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Mol	Chain	Res	Type
1	C	100	ASP
1	C	127	GLU
1	C	141	GLN
1	D	16	GLU
1	D	49	LEU
1	D	54	GLU
1	D	84	LEU
1	D	95	PHE
1	D	127	GLU
1	D	141	GLN
1	E	16	GLU
1	E	49	LEU
1	E	54	GLU
1	E	84	LEU
1	E	95	PHE
1	E	100	ASP
1	E	127	GLU
1	E	141	GLN
1	F	16	GLU
1	F	49	LEU
1	F	54	GLU
1	F	84	LEU
1	F	95	PHE
1	F	100	ASP
1	F	127	GLU
1	F	141	GLN
1	G	16	GLU
1	G	49	LEU
1	G	54	GLU
1	G	84	LEU
1	G	95	PHE
1	G	127	GLU
1	G	141	GLN
1	H	16	GLU
1	H	49	LEU
1	H	54	GLU
1	H	84	LEU
1	H	95	PHE
1	H	127	GLU
1	H	141	GLN
1	I	16	GLU
1	I	49	LEU

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Mol	Chain	Res	Type
1	I	54	GLU
1	I	84	LEU
1	I	95	PHE
1	I	127	GLU
1	I	141	GLN
1	J	16	GLU
1	J	49	LEU
1	J	54	GLU
1	J	84	LEU
1	J	95	PHE
1	J	100	ASP
1	J	127	GLU
1	J	139	LYS
1	J	141	GLN
1	K	16	GLU
1	K	49	LEU
1	K	54	GLU
1	K	84	LEU
1	K	95	PHE
1	K	127	GLU
1	K	141	GLN
1	L	11	ASN
1	L	16	GLU
1	L	49	LEU
1	L	54	GLU
1	L	84	LEU
1	L	95	PHE
1	L	99	LYS
1	L	127	GLU
1	L	141	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	86	ASN
1	A	141	GLN
1	B	81	GLN
1	B	141	GLN
1	C	81	GLN
1	C	86	ASN
1	C	141	GLN

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Mol	Chain	Res	Type
1	D	81	GLN
1	D	86	ASN
1	D	141	GLN
1	E	81	GLN
1	E	141	GLN
1	F	81	GLN
1	F	141	GLN
1	G	81	GLN
1	G	141	GLN
1	H	81	GLN
1	H	86	ASN
1	H	141	GLN
1	I	11	ASN
1	I	81	GLN
1	I	86	ASN
1	I	141	GLN
1	J	11	ASN
1	J	81	GLN
1	J	141	GLN
1	K	81	GLN
1	K	141	GLN
1	L	81	GLN
1	L	86	ASN
1	L	141	GLN

### 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 ⓘ

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	149/161 (92%)	-0.25	4 (2%) 58 46	17, 38, 90, 134	0
1	B	149/161 (92%)	-0.30	1 (0%) 89 84	21, 40, 76, 116	0
1	C	151/161 (93%)	-0.17	2 (1%) 79 71	22, 45, 94, 122	0
1	D	149/161 (92%)	-0.21	1 (0%) 89 84	18, 44, 104, 153	0
1	E	149/161 (92%)	-0.17	2 (1%) 79 71	18, 41, 98, 129	0
1	F	149/161 (92%)	-0.29	2 (1%) 79 71	22, 39, 81, 125	0
1	G	147/161 (91%)	2.35	66 (44%) 0 0	76, 151, 187, 198	0
1	H	147/161 (91%)	2.20	74 (50%) 0 0	72, 159, 186, 199	0
1	I	147/161 (91%)	0.83	22 (14%) 3 2	43, 98, 152, 171	0
1	J	147/161 (91%)	1.13	30 (20%) 1 1	53, 121, 169, 200	0
1	K	147/161 (91%)	2.92	95 (64%) 0 0	108, 171, 197, 200	0
1	L	147/161 (91%)	3.24	96 (65%) 0 0	89, 172, 196, 200	0
All	All	1778/1932 (92%)	0.93	395 (22%) 1 1	17, 84, 186, 200	0

All (395) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	94	ALA	19.0
1	K	130	GLY	13.4
1	L	154	LEU	12.4
1	L	153	ALA	10.9
1	K	129	SER	10.4
1	J	127	GLU	9.3
1	G	124	ASP	8.7
1	K	92	VAL	8.7
1	G	153	ALA	8.6
1	L	93	ILE	8.3
1	H	52	ASP	8.0

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Mol	Chain	Res	Type	RSRZ
1	G	86	ASN	7.7
1	L	119	VAL	7.7
1	L	79	VAL	7.6
1	L	96	PHE	7.4
1	H	21	GLY	7.1
1	G	158	THR	6.8
1	K	21	GLY	6.8
1	L	121	GLU	6.7
1	G	159	PRO	6.7
1	L	25	GLU	6.6
1	K	159	PRO	6.6
1	K	137	GLU	6.5
1	L	86	ASN	6.3
1	L	111	ASP	6.3
1	L	13	ILE	6.2
1	H	24	ILE	6.1
1	L	31	VAL	6.1
1	G	20	ILE	6.0
1	K	155	ILE	6.0
1	K	122	LYS	6.0
1	L	17	SER	5.9
1	G	131	VAL	5.9
1	G	87	TYR	5.9
1	K	22	GLU	5.9
1	K	20	ILE	5.9
1	K	13	ILE	5.9
1	K	61	PHE	5.8
1	K	111	ASP	5.8
1	L	130	GLY	5.8
1	G	23	LYS	5.7
1	H	45	ASP	5.6
1	G	139	LYS	5.6
1	H	127	GLU	5.6
1	G	26	GLY	5.5
1	L	91	SER	5.5
1	L	127	GLU	5.5
1	G	128	LYS	5.4
1	G	29	ARG	5.3
1	L	141	GLN	5.3
1	K	121	GLU	5.2
1	L	159	PRO	5.2
1	G	154	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	L	131	VAL	5.2
1	G	125	PHE	5.2
1	L	124	ASP	5.2
1	L	97	GLY	5.1
1	K	11	ASN	5.1
1	L	155	ILE	5.1
1	G	94	ALA	5.1
1	K	117	ALA	5.1
1	K	134	TYR	5.1
1	K	128	LYS	5.1
1	G	14	TYR	5.0
1	K	145	LEU	5.0
1	K	94	ALA	5.0
1	K	89	VAL	5.0
1	G	16	GLU	5.0
1	L	23	LYS	5.0
1	L	95	PHE	5.0
1	K	150	LEU	5.0
1	J	124	ASP	5.0
1	L	120	VAL	4.9
1	G	28	PRO	4.9
1	L	20	ILE	4.9
1	K	17	SER	4.9
1	L	11	ASN	4.8
1	L	26	GLY	4.8
1	K	127	GLU	4.8
1	K	14	TYR	4.8
1	H	53	VAL	4.8
1	H	54	GLU	4.8
1	H	156	ARG	4.7
1	G	18	ILE	4.7
1	L	143	GLY	4.7
1	H	124	ASP	4.7
1	L	82	VAL	4.7
1	L	12	PRO	4.7
1	I	11	ASN	4.7
1	H	96	PHE	4.7
1	L	89	VAL	4.7
1	H	159	PRO	4.7
1	G	19	GLN	4.7
1	J	123	GLN	4.6
1	L	15	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	K	99	LYS	4.6
1	L	156	ARG	4.6
1	K	96	PHE	4.6
1	L	104	LEU	4.6
1	L	88	ASP	4.6
1	L	87	TYR	4.6
1	H	14	TYR	4.5
1	K	119	VAL	4.5
1	G	113	ILE	4.5
1	L	125	PHE	4.5
1	G	11	ASN	4.5
1	G	99	LYS	4.5
1	I	12	PRO	4.5
1	H	128	LYS	4.4
1	K	143	GLY	4.4
1	L	152	SER	4.4
1	H	17	SER	4.4
1	J	14	TYR	4.4
1	L	146	VAL	4.4
1	G	114	ALA	4.3
1	K	123	GLN	4.2
1	J	159	PRO	4.2
1	K	62	GLY	4.2
1	K	95	PHE	4.2
1	L	16	GLU	4.2
1	L	148	THR	4.2
1	L	118	GLU	4.2
1	H	144	GLU	4.2
1	L	102	ARG	4.2
1	L	122	LYS	4.2
1	K	76	LEU	4.2
1	J	122	LYS	4.1
1	H	104	LEU	4.1
1	K	103	PHE	4.1
1	K	133	THR	4.1
1	I	57	LYS	4.1
1	H	131	VAL	4.1
1	H	63	LYS	4.0
1	G	112	THR	4.0
1	H	145	LEU	4.0
1	J	125	PHE	4.0
1	L	158	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	K	104	LEU	3.9
1	I	142	ARG	3.9
1	G	37	TRP	3.9
1	K	120	VAL	3.9
1	H	122	LYS	3.9
1	L	67	GLN	3.9
1	L	133	THR	3.9
1	G	127	GLU	3.9
1	G	61	PHE	3.8
1	K	106	PRO	3.8
1	K	60	ILE	3.8
1	J	25	GLU	3.8
1	G	156	ARG	3.8
1	L	135	LYS	3.8
1	K	50	HIS	3.8
1	L	110	GLY	3.8
1	G	30	THR	3.8
1	H	22	GLU	3.8
1	K	131	VAL	3.8
1	L	52	ASP	3.7
1	K	142	ARG	3.7
1	H	139	LYS	3.7
1	K	144	GLU	3.7
1	K	135	LYS	3.7
1	F	9	ALA	3.7
1	H	125	PHE	3.7
1	L	115	ALA	3.7
1	H	19	GLN	3.6
1	E	11	ASN	3.6
1	J	154	LEU	3.6
1	J	93	ILE	3.6
1	L	109	ILE	3.6
1	H	106	PRO	3.5
1	K	157	LYS	3.5
1	L	63	LYS	3.5
1	K	73	SER	3.5
1	G	27	LEU	3.5
1	K	146	VAL	3.5
1	K	25	GLU	3.4
1	B	9	ALA	3.4
1	G	96	PHE	3.4
1	L	30	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	149	ALA	3.4
1	H	129	SER	3.4
1	K	48	PRO	3.4
1	L	92	VAL	3.3
1	K	47	PHE	3.3
1	G	155	ILE	3.3
1	L	80	ASP	3.3
1	I	105	ARG	3.3
1	H	44	ALA	3.3
1	L	71	VAL	3.3
1	K	66	ALA	3.3
1	K	91	SER	3.3
1	L	116	SER	3.3
1	K	26	GLY	3.3
1	H	120	VAL	3.3
1	K	24	ILE	3.3
1	H	12	PRO	3.3
1	K	151	TYR	3.3
1	A	9	ALA	3.2
1	H	43	THR	3.2
1	H	130	GLY	3.2
1	H	18	ILE	3.2
1	L	50	HIS	3.2
1	F	11	ASN	3.2
1	G	140	ASN	3.2
1	L	114	ALA	3.2
1	J	11	ASN	3.2
1	G	17	SER	3.2
1	L	145	LEU	3.2
1	H	23	LYS	3.2
1	J	139	LYS	3.1
1	H	123	GLN	3.1
1	H	134	TYR	3.1
1	K	132	VAL	3.1
1	H	38	THR	3.1
1	H	100	ASP	3.1
1	K	105	ARG	3.1
1	G	135	LYS	3.1
1	K	63	LYS	3.1
1	L	32	THR	3.1
1	L	64	PRO	3.1
1	K	84	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	45	ASP	3.1
1	G	56	ALA	3.1
1	J	23	LYS	3.1
1	H	27	LEU	3.1
1	H	97	GLY	3.0
1	H	68	GLY	3.0
1	K	156	ARG	3.0
1	L	157	LYS	3.0
1	I	52	ASP	3.0
1	L	37	TRP	3.0
1	J	105	ARG	3.0
1	G	68	GLY	3.0
1	G	102	ARG	3.0
1	L	129	SER	3.0
1	G	101	VAL	3.0
1	G	118	GLU	2.9
1	G	121	GLU	2.9
1	J	22	GLU	2.9
1	L	105	ARG	2.9
1	I	141	GLN	2.9
1	K	116	SER	2.9
1	L	58	LYS	2.9
1	K	101	VAL	2.9
1	G	12	PRO	2.9
1	G	60	ILE	2.9
1	G	13	ILE	2.9
1	G	152	SER	2.9
1	L	142	ARG	2.9
1	I	27	LEU	2.9
1	K	19	GLN	2.8
1	J	85	SER	2.8
1	L	144	GLU	2.8
1	K	126	ASP	2.8
1	K	148	THR	2.8
1	H	61	PHE	2.8
1	L	99	LYS	2.8
1	L	101	VAL	2.8
1	L	27	LEU	2.8
1	H	113	ILE	2.8
1	E	9	ALA	2.8
1	K	114	ALA	2.8
1	L	51	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	61	PHE	2.7
1	L	18	ILE	2.7
1	G	59	THR	2.7
1	J	129	SER	2.7
1	G	132	VAL	2.7
1	H	132	VAL	2.7
1	K	53	VAL	2.7
1	K	90	SER	2.7
1	J	140	ASN	2.7
1	A	10	ARG	2.7
1	L	126	ASP	2.7
1	I	54	GLU	2.7
1	G	141	GLN	2.7
1	H	47	PHE	2.6
1	L	98	ILE	2.6
1	G	130	GLY	2.6
1	K	49	LEU	2.6
1	I	87	TYR	2.6
1	H	119	VAL	2.6
1	G	65	ILE	2.6
1	K	23	LYS	2.6
1	H	11	ASN	2.6
1	H	55	PHE	2.6
1	H	102	ARG	2.6
1	H	115	ALA	2.6
1	J	19	GLN	2.6
1	C	7	ILE	2.5
1	H	108	PHE	2.5
1	J	20	ILE	2.5
1	L	56	ALA	2.5
1	G	105	ARG	2.5
1	J	21	GLY	2.5
1	J	45	ASP	2.5
1	L	29	ARG	2.5
1	K	98	ILE	2.5
1	L	24	ILE	2.5
1	I	55	PHE	2.5
1	H	154	LEU	2.5
1	H	13	ILE	2.5
1	J	17	SER	2.5
1	H	138	VAL	2.5
1	H	16	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	28	PRO	2.4
1	H	133	THR	2.4
1	J	87	TYR	2.4
1	H	105	ARG	2.4
1	K	118	GLU	2.4
1	I	109	ILE	2.4
1	H	121	GLU	2.4
1	L	128	LYS	2.4
1	K	115	ALA	2.4
1	J	54	GLU	2.4
1	K	108	PHE	2.4
1	G	89	VAL	2.4
1	K	56	ALA	2.4
1	K	97	GLY	2.4
1	J	126	ASP	2.4
1	L	90	SER	2.4
1	K	158	THR	2.4
1	K	67	GLN	2.4
1	H	137	GLU	2.4
1	G	95	PHE	2.4
1	L	123	GLN	2.3
1	H	62	GLY	2.3
1	H	95	PHE	2.3
1	I	108	PHE	2.3
1	J	153	ALA	2.3
1	H	143	GLY	2.3
1	G	90	SER	2.3
1	K	136	LEU	2.3
1	L	150	LEU	2.3
1	I	60	ILE	2.3
1	K	72	LEU	2.3
1	K	88	ASP	2.3
1	G	134	TYR	2.3
1	H	20	ILE	2.3
1	H	46	PHE	2.3
1	G	133	THR	2.3
1	H	92	VAL	2.3
1	K	38	THR	2.3
1	H	57	LYS	2.3
1	G	54	GLU	2.2
1	J	86	ASN	2.2
1	I	145	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	9	ALA	2.2
1	G	24	ILE	2.2
1	G	84	LEU	2.2
1	K	100	ASP	2.2
1	K	83	ILE	2.2
1	L	151	TYR	2.2
1	K	68	GLY	2.2
1	H	158	THR	2.2
1	I	143	GLY	2.2
1	H	51	THR	2.2
1	L	28	PRO	2.2
1	K	27	LEU	2.2
1	H	39	PHE	2.2
1	L	106	PRO	2.2
1	K	18	ILE	2.2
1	K	74	ILE	2.2
1	H	112	THR	2.2
1	K	154	LEU	2.1
1	K	54	GLU	2.1
1	I	37	TRP	2.1
1	A	127	GLU	2.1
1	H	153	ALA	2.1
1	I	14	TYR	2.1
1	L	81	GLN	2.1
1	A	99	LYS	2.1
1	H	65	ILE	2.1
1	G	48	PRO	2.1
1	I	144	GLU	2.1
1	H	42	LEU	2.1
1	I	159	PRO	2.1
1	C	63	LYS	2.0
1	G	137	GLU	2.0
1	K	40	ALA	2.0
1	K	153	ALA	2.0
1	K	15	PHE	2.0
1	L	21	GLY	2.0
1	K	107	VAL	2.0
1	I	63	LYS	2.0
1	L	73	SER	2.0
1	L	117	ALA	2.0
1	L	62	GLY	2.0
1	J	144	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	57	LYS	2.0
1	G	120	VAL	2.0
1	H	41	TYR	2.0
1	L	134	TYR	2.0
1	G	25	GLU	2.0
1	L	47	PHE	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 carbohydrates 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.