



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:05 am BST

PDB ID : 2YBV  
Title : STRUCTURE OF RUBISCO FROM THERMOSYNECHOCOCCUS ELONGATUS  
Authors : Terlecka, B.; Wilhelmi, V.; Bialek, W.; Gubernator, B.; Szczepaniak, A.; Hofmann, E.  
Deposited on : 2011-03-10  
Resolution : 2.30 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.

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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)	:	1.13
EDS	:	2.11
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)	:	2.11

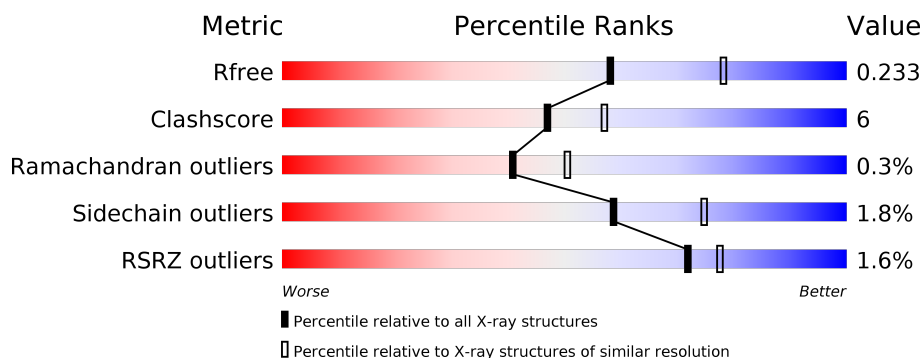
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	475	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>10%</div> </div> </div>
1	C	475	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>
1	E	475	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>• 10%</div> </div> </div>
1	G	475	<div> <div></div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>
1	I	475	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>• 10%</div> </div> </div>
1	K	475	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	M	475	
1	O	475	
2	B	118	
2	D	118	
2	F	118	
2	H	118	
2	J	118	
2	L	118	
2	N	118	
2	P	118	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34583 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 RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3348	2123	588	616	21			
1	C	428	Total	C	N	O	S	0	0	0
			3348	2123	588	616	21			
1	E	428	Total	C	N	O	S	0	0	0
			3348	2123	588	616	21			
1	G	428	Total	C	N	O	S	0	0	0
			3348	2123	588	616	21			
1	I	428	Total	C	N	O	S	0	0	0
			3348	2123	588	616	21			
1	K	428	Total	C	N	O	S	0	0	0
			3348	2123	588	616	21			
1	M	428	Total	C	N	O	S	0	0	0
			3348	2123	588	616	21			
1	O	428	Total	C	N	O	S	0	0	0
			3348	2123	588	616	21			

- Molecule 2 is a protein called RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			869	557	146	159	7			
2	D	104	Total	C	N	O	S	0	0	0
			869	557	146	159	7			
2	F	104	Total	C	N	O	S	0	0	0
			869	557	146	159	7			
2	H	104	Total	C	N	O	S	0	0	0
			869	557	146	159	7			
2	J	104	Total	C	N	O	S	0	0	0
			869	557	146	159	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	104	Total 869	C 557	N 146	O 159	S 7	0	0	0
2	N	104	Total 869	C 557	N 146	O 159	S 7	0	0	0
2	P	104	Total 869	C 557	N 146	O 159	S 7	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total 2	Cl 2	0	0
3	K	2	Total 2	Cl 2	0	0
3	E	1	Total 1	Cl 1	0	0
3	I	2	Total 2	Cl 2	0	0
3	C	2	Total 2	Cl 2	0	0
3	A	2	Total 2	Cl 2	0	0
3	O	2	Total 2	Cl 2	0	0
3	M	2	Total 2	Cl 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total 106	O 106	0	0
4	B	3	Total 3	O 3	0	0
4	C	119	Total 119	O 119	0	0
4	D	7	Total 7	O 7	0	0
4	E	118	Total 118	O 118	0	0
4	F	8	Total 8	O 8	0	0

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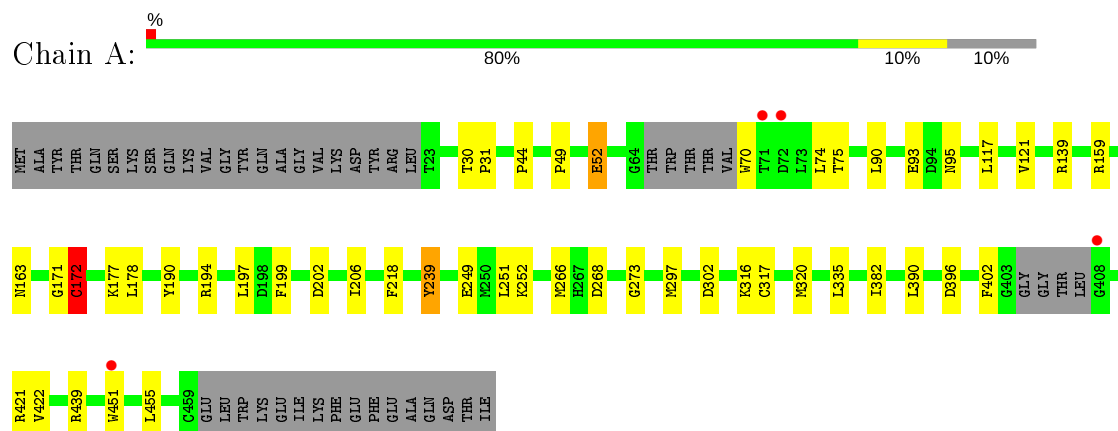
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	112	Total 112	O 112	0	0
4	H	4	Total 4	O 4	0	0
4	I	87	Total 87	O 87	0	0
4	J	16	Total 16	O 16	0	0
4	K	73	Total 73	O 73	0	0
4	L	7	Total 7	O 7	0	0
4	M	77	Total 77	O 77	0	0
4	N	9	Total 9	O 9	0	0
4	O	80	Total 80	O 80	0	0
4	P	6	Total 6	O 6	0	0

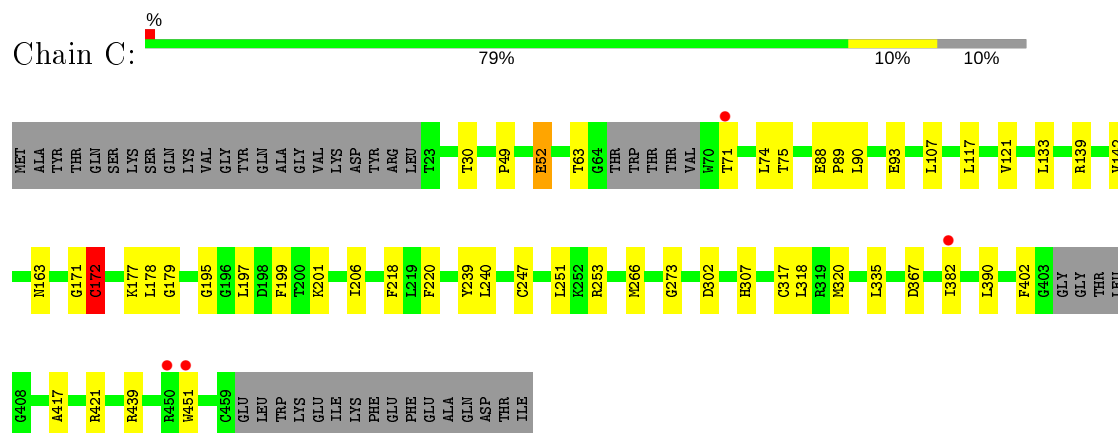
### 3 Residue-property plots [i](#)

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

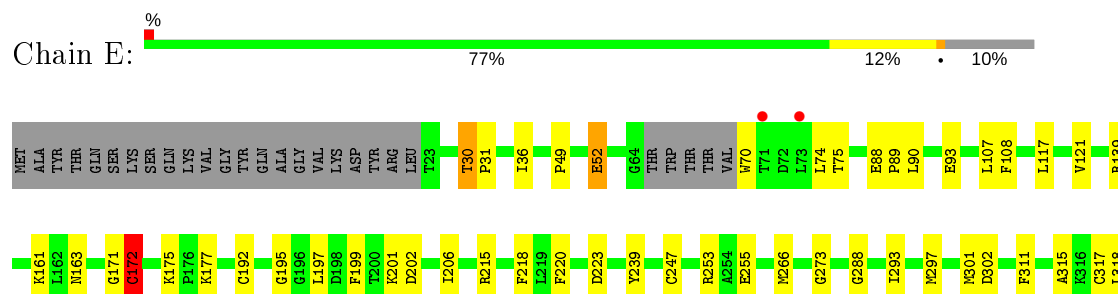
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

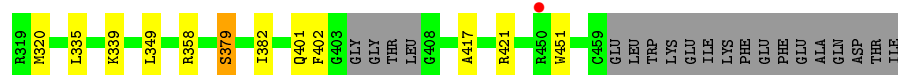


#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



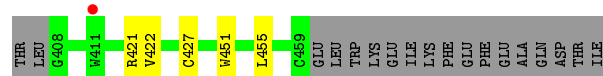
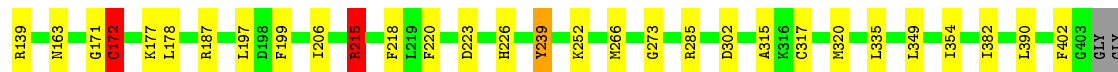
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN





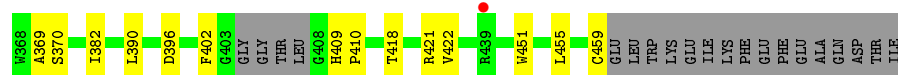
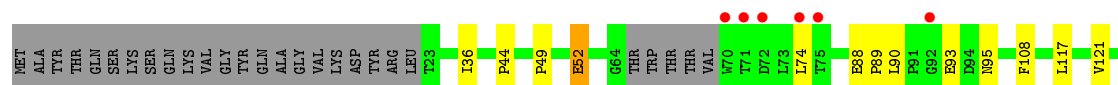
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain G: 79% 10% 10%



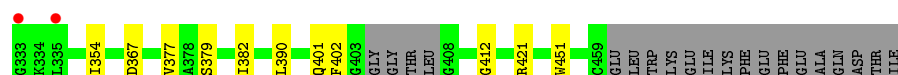
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain I: 2% 78% 12% 10%



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

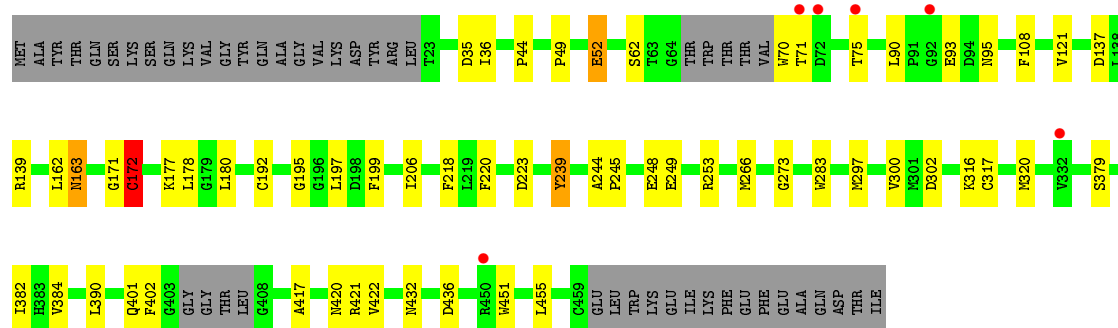
Chain K: % 78% 12% 10%



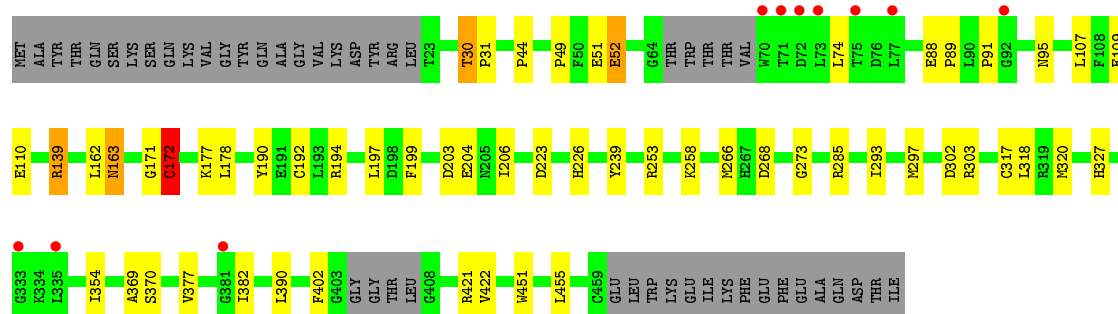
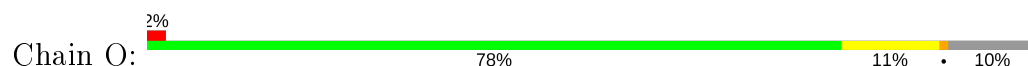
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain M: % 77% 12% 10%

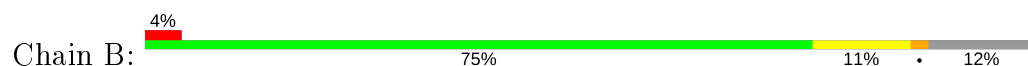




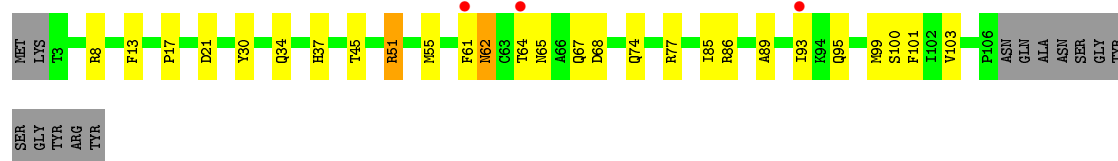
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



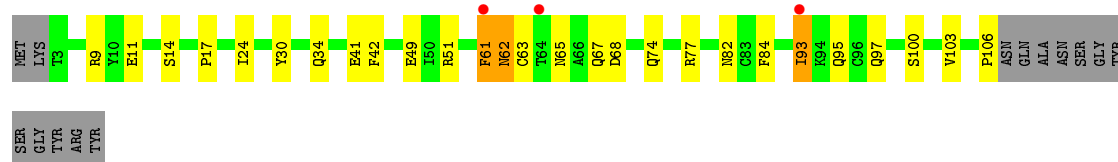
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT




• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT



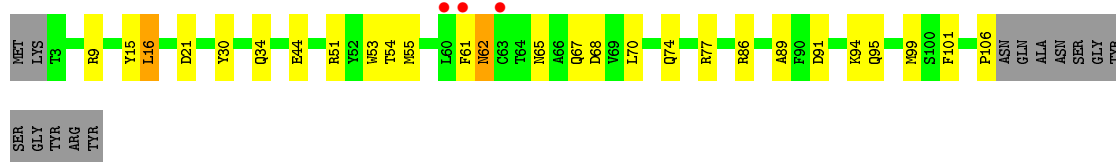
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT

Chain H: 



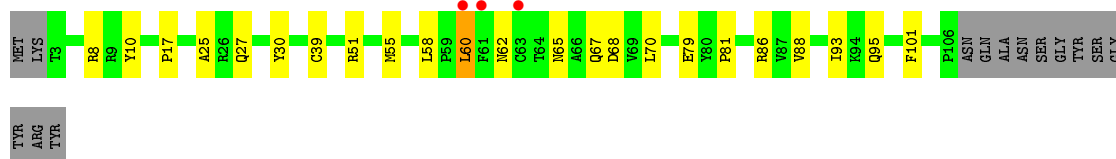
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT

Chain J: 




- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT

Chain L: 



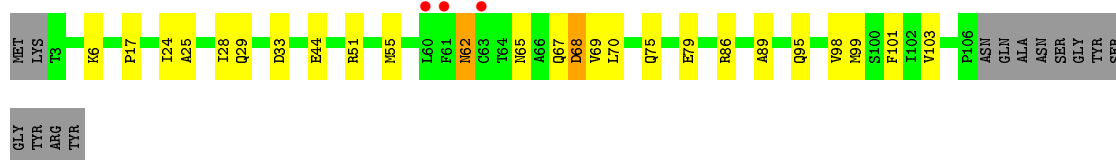
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT

Chain N: 



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT

Chain P: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.48Å 163.47Å 163.54Å 90.00° 108.96° 90.00°	Depositor
Resolution (Å)	39.84 – 2.30 39.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.84-2.30) 100.0 (39.83-2.30)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.196 , 0.232 0.196 , 0.233	Depositor DCC
$R_{free}$ test set	12993 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.8	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 14.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	34583	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.12	9/3427 (0.3%)	0.99	10/4642 (0.2%)
1	C	1.11	8/3427 (0.2%)	0.93	7/4642 (0.2%)
1	E	1.11	11/3427 (0.3%)	0.97	9/4642 (0.2%)
1	G	1.11	7/3427 (0.2%)	0.99	9/4642 (0.2%)
1	I	1.07	6/3427 (0.2%)	0.96	6/4642 (0.1%)
1	K	1.09	5/3427 (0.1%)	0.93	7/4642 (0.2%)
1	M	1.09	9/3427 (0.3%)	0.94	10/4642 (0.2%)
1	O	1.08	3/3427 (0.1%)	0.92	7/4642 (0.2%)
2	B	0.90	0/893	0.85	0/1215
2	D	0.94	0/893	0.83	0/1215
2	F	0.99	2/893 (0.2%)	0.86	0/1215
2	H	0.98	1/893 (0.1%)	0.85	0/1215
2	J	1.02	0/893	0.84	0/1215
2	L	0.95	0/893	0.86	0/1215
2	N	0.91	0/893	0.83	0/1215
2	P	0.94	0/893	0.81	0/1215
All	All	1.07	61/34560 (0.2%)	0.93	65/46856 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	172	CYS	CB-SG	10.14	1.99	1.82
1	M	218	PHE	CE2-CZ	-9.31	1.19	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	ARG	CZ-NH1	-8.98	1.21	1.33
1	M	218	PHE	CG-CD2	-8.66	1.25	1.38
1	A	139	ARG	CZ-NH2	-8.63	1.21	1.33
1	A	218	PHE	CG-CD2	-8.46	1.26	1.38
1	I	421	ARG	CZ-NH2	-8.42	1.22	1.33
1	C	172	CYS	CB-SG	8.41	1.96	1.82
1	C	218	PHE	CG-CD2	-8.24	1.26	1.38
1	O	172	CYS	CB-SG	8.10	1.96	1.82
1	M	218	PHE	CE1-CZ	-7.97	1.22	1.37
1	E	139	ARG	CZ-NH2	-7.74	1.23	1.33
1	G	172	CYS	CB-SG	7.72	1.95	1.82
1	G	421	ARG	CZ-NH2	-7.56	1.23	1.33
1	E	139	ARG	CZ-NH1	-7.54	1.23	1.33
1	A	218	PHE	CE2-CZ	-7.39	1.23	1.37
1	C	218	PHE	CE1-CZ	-7.30	1.23	1.37
1	I	172	CYS	CB-SG	7.25	1.94	1.82
1	A	172	CYS	CB-SG	6.98	1.94	1.82
1	G	421	ARG	CZ-NH1	-6.81	1.24	1.33
1	M	421	ARG	CZ-NH2	-6.77	1.24	1.33
1	A	218	PHE	CG-CD1	-6.68	1.28	1.38
1	A	218	PHE	CE1-CZ	-6.65	1.24	1.37
2	F	41	GLU	CG-CD	6.46	1.61	1.51
1	C	218	PHE	CG-CD1	-6.41	1.29	1.38
1	E	172	CYS	CB-SG	6.37	1.93	1.82
1	K	218	PHE	CE2-CZ	-6.31	1.25	1.37
1	E	311	PHE	CE2-CZ	6.22	1.49	1.37
1	E	421	ARG	CZ-NH1	-6.22	1.25	1.33
1	E	218	PHE	CE1-CZ	-5.99	1.25	1.37
1	C	421	ARG	CZ-NH1	-5.96	1.25	1.33
1	I	421	ARG	CZ-NH1	-5.96	1.25	1.33
2	F	11	GLU	CG-CD	5.93	1.60	1.51
1	O	109	GLU	CB-CG	5.92	1.63	1.52
1	G	218	PHE	CG-CD2	-5.90	1.29	1.38
1	E	218	PHE	CG-CD2	-5.87	1.29	1.38
1	M	172	CYS	CB-SG	5.76	1.92	1.82
1	M	218	PHE	CG-CD1	-5.71	1.30	1.38
2	H	41	GLU	CG-CD	5.66	1.60	1.51
1	K	249	GLU	CB-CG	-5.64	1.41	1.52
1	C	247	CYS	CB-SG	5.63	1.91	1.82
1	A	421	ARG	CZ-NH2	-5.60	1.25	1.33
1	M	421	ARG	CZ-NH1	-5.53	1.25	1.33
1	K	248	GLU	CG-CD	5.50	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	247	CYS	CB-SG	5.50	1.91	1.82
1	I	218	PHE	CE1-CZ	-5.46	1.26	1.37
1	I	125	PHE	CE1-CZ	5.33	1.47	1.37
1	M	283	TRP	CG-CD1	5.32	1.44	1.36
1	K	218	PHE	CG-CD2	-5.24	1.30	1.38
1	A	249	GLU	CB-CG	-5.23	1.42	1.52
1	G	427	CYS	CB-SG	-5.21	1.73	1.81
1	E	255	GLU	CG-CD	5.21	1.59	1.51
1	E	218	PHE	CG-CD1	-5.16	1.31	1.38
1	O	110	GLU	CB-CG	5.15	1.61	1.52
1	E	218	PHE	CE2-CZ	-5.14	1.27	1.37
1	C	218	PHE	CE2-CZ	-5.14	1.27	1.37
1	G	110	GLU	CG-CD	5.12	1.59	1.51
1	G	187	ARG	CG-CD	5.11	1.64	1.51
1	I	459	CYS	CB-SG	5.10	1.91	1.82
1	C	142	VAL	CB-CG2	5.04	1.63	1.52
1	M	248	GLU	CG-CD	5.02	1.59	1.51

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	215	ARG	NE-CZ-NH1	19.10	129.85	120.30
1	I	421	ARG	NE-CZ-NH1	15.58	128.09	120.30
1	E	139	ARG	NE-CZ-NH2	14.95	127.77	120.30
1	M	421	ARG	NE-CZ-NH1	13.97	127.28	120.30
1	A	139	ARG	NE-CZ-NH2	13.84	127.22	120.30
1	A	139	ARG	NE-CZ-NH1	13.75	127.17	120.30
1	G	215	ARG	NE-CZ-NH2	-13.10	113.75	120.30
1	A	139	ARG	NH1-CZ-NH2	-12.55	105.60	119.40
1	E	139	ARG	NH1-CZ-NH2	-12.39	105.77	119.40
1	E	139	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	I	421	ARG	NH1-CZ-NH2	-11.81	106.41	119.40
1	G	215	ARG	CD-NE-CZ	11.28	139.39	123.60
1	G	421	ARG	NE-CZ-NH1	10.77	125.69	120.30
1	I	421	ARG	NE-CZ-NH2	10.39	125.50	120.30
1	M	421	ARG	NH1-CZ-NH2	-9.66	108.77	119.40
1	K	139	ARG	NE-CZ-NH2	9.56	125.08	120.30
1	E	421	ARG	NE-CZ-NH2	8.76	124.68	120.30
1	A	421	ARG	NE-CZ-NH2	8.69	124.65	120.30
1	G	421	ARG	NH1-CZ-NH2	-8.33	110.24	119.40
1	C	421	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	O	421	ARG	NE-CZ-NH1	8.16	124.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	421	ARG	NE-CZ-NH2	8.11	124.36	120.30
1	M	139	ARG	NE-CZ-NH2	8.06	124.33	120.30
1	G	421	ARG	NE-CZ-NH2	7.53	124.07	120.30
1	C	253	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	268	ASP	CB-CG-OD2	7.27	124.85	118.30
1	M	421	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	E	421	ARG	NH1-CZ-NH2	-7.21	111.46	119.40
1	K	421	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	O	139	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	C	139	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	E	421	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	K	421	ARG	NH1-CZ-NH2	-6.98	111.72	119.40
1	A	421	ARG	NH1-CZ-NH2	-6.79	111.94	119.40
1	C	253	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	I	367	ASP	CB-CG-OD1	6.25	123.93	118.30
1	I	139	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	A	421	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	202	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	O	421	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
1	O	268	ASP	CB-CG-OD2	5.88	123.59	118.30
1	G	139	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	E	358	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	K	303	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	M	218	PHE	CD1-CG-CD2	-5.76	110.81	118.30
1	E	215	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	M	218	PHE	CB-CG-CD2	5.54	124.67	120.80
1	C	421	ARG	NH1-CZ-NH2	-5.49	113.36	119.40
1	E	253	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	I	215	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	C	367	ASP	CB-CG-OD1	5.24	123.01	118.30
1	O	258	LYS	CD-CE-NZ	-5.23	99.68	111.70
1	A	218	PHE	CB-CG-CD1	5.22	124.45	120.80
1	G	252	LYS	CD-CE-NZ	-5.20	99.73	111.70
1	M	137	ASP	CB-CG-OD1	5.20	122.98	118.30
1	M	218	PHE	CB-CG-CD1	5.19	124.43	120.80
1	M	218	PHE	CZ-CE2-CD2	5.16	126.29	120.10
1	O	253	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	O	303	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	240	LEU	CB-CG-CD1	-5.13	102.29	111.00
1	K	252	LYS	CD-CE-NZ	-5.12	99.94	111.70
1	G	215	ARG	CG-CD-NE	-5.11	101.06	111.80
1	A	252	LYS	CD-CE-NZ	-5.11	99.96	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	367	ASP	CB-CG-OD1	5.10	122.89	118.30
1	M	35	ASP	CB-CG-OD1	5.06	122.86	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	215	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3348	0	3273	35	2
1	C	3348	0	3273	41	2
1	E	3348	0	3273	44	0
1	G	3348	0	3273	37	0
1	I	3348	0	3273	45	0
1	K	3348	0	3273	45	0
1	M	3348	0	3273	47	0
1	O	3348	0	3273	44	0
2	B	869	0	836	12	0
2	D	869	0	836	22	0
2	F	869	0	836	18	0
2	H	869	0	836	10	0
2	J	869	0	836	22	0
2	L	869	0	836	19	0
2	N	869	0	836	16	0
2	P	869	0	836	21	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
3	E	1	0	0	0	0
3	G	2	0	0	0	0
3	I	2	0	0	0	0
3	K	2	0	0	0	0
3	M	2	0	0	0	0
3	O	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	106	0	0	2	0
4	B	3	0	0	0	0
4	C	119	0	0	3	0
4	D	7	0	0	1	0
4	E	118	0	0	4	0
4	F	8	0	0	0	0
4	G	112	0	0	3	0
4	H	4	0	0	0	0
4	I	87	0	0	2	0
4	J	16	0	0	0	0
4	K	73	0	0	4	0
4	L	7	0	0	0	0
4	M	77	0	0	0	0
4	N	9	0	0	0	0
4	O	80	0	0	5	0
4	P	6	0	0	0	0
All	All	34583	0	32872	412	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (412) 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:C:49:PRO:HD2	1:C:52:GLU:HG3	1.37	1.06
1:O:177:LYS:O	1:O:206:ILE:HD11	1.63	0.99
4:C:2011:HOH:O	1:K:178:LEU:HD12	1.63	0.98
1:I:49:PRO:HD2	1:I:52:GLU:HG3	1.45	0.98
2:D:51:ARG:HD2	1:E:223:ASP:OD2	1.63	0.98
1:O:223:ASP:OD2	2:P:51:ARG:HD2	1.63	0.97
4:E:2010:HOH:O	1:M:178:LEU:HD12	1.61	0.97
1:E:49:PRO:HD2	1:E:52:GLU:HG3	1.47	0.97
1:I:223:ASP:OD2	2:J:51:ARG:HD2	1.64	0.96
1:A:49:PRO:HD2	1:A:52:GLU:HG3	1.46	0.96
1:O:49:PRO:HD2	1:O:52:GLU:HG3	1.48	0.95
1:M:177:LYS:O	1:M:206:ILE:HD11	1.66	0.94
1:O:317:CYS:HA	1:O:320:MET:HE2	1.47	0.94
1:G:49:PRO:HD2	1:G:52:GLU:HG3	1.50	0.94
1:A:178:LEU:HD12	4:I:2007:HOH:O	1.68	0.94
1:M:49:PRO:HD2	1:M:52:GLU:HG3	1.50	0.94
1:K:223:ASP:OD2	2:L:51:ARG:HD2	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:ASN:HD21	2:D:67:GLN:HB3	1.38	0.88
1:K:177:LYS:O	1:K:206:ILE:HD11	1.75	0.87
1:I:177:LYS:O	1:I:206:ILE:HD11	1.73	0.86
1:C:178:LEU:HD12	4:K:2012:HOH:O	1.76	0.86
1:I:317:CYS:HA	1:I:320:MET:HE2	1.58	0.85
2:N:95:GLN:HG3	2:N:95:GLN:O	1.73	0.85
2:J:65:ASN:HD21	2:J:67:GLN:HB3	1.41	0.85
2:N:65:ASN:HD21	2:N:67:GLN:HB3	1.42	0.84
1:K:317:CYS:HA	1:K:320:MET:HE2	1.59	0.84
1:K:49:PRO:HD2	1:K:52:GLU:HG3	1.58	0.84
1:A:177:LYS:O	1:A:206:ILE:HD11	1.78	0.84
1:M:317:CYS:HA	1:M:320:MET:CE	2.08	0.84
1:E:317:CYS:HA	1:E:320:MET:HE2	1.59	0.84
1:O:317:CYS:HA	1:O:320:MET:CE	2.07	0.83
1:K:317:CYS:HA	1:K:320:MET:CE	2.08	0.83
1:A:317:CYS:HA	1:A:320:MET:HE2	1.62	0.81
1:E:382:ILE:HG22	1:E:402:PHE:CE1	2.15	0.81
1:E:177:LYS:O	1:E:206:ILE:HD11	1.81	0.81
1:C:317:CYS:HA	1:C:320:MET:HE2	1.62	0.81
1:O:226:HIS:HB2	4:O:2051:HOH:O	1.81	0.81
1:I:317:CYS:HA	1:I:320:MET:CE	2.11	0.81
4:A:2011:HOH:O	1:I:178:LEU:HD12	1.80	0.80
1:E:382:ILE:HG22	1:E:402:PHE:HE1	1.45	0.79
2:N:65:ASN:ND2	2:N:67:GLN:HB3	1.97	0.79
1:C:317:CYS:HA	1:C:320:MET:CE	2.14	0.78
1:G:382:ILE:HG22	1:G:402:PHE:HE1	1.49	0.78
1:G:382:ILE:HG22	1:G:402:PHE:CE1	2.18	0.78
1:G:317:CYS:HA	1:G:320:MET:HE2	1.67	0.78
1:C:177:LYS:O	1:C:206:ILE:HD11	1.84	0.77
1:C:172:CYS:HB3	1:C:197:LEU:HD13	1.67	0.77
1:G:177:LYS:O	1:G:206:ILE:HD11	1.85	0.76
2:L:60:LEU:H	2:L:60:LEU:HD12	1.51	0.76
1:O:204:GLU:OE1	4:O:2043:HOH:O	2.05	0.75
2:F:51:ARG:HH11	1:G:220:PHE:HE1	1.35	0.73
1:A:172:CYS:HB3	1:A:197:LEU:HD13	1.70	0.73
1:M:317:CYS:HA	1:M:320:MET:HE2	1.69	0.73
1:K:382:ILE:HG22	1:K:402:PHE:CE1	2.24	0.73
1:E:317:CYS:HA	1:E:320:MET:CE	2.19	0.72
1:M:382:ILE:HG22	1:M:402:PHE:HE1	1.54	0.72
1:K:382:ILE:HG22	1:K:402:PHE:HE1	1.53	0.71
1:M:382:ILE:HG22	1:M:402:PHE:CE1	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:CYS:HB3	1:G:197:LEU:HD13	1.73	0.70
1:A:317:CYS:HA	1:A:320:MET:CE	2.20	0.70
1:K:172:CYS:HB3	1:K:197:LEU:HD13	1.74	0.70
1:M:177:LYS:O	1:M:206:ILE:CD1	2.39	0.70
1:A:178:LEU:CD1	4:I:2007:HOH:O	2.33	0.69
1:C:382:ILE:HG22	1:C:402:PHE:CE2	2.26	0.69
2:L:95:GLN:HG3	2:L:95:GLN:O	1.93	0.69
1:M:172:CYS:HB3	1:M:197:LEU:CD1	2.22	0.69
1:M:172:CYS:HB3	1:M:197:LEU:HD13	1.74	0.69
1:A:172:CYS:HB3	1:A:197:LEU:CD1	2.24	0.68
1:O:177:LYS:O	1:O:206:ILE:CD1	2.40	0.67
1:C:382:ILE:HG22	1:C:402:PHE:HE2	1.59	0.67
1:I:177:LYS:O	1:I:206:ILE:CD1	2.42	0.67
2:F:51:ARG:NH1	1:G:220:PHE:HE1	1.93	0.67
1:A:382:ILE:HG22	1:A:402:PHE:CE1	2.30	0.67
1:G:317:CYS:HA	1:G:320:MET:CE	2.26	0.66
4:G:2107:HOH:O	2:H:4:LEU:HD21	1.96	0.66
1:E:382:ILE:CG2	1:E:402:PHE:CE1	2.78	0.65
1:G:74:LEU:O	2:P:95:GLN:NE2	2.30	0.65
1:I:382:ILE:HG22	1:I:402:PHE:CE2	2.32	0.65
1:A:382:ILE:HG22	1:A:402:PHE:HE1	1.60	0.64
1:C:172:CYS:HB3	1:C:197:LEU:CD1	2.28	0.63
1:A:177:LYS:O	1:A:206:ILE:CD1	2.46	0.63
1:C:49:PRO:HD2	1:C:52:GLU:CG	2.23	0.63
1:I:172:CYS:HB3	1:I:197:LEU:HD13	1.80	0.63
1:E:172:CYS:HB3	1:E:197:LEU:HD13	1.79	0.62
1:G:382:ILE:CG2	1:G:402:PHE:CE1	2.82	0.62
1:O:382:ILE:HG22	1:O:402:PHE:CE1	2.33	0.62
1:M:317:CYS:HA	1:M:320:MET:HE3	1.81	0.62
1:I:382:ILE:HG22	1:I:402:PHE:HE2	1.65	0.62
1:E:74:LEU:O	2:N:95:GLN:NE2	2.32	0.62
1:C:172:CYS:HB2	4:C:2058:HOH:O	2.00	0.61
1:I:172:CYS:HB3	1:I:197:LEU:CD1	2.30	0.61
1:E:172:CYS:HB3	1:E:197:LEU:CD1	2.31	0.61
1:M:382:ILE:CG2	1:M:402:PHE:CE1	2.85	0.60
1:K:382:ILE:CG2	1:K:402:PHE:CE1	2.85	0.59
1:G:172:CYS:HB3	1:G:197:LEU:CD1	2.31	0.59
1:C:177:LYS:O	1:C:206:ILE:CD1	2.51	0.59
2:F:61:PHE:O	2:F:62:ASN:HB3	2.01	0.59
1:A:422:VAL:HG23	1:A:455:LEU:HD22	1.85	0.59
2:F:65:ASN:HD21	2:F:67:GLN:HB3	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LEU:CD1	4:K:2012:HOH:O	2.41	0.58
1:E:177:LYS:O	1:E:206:ILE:CD1	2.50	0.58
2:L:60:LEU:N	2:L:60:LEU:HD12	2.16	0.58
1:O:172:CYS:HB3	1:O:197:LEU:CD1	2.33	0.58
2:F:95:GLN:HG3	2:F:95:GLN:O	2.03	0.58
2:H:95:GLN:NE2	1:I:74:LEU:O	2.37	0.58
1:G:239:TYR:HB3	1:G:266:MET:HB2	1.85	0.58
1:K:172:CYS:HB3	1:K:197:LEU:CD1	2.33	0.58
1:O:382:ILE:HG22	1:O:402:PHE:HE1	1.68	0.58
1:O:51:GLU:HG3	4:O:2012:HOH:O	2.04	0.58
1:C:382:ILE:CG2	1:C:402:PHE:CE2	2.87	0.58
2:P:95:GLN:HG3	2:P:95:GLN:O	2.04	0.58
2:F:51:ARG:HD2	1:G:223:ASP:OD2	2.03	0.57
2:B:51:ARG:HD3	1:C:220:PHE:CE1	2.39	0.57
2:F:95:GLN:NE2	1:O:74:LEU:O	2.38	0.57
1:E:161:LYS:HA	2:F:51:ARG:HH12	1.70	0.56
2:D:95:GLN:HG3	2:D:95:GLN:O	2.04	0.56
1:K:239:TYR:HB3	1:K:266:MET:HB2	1.86	0.56
2:D:95:GLN:NE2	1:M:75:THR:HG22	2.20	0.56
1:O:302:ASP:C	1:O:302:ASP:OD1	2.44	0.56
2:J:61:PHE:O	2:J:62:ASN:HB3	2.05	0.56
1:G:285:ARG:NH2	4:G:2045:HOH:O	2.36	0.56
1:C:49:PRO:CD	1:C:52:GLU:HG3	2.24	0.56
2:D:51:ARG:CD	1:E:223:ASP:OD2	2.46	0.56
1:I:212:GLN:OE1	1:I:217:ARG:HD3	2.06	0.55
1:A:74:LEU:O	2:J:95:GLN:NE2	2.39	0.55
2:J:16:LEU:HD12	1:K:451:TRP:CH2	2.41	0.55
1:A:382:ILE:CG2	1:A:402:PHE:CE1	2.89	0.55
1:C:63:THR:HG22	4:K:2033:HOH:O	2.07	0.55
1:E:339:LYS:HB2	4:E:2097:HOH:O	2.06	0.55
1:I:317:CYS:CA	1:I:320:MET:HE2	2.34	0.55
1:E:302:ASP:OD1	1:E:302:ASP:C	2.46	0.54
1:G:177:LYS:O	1:G:206:ILE:CD1	2.54	0.54
4:C:2011:HOH:O	1:K:178:LEU:CD1	2.37	0.54
2:H:30:TYR:O	2:H:34:GLN:HG2	2.07	0.54
1:M:44:PRO:HD2	1:M:95:ASN:O	2.07	0.54
2:P:89:ALA:HB3	2:P:99:MET:HB2	1.90	0.54
1:C:317:CYS:CA	1:C:320:MET:HE2	2.37	0.54
2:J:95:GLN:O	2:J:95:GLN:HG3	2.08	0.54
1:I:172:CYS:SG	1:I:200:THR:HG22	2.47	0.54
2:L:39:CYS:HB3	2:L:88:VAL:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:25:ALA:HB2	2:L:70:LEU:HD22	1.90	0.54
1:A:171:GLY:HA2	1:A:199:PHE:O	2.08	0.54
1:O:203:ASP:HB3	1:O:206:ILE:HD12	1.91	0.53
1:G:70:TRP:CH2	2:P:55:MET:HE1	2.44	0.53
2:N:60:LEU:H	2:N:60:LEU:HD12	1.72	0.53
2:N:97:GLN:HE21	2:N:100:SER:HB2	1.74	0.53
2:L:65:ASN:HD21	2:L:67:GLN:HB3	1.73	0.53
2:H:89:ALA:HB3	2:H:99:MET:HB2	1.90	0.53
2:B:95:GLN:NE2	1:K:74:LEU:O	2.42	0.53
2:D:21:ASP:OD2	2:D:74:GLN:NE2	2.32	0.53
2:D:37:HIS:HE1	4:D:2002:HOH:O	1.92	0.53
1:G:451:TRP:CZ2	2:H:17:PRO:HD3	2.43	0.52
1:C:273:GLY:HA3	1:K:273:GLY:HA3	1.92	0.52
1:G:422:VAL:HG23	1:G:455:LEU:HD22	1.92	0.52
1:E:239:TYR:HB3	1:E:266:MET:HB2	1.92	0.52
2:N:44:GLU:H	2:N:44:GLU:CD	2.12	0.52
1:C:117:LEU:O	1:C:121:VAL:HG22	2.10	0.52
2:J:91:ASP:OD2	2:J:94:LYS:HE3	2.10	0.52
1:C:178:LEU:HD23	1:C:206:ILE:HG13	1.92	0.52
1:C:451:TRP:CZ2	2:D:17:PRO:HD3	2.44	0.52
1:E:273:GLY:HA3	1:M:273:GLY:HA3	1.92	0.51
1:C:171:GLY:HA2	1:C:199:PHE:O	2.11	0.51
1:A:317:CYS:CA	1:A:320:MET:HE2	2.38	0.51
1:G:171:GLY:HA2	1:G:199:PHE:O	2.10	0.51
1:O:172:CYS:HB3	1:O:197:LEU:HD13	1.90	0.51
1:O:317:CYS:CA	1:O:320:MET:HE2	2.29	0.51
1:E:451:TRP:CZ2	2:F:17:PRO:HD3	2.45	0.51
1:A:75:THR:HG22	2:J:95:GLN:NE2	2.26	0.51
1:A:121:VAL:HG23	1:I:297:MET:HG3	1.92	0.51
1:G:317:CYS:CA	1:G:320:MET:HE2	2.40	0.51
1:M:36:ILE:HD12	1:M:108:PHE:CE2	2.46	0.51
1:E:317:CYS:CA	1:E:320:MET:HE2	2.37	0.50
1:G:107:LEU:HD22	1:O:178:LEU:HD13	1.92	0.50
1:K:302:ASP:OD1	1:K:302:ASP:C	2.50	0.50
1:K:44:PRO:HD2	1:K:95:ASN:O	2.11	0.50
2:D:74:GLN:HG2	2:D:77:ARG:NH2	2.26	0.50
2:D:65:ASN:ND2	2:D:67:GLN:HB3	2.18	0.50
1:A:273:GLY:HA3	1:I:273:GLY:HA3	1.93	0.50
2:P:25:ALA:HB2	2:P:70:LEU:HD22	1.94	0.50
2:N:44:GLU:N	2:N:44:GLU:OE1	2.43	0.50
1:A:451:TRP:CZ2	2:B:17:PRO:HD3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:74:GLN:HG2	2:H:77:ARG:NH2	2.26	0.50
2:D:55:MET:HE1	1:M:70:TRP:CH2	2.47	0.50
1:I:451:TRP:CZ2	2:P:17:PRO:HD3	2.47	0.49
1:I:302:ASP:C	1:I:302:ASP:OD1	2.50	0.49
2:L:17:PRO:HD3	1:M:451:TRP:CZ2	2.46	0.49
1:C:75:THR:CG2	1:K:180:LEU:HD23	2.43	0.49
1:E:171:GLY:HA2	1:E:199:PHE:O	2.13	0.49
1:I:382:ILE:CG2	1:I:402:PHE:CE2	2.94	0.49
1:C:133:LEU:O	1:C:307:HIS:HA	2.12	0.49
1:A:302:ASP:OD1	1:A:302:ASP:C	2.49	0.49
1:K:317:CYS:CA	1:K:320:MET:HE2	2.36	0.49
1:G:273:GLY:HA3	1:O:273:GLY:HA3	1.93	0.49
2:B:26:ARG:HH11	2:B:26:ARG:HG3	1.77	0.49
1:I:44:PRO:HD2	1:I:95:ASN:O	2.13	0.49
1:K:77:LEU:HB2	4:K:2011:HOH:O	2.13	0.49
1:M:162:LEU:O	1:M:163:ASN:CB	2.61	0.49
2:D:30:TYR:O	2:D:34:GLN:HG2	2.13	0.48
1:O:91:PRO:HG3	4:O:2018:HOH:O	2.13	0.48
1:C:302:ASP:OD1	1:C:302:ASP:C	2.48	0.48
1:M:382:ILE:CG2	1:M:390:LEU:HD11	2.43	0.48
2:H:8:ARG:HG2	2:H:10:TYR:CZ	2.47	0.48
1:K:171:GLY:HA2	1:K:199:PHE:O	2.13	0.48
2:L:27:GLN:OE1	1:M:432:ASN:CB	2.62	0.48
2:N:95:GLN:CG	2:N:95:GLN:O	2.50	0.48
2:D:61:PHE:O	2:D:62:ASN:HB3	2.14	0.48
2:D:65:ASN:ND2	2:D:67:GLN:H	2.11	0.48
2:L:39:CYS:HB3	2:L:88:VAL:HG23	1.94	0.48
1:O:382:ILE:CG2	1:O:402:PHE:CE1	2.96	0.48
2:P:44:GLU:H	2:P:44:GLU:CD	2.17	0.48
1:K:382:ILE:CG2	1:K:390:LEU:HD11	2.44	0.48
1:M:317:CYS:CA	1:M:320:MET:HE2	2.40	0.48
2:B:61:PHE:O	2:B:62:ASN:HB3	2.13	0.48
1:O:382:ILE:CG2	1:O:390:LEU:HD11	2.43	0.48
1:C:239:TYR:HB3	1:C:266:MET:HB2	1.96	0.48
1:M:379:SER:HB3	1:M:401:GLN:HB3	1.95	0.48
1:G:121:VAL:HG23	1:O:297:MET:HG3	1.95	0.47
1:I:382:ILE:CG2	1:I:390:LEU:HD11	2.44	0.47
2:L:30:TYR:HB2	1:M:432:ASN:O	2.14	0.47
2:P:24:ILE:HG12	2:P:103:VAL:HG12	1.96	0.47
1:G:315:ALA:HB1	1:G:349:LEU:HD21	1.96	0.47
2:J:53:TRP:CZ3	2:J:86:ARG:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:ARG:HD3	1:E:220:PHE:CD1	2.49	0.47
1:M:223:ASP:OD2	2:N:51:ARG:HD2	2.13	0.47
1:E:70:TRP:CH2	2:N:55:MET:HE1	2.50	0.47
1:C:74:LEU:O	2:L:95:GLN:NE2	2.47	0.47
1:I:162:LEU:O	1:I:163:ASN:CB	2.62	0.47
1:I:178:LEU:HD23	1:I:206:ILE:HG13	1.97	0.47
1:A:382:ILE:CG2	1:A:390:LEU:HD11	2.45	0.47
2:P:65:ASN:O	2:P:68:ASP:OD1	2.33	0.47
1:M:239:TYR:HB3	1:M:266:MET:HB2	1.96	0.47
1:O:171:GLY:HA2	1:O:199:PHE:O	2.15	0.47
2:B:51:ARG:HD3	1:C:220:PHE:HE1	1.79	0.47
1:E:288:GLY:HA3	1:G:215:ARG:HH21	1.79	0.47
1:I:171:GLY:HA2	1:I:199:PHE:O	2.14	0.47
2:J:61:PHE:O	2:J:62:ASN:CB	2.63	0.47
1:K:212:GLN:OE1	1:K:217:ARG:HD3	2.15	0.47
1:A:239:TYR:HB3	1:A:266:MET:HB2	1.95	0.47
1:C:71:THR:OG1	1:K:175:LYS:O	2.22	0.47
2:B:95:GLN:HG2	1:C:179:GLY:O	2.15	0.46
1:G:226:HIS:HB2	4:G:2067:HOH:O	2.14	0.46
1:C:318:LEU:C	1:C:318:LEU:HD13	2.35	0.46
2:F:24:ILE:HG12	2:F:103:VAL:HG12	1.98	0.46
1:M:422:VAL:HG23	1:M:455:LEU:HD22	1.97	0.46
1:M:436:ASP:C	1:M:436:ASP:OD1	2.54	0.46
1:I:52:GLU:HG2	1:I:52:GLU:H	1.57	0.46
1:K:354:ILE:HD12	1:K:354:ILE:N	2.31	0.46
1:E:293:ILE:HG13	1:E:318:LEU:HD21	1.98	0.46
2:J:86:ARG:HB2	2:J:101:PHE:O	2.16	0.46
1:M:249:GLU:O	1:M:253:ARG:HG3	2.16	0.46
1:C:195:GLY:HA3	1:C:417:ALA:HB3	1.99	0.46
2:B:9:ARG:NH1	2:B:15:TYR:HA	2.31	0.45
1:G:75:THR:HG22	2:P:95:GLN:NE2	2.29	0.45
1:I:159:ARG:NH2	1:I:396:ASP:O	2.49	0.45
2:L:60:LEU:CD1	2:L:60:LEU:H	2.23	0.45
1:M:195:GLY:HA3	1:M:417:ALA:HB3	1.98	0.45
1:O:178:LEU:HD23	1:O:206:ILE:HG13	1.98	0.45
2:F:74:GLN:HG2	2:F:77:ARG:NH2	2.31	0.45
1:E:175:LYS:O	1:M:71:THR:OG1	2.26	0.45
2:F:49:GLU:N	2:F:49:GLU:CD	2.70	0.45
2:H:97:GLN:HE21	2:H:100:SER:HB2	1.82	0.45
1:I:422:VAL:HG23	1:I:455:LEU:HD22	1.98	0.45
1:O:318:LEU:C	1:O:318:LEU:HD13	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:98:VAL:O	2:P:99:MET:HG3	2.16	0.45
4:A:2011:HOH:O	1:I:178:LEU:CD1	2.52	0.45
1:A:70:TRP:CH2	2:J:55:MET:HE1	2.52	0.45
1:K:52:GLU:HG2	1:K:52:GLU:H	1.56	0.45
2:D:61:PHE:O	2:D:62:ASN:CB	2.65	0.45
1:A:297:MET:HG3	1:I:121:VAL:HG23	1.99	0.45
1:O:293:ILE:HG13	1:O:318:LEU:HD21	1.99	0.45
1:A:178:LEU:HD23	1:A:206:ILE:HG13	1.99	0.45
1:A:316:LYS:O	1:A:320:MET:HE2	2.17	0.45
2:J:54:THR:OG1	2:P:6:LYS:HE2	2.17	0.45
1:C:88:GLU:HA	1:C:89:PRO:HD2	1.89	0.44
2:D:86:ARG:HA	2:D:103:VAL:HG22	1.99	0.44
2:J:74:GLN:HG2	2:J:77:ARG:NH2	2.32	0.44
1:E:75:THR:CG2	1:M:180:LEU:HD23	2.46	0.44
2:P:65:ASN:ND2	2:P:67:GLN:HB3	2.32	0.44
2:D:13:PHE:HD2	2:D:101:PHE:HB2	1.82	0.44
2:D:85:ILE:HG22	2:D:86:ARG:N	2.32	0.44
1:E:195:GLY:HA3	1:E:417:ALA:HB3	1.99	0.44
1:G:382:ILE:CG2	1:G:390:LEU:HD11	2.47	0.44
1:K:177:LYS:O	1:K:206:ILE:CD1	2.55	0.44
2:B:61:PHE:O	2:B:62:ASN:CB	2.66	0.44
2:D:51:ARG:HG3	2:D:51:ARG:HH11	1.83	0.44
1:G:44:PRO:HD2	1:G:95:ASN:O	2.17	0.44
1:I:220:PHE:CE1	2:J:51:ARG:HD3	2.53	0.44
1:A:90:LEU:HB3	1:A:93:GLU:HG3	1.99	0.44
1:C:201:LYS:HB2	1:C:239:TYR:CD2	2.53	0.44
1:G:354:ILE:N	1:G:354:ILE:HD12	2.32	0.44
2:F:49:GLU:H	2:F:49:GLU:CD	2.21	0.44
1:A:30:THR:HA	1:A:31:PRO:HD3	1.86	0.44
1:E:107:LEU:HD22	1:M:178:LEU:HD13	1.98	0.44
1:K:379:SER:HB3	1:K:401:GLN:HB3	2.00	0.44
1:I:90:LEU:HB3	1:I:93:GLU:HG3	1.99	0.44
1:O:88:GLU:HA	1:O:89:PRO:HD2	1.73	0.44
2:F:30:TYR:O	2:F:34:GLN:HG2	2.17	0.43
2:N:17:PRO:HD3	1:O:451:TRP:CH2	2.53	0.43
1:O:44:PRO:HD2	1:O:95:ASN:O	2.18	0.43
2:P:75:GLN:HG2	2:P:79:GLU:OE2	2.18	0.43
1:E:49:PRO:CD	1:E:52:GLU:HG3	2.33	0.43
1:E:88:GLU:HA	1:E:89:PRO:HD2	1.87	0.43
2:L:86:ARG:HB2	2:L:101:PHE:O	2.18	0.43
2:P:86:ARG:HA	2:P:103:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:62:ASN:N	2:P:62:ASN:OD1	2.50	0.43
1:A:190:TYR:CZ	1:A:194:ARG:HD3	2.53	0.43
1:O:318:LEU:O	1:O:318:LEU:HD13	2.18	0.43
1:O:422:VAL:HG23	1:O:455:LEU:HD22	1.99	0.43
1:A:49:PRO:CD	1:A:52:GLU:HG3	2.33	0.43
1:C:382:ILE:CG2	1:C:390:LEU:HD11	2.49	0.43
1:G:178:LEU:HD13	1:O:107:LEU:HD22	2.00	0.43
2:H:42:PHE:HA	2:H:84:PHE:O	2.19	0.43
1:O:327:HIS:HA	1:O:377:VAL:HB	2.00	0.43
1:G:30:THR:HA	1:G:31:PRO:HD3	1.89	0.43
1:I:117:LEU:O	1:I:121:VAL:HG22	2.19	0.43
1:I:369:ALA:O	1:I:370:SER:HB2	2.19	0.43
1:O:382:ILE:HG21	1:O:390:LEU:HD11	2.00	0.43
1:I:49:PRO:CD	1:I:52:GLU:HG3	2.31	0.43
1:K:317:CYS:HA	1:K:320:MET:HE3	1.94	0.43
2:B:92:ASN:HA	1:K:74:LEU:O	2.19	0.43
1:I:244:ALA:HB1	1:I:245:PRO:HD2	2.01	0.43
1:K:190:TYR:CZ	1:K:194:ARG:HD3	2.53	0.43
1:M:90:LEU:HB3	1:M:93:GLU:HG3	2.00	0.43
1:E:315:ALA:HB1	1:E:349:LEU:HD21	2.01	0.42
1:I:36:ILE:HD12	1:I:108:PHE:CE2	2.54	0.42
1:K:117:LEU:O	1:K:121:VAL:HG22	2.18	0.42
1:C:107:LEU:HD22	1:K:178:LEU:HD13	2.01	0.42
1:O:30:THR:HA	1:O:31:PRO:HD3	1.88	0.42
2:F:9:ARG:NH1	2:F:14:SER:O	2.52	0.42
1:A:251:LEU:HA	1:A:251:LEU:HD23	1.80	0.42
1:E:339:LYS:HD2	4:E:2097:HOH:O	2.19	0.42
1:E:379:SER:CB	1:E:401:GLN:HB3	2.49	0.42
2:L:55:MET:HB2	2:L:55:MET:HE2	1.81	0.42
2:F:82:ASN:HA	2:F:106:PRO:HB3	2.00	0.42
1:G:49:PRO:CD	1:G:52:GLU:HG3	2.34	0.42
2:J:16:LEU:HD12	1:K:451:TRP:CZ2	2.54	0.42
2:N:55:MET:HE2	2:N:55:MET:HB2	1.92	0.42
1:I:354:ILE:HD12	1:I:354:ILE:N	2.34	0.42
1:I:418:THR:O	1:I:422:VAL:HG13	2.20	0.42
1:O:139:ARG:C	1:O:139:ARG:HD2	2.40	0.42
1:E:301:MET:HG2	1:M:300:VAL:HG12	2.01	0.42
1:M:302:ASP:C	1:M:302:ASP:OD1	2.58	0.42
1:A:117:LEU:O	1:A:121:VAL:HG22	2.19	0.42
2:B:102:ILE:HD12	2:B:102:ILE:HA	1.76	0.42
2:F:42:PHE:HA	2:F:84:PHE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:190:TYR:CZ	1:I:194:ARG:HD3	2.55	0.42
2:J:16:LEU:HD12	1:K:451:TRP:HH2	1.84	0.42
1:K:36:ILE:HD12	1:K:108:PHE:CE2	2.55	0.42
1:M:384:VAL:HG13	1:M:420:ASN:OD1	2.20	0.42
1:E:201:LYS:HG3	1:E:202:ASP:O	2.20	0.42
2:F:97:GLN:HE21	2:F:100:SER:HB2	1.85	0.42
2:J:44:GLU:H	2:J:44:GLU:CD	2.23	0.42
1:M:316:LYS:O	1:M:320:MET:HE2	2.20	0.42
1:C:251:LEU:HA	1:C:251:LEU:HD23	1.83	0.42
2:H:92:ASN:HA	1:I:74:LEU:O	2.20	0.42
1:K:30:THR:HA	1:K:31:PRO:HD3	1.91	0.42
1:M:177:LYS:HB3	1:M:177:LYS:HE3	1.88	0.42
2:N:17:PRO:HA	2:N:18:PRO:HD2	1.92	0.42
2:P:65:ASN:ND2	2:P:67:GLN:CB	2.83	0.42
1:O:162:LEU:O	1:O:163:ASN:CB	2.67	0.41
1:O:239:TYR:HB3	1:O:266:MET:HB2	2.01	0.41
2:P:28:ILE:HG21	2:P:69:VAL:HB	2.02	0.41
2:D:51:ARG:NH1	2:D:51:ARG:HG3	2.35	0.41
1:K:244:ALA:HB1	1:K:245:PRO:HD2	2.02	0.41
1:K:382:ILE:HG23	1:K:390:LEU:HD11	2.02	0.41
1:M:49:PRO:CD	1:M:52:GLU:HG3	2.36	0.41
1:A:159:ARG:NH2	1:A:396:ASP:O	2.54	0.41
1:G:302:ASP:C	1:G:302:ASP:OD1	2.59	0.41
1:G:90:LEU:HB3	1:G:93:GLU:HG3	2.02	0.41
2:L:27:GLN:OE1	1:M:432:ASN:HB3	2.19	0.41
1:M:220:PHE:CE1	2:N:51:ARG:HD3	2.56	0.41
1:E:297:MET:HG3	1:M:121:VAL:HG23	2.01	0.41
1:I:317:CYS:HA	1:I:320:MET:HE3	1.98	0.41
2:J:9:ARG:HD2	2:J:15:TYR:CE1	2.55	0.41
1:K:327:HIS:HA	1:K:377:VAL:HB	2.03	0.41
1:O:190:TYR:CZ	1:O:194:ARG:HD3	2.55	0.41
1:O:354:ILE:N	1:O:354:ILE:HD12	2.36	0.41
1:M:382:ILE:HG23	1:M:390:LEU:HD11	2.02	0.41
1:E:318:LEU:HD13	1:E:318:LEU:C	2.40	0.41
2:J:89:ALA:HB3	2:J:99:MET:HB2	2.02	0.41
1:O:369:ALA:O	1:O:370:SER:HB2	2.21	0.41
1:I:88:GLU:HA	1:I:89:PRO:HD2	1.84	0.41
2:L:8:ARG:HG2	2:L:10:TYR:CZ	2.55	0.41
2:L:79:GLU:O	2:L:81:PRO:HD3	2.20	0.41
2:P:86:ARG:HB2	2:P:101:PHE:O	2.21	0.41
1:G:88:GLU:HA	1:G:89:PRO:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:409:HIS:HA	1:I:410:PRO:HD3	1.95	0.41
2:J:30:TYR:O	2:J:34:GLN:HG2	2.21	0.41
2:J:21:ASP:HB3	2:J:70:LEU:HD21	2.03	0.41
1:E:90:LEU:HB3	1:E:93:GLU:HG3	2.03	0.41
1:K:412:GLY:HA3	2:L:58:LEU:HD21	2.03	0.41
1:C:382:ILE:HG23	1:C:390:LEU:HD11	2.04	0.40
1:E:117:LEU:O	1:E:121:VAL:HG22	2.21	0.40
1:E:339:LYS:CD	4:E:2097:HOH:O	2.68	0.40
1:M:171:GLY:HA2	1:M:199:PHE:O	2.20	0.40
1:M:244:ALA:HB1	1:M:245:PRO:HD2	2.03	0.40
2:N:60:LEU:N	2:N:60:LEU:HD12	2.33	0.40
1:A:44:PRO:HD2	1:A:95:ASN:O	2.21	0.40
1:C:90:LEU:HB3	1:C:93:GLU:HG3	2.03	0.40
1:K:49:PRO:CD	1:K:52:GLU:HG3	2.39	0.40
1:K:90:LEU:HB3	1:K:93:GLU:HG3	2.03	0.40
1:E:121:VAL:HG23	1:M:297:MET:HG3	2.03	0.40
1:O:285:ARG:NH2	4:O:2032:HOH:O	2.53	0.40
2:P:29:GLN:NE2	2:P:33:ASP:OD1	2.52	0.40
2:B:65:ASN:ND2	2:B:67:GLN:HB3	2.37	0.40
1:I:49:PRO:HD2	1:I:52:GLU:CG	2.32	0.40
1:K:316:LYS:O	1:K:320:MET:HE2	2.21	0.40
2:D:89:ALA:HB3	2:D:99:MET:HB2	2.03	0.40
1:E:30:THR:HA	1:E:31:PRO:HD3	1.85	0.40
1:C:177:LYS:HB3	1:C:177:LYS:HE3	1.89	0.40
1:E:36:ILE:HD12	1:E:108:PHE:CE2	2.56	0.40
1:O:52:GLU:HG2	1:O:52:GLU:H	1.51	0.40

All (2) 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:439:ARG:NH2	1:C:52:GLU:OE2[2_656]	2.07	0.13
1:A:52:GLU:OE2	1:C:439:ARG:NH2[2_656]	2.18	0.02

## 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	422/475 (89%)	412 (98%)	10 (2%)	0	100	100
1	C	422/475 (89%)	410 (97%)	12 (3%)	0	100	100
1	E	422/475 (89%)	411 (97%)	11 (3%)	0	100	100
1	G	422/475 (89%)	411 (97%)	11 (3%)	0	100	100
1	I	422/475 (89%)	414 (98%)	8 (2%)	0	100	100
1	K	422/475 (89%)	412 (98%)	10 (2%)	0	100	100
1	M	422/475 (89%)	411 (97%)	10 (2%)	1 (0%)	47	58
1	O	422/475 (89%)	411 (97%)	11 (3%)	0	100	100
2	B	102/118 (86%)	95 (93%)	4 (4%)	3 (3%)	4	3
2	D	102/118 (86%)	95 (93%)	4 (4%)	3 (3%)	4	3
2	F	102/118 (86%)	92 (90%)	8 (8%)	2 (2%)	7	6
2	H	102/118 (86%)	96 (94%)	5 (5%)	1 (1%)	15	17
2	J	102/118 (86%)	94 (92%)	7 (7%)	1 (1%)	15	17
2	L	102/118 (86%)	92 (90%)	8 (8%)	2 (2%)	7	6
2	N	102/118 (86%)	92 (90%)	9 (9%)	1 (1%)	15	17
2	P	102/118 (86%)	92 (90%)	10 (10%)	0	100	100
All	All	4192/4744 (88%)	4040 (96%)	138 (3%)	14 (0%)	41	50

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	62	ASN
2	D	62	ASN
2	F	93	ILE
2	J	62	ASN
2	L	93	ILE
2	B	100	SER
2	F	62	ASN
2	H	93	ILE
2	D	93	ILE
2	D	100	SER
2	L	62	ASN
1	M	62	SER

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Mol	Chain	Res	Type
2	B	93	ILE
2	N	93	ILE

### 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	346/386 (90%)	341 (99%)	5 (1%)	67	81
1	C	346/386 (90%)	341 (99%)	5 (1%)	67	81
1	E	346/386 (90%)	339 (98%)	7 (2%)	55	72
1	G	346/386 (90%)	340 (98%)	6 (2%)	60	76
1	I	346/386 (90%)	342 (99%)	4 (1%)	71	84
1	K	346/386 (90%)	341 (99%)	5 (1%)	67	81
1	M	346/386 (90%)	341 (99%)	5 (1%)	67	81
1	O	346/386 (90%)	341 (99%)	5 (1%)	67	81
2	B	97/108 (90%)	95 (98%)	2 (2%)	53	70
2	D	97/108 (90%)	92 (95%)	5 (5%)	23	32
2	F	97/108 (90%)	93 (96%)	4 (4%)	30	43
2	H	97/108 (90%)	96 (99%)	1 (1%)	76	87
2	J	97/108 (90%)	94 (97%)	3 (3%)	40	55
2	L	97/108 (90%)	95 (98%)	2 (2%)	53	70
2	N	97/108 (90%)	95 (98%)	2 (2%)	53	70
2	P	97/108 (90%)	95 (98%)	2 (2%)	53	70
All	All	3544/3952 (90%)	3481 (98%)	63 (2%)	59	75

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	163	ASN

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Mol	Chain	Res	Type
1	A	172	CYS
1	A	239	TYR
1	A	335	LEU
2	B	61	PHE
2	B	68	ASP
1	C	30	THR
1	C	52	GLU
1	C	163	ASN
1	C	172	CYS
1	C	335	LEU
2	D	8	ARG
2	D	45	THR
2	D	51	ARG
2	D	64	THR
2	D	68	ASP
1	E	30	THR
1	E	52	GLU
1	E	163	ASN
1	E	172	CYS
1	E	192	CYS
1	E	335	LEU
1	E	379	SER
2	F	61	PHE
2	F	63	CYS
2	F	68	ASP
2	F	93	ILE
1	G	52	GLU
1	G	163	ASN
1	G	172	CYS
1	G	215	ARG
1	G	239	TYR
1	G	335	LEU
2	H	45	THR
1	I	52	GLU
1	I	163	ASN
1	I	192	CYS
1	I	239	TYR
2	J	16	LEU
2	J	68	ASP
2	J	106	PRO
1	K	52	GLU
1	K	71	THR

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Mol	Chain	Res	Type
1	K	163	ASN
1	K	172	CYS
1	K	192	CYS
2	L	60	LEU
2	L	68	ASP
1	M	52	GLU
1	M	163	ASN
1	M	172	CYS
1	M	192	CYS
1	M	239	TYR
2	N	60	LEU
2	N	68	ASP
1	O	30	THR
1	O	52	GLU
1	O	163	ASN
1	O	172	CYS
1	O	192	CYS
2	P	62	ASN
2	P	68	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	37	HIS
2	D	65	ASN
2	F	65	ASN
1	I	156	GLN
2	J	65	ASN
1	K	163	ASN
1	K	226	HIS
2	L	75	GLN
2	N	65	ASN
2	N	97	GLN
1	O	156	GLN
2	P	65	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	428/475 (90%)	-0.28	4 (0%) 84 88	2, 11, 39, 53	0
1	C	428/475 (90%)	-0.30	4 (0%) 84 88	2, 11, 39, 53	0
1	E	428/475 (90%)	-0.30	3 (0%) 87 91	2, 11, 39, 53	0
1	G	428/475 (90%)	-0.27	2 (0%) 91 94	2, 11, 38, 53	0
1	I	428/475 (90%)	-0.31	9 (2%) 63 70	2, 11, 39, 53	0
1	K	428/475 (90%)	-0.30	7 (1%) 72 77	2, 11, 39, 53	0
1	M	428/475 (90%)	-0.32	6 (1%) 75 80	2, 11, 39, 53	0
1	O	428/475 (90%)	-0.29	10 (2%) 60 67	2, 11, 39, 53	0
2	B	104/118 (88%)	0.13	5 (4%) 30 37	19, 33, 52, 64	0
2	D	104/118 (88%)	0.17	3 (2%) 51 58	17, 32, 48, 59	0
2	F	104/118 (88%)	-0.01	3 (2%) 51 58	15, 27, 44, 57	0
2	H	104/118 (88%)	0.08	3 (2%) 51 58	16, 28, 51, 62	0
2	J	104/118 (88%)	0.08	3 (2%) 51 58	15, 30, 47, 59	0
2	L	104/118 (88%)	0.20	3 (2%) 51 58	17, 32, 52, 63	0
2	N	104/118 (88%)	0.13	1 (0%) 82 86	18, 33, 53, 62	0
2	P	104/118 (88%)	0.08	3 (2%) 51 58	15, 31, 52, 63	0
All	All	4256/4744 (89%)	-0.22	69 (1%) 72 77	2, 14, 42, 64	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	332	VAL	4.1
2	L	60	LEU	3.9
1	C	451	TRP	3.8
1	O	72	ASP	3.8
1	I	74	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	P	61	PHE	3.7
1	O	70	TRP	3.5
1	K	70	TRP	3.4
2	B	63	CYS	3.3
2	B	61	PHE	3.3
1	G	72	ASP	3.3
1	O	71	THR	3.2
1	M	72	ASP	3.2
1	I	72	ASP	3.2
1	K	73	LEU	3.1
1	M	75	THR	3.1
1	O	92	GLY	3.1
2	P	60	LEU	3.1
1	K	333	GLY	3.0
2	J	61	PHE	3.0
1	E	73	LEU	2.9
1	K	92	GLY	2.9
2	P	63	CYS	2.9
2	N	61	PHE	2.9
1	A	72	ASP	2.9
2	F	64	THR	2.8
2	L	61	PHE	2.8
1	M	450	ARG	2.8
1	O	333	GLY	2.7
1	I	75	THR	2.7
1	I	70	TRP	2.7
2	D	61	PHE	2.7
1	E	450	ARG	2.6
2	F	61	PHE	2.6
2	L	63	CYS	2.6
2	H	61	PHE	2.6
1	A	71	THR	2.6
2	H	64	THR	2.5
1	O	335	LEU	2.5
1	K	72	ASP	2.5
1	O	77	LEU	2.5
1	K	335	LEU	2.4
1	I	71	THR	2.4
2	F	93	ILE	2.4
2	H	62	ASN	2.4
2	J	60	LEU	2.4
1	I	333	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	59	PRO	2.3
2	B	62	ASN	2.3
1	E	71	THR	2.3
2	B	64	THR	2.3
1	I	439	ARG	2.3
2	D	93	ILE	2.3
1	O	73	LEU	2.3
1	C	71	THR	2.2
1	A	451	TRP	2.2
1	G	411	TRP	2.2
1	I	92	GLY	2.2
2	J	63	CYS	2.2
2	D	64	THR	2.2
1	C	382	ILE	2.1
1	A	408	GLY	2.1
1	M	92	GLY	2.1
1	O	381	GLY	2.1
1	O	75	THR	2.0
1	C	450	ARG	2.0
1	M	71	THR	2.0
1	K	332	VAL	2.0
1	M	332	VAL	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	I	1461	1/1	0.94	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	O	1461	1/1	0.94	0.12	35,35,35,35	0
3	CL	M	1461	1/1	0.95	0.14	34,34,34,34	0
3	CL	A	1460	1/1	0.95	0.10	36,36,36,36	0
3	CL	K	1461	1/1	0.96	0.18	31,31,31,31	0
3	CL	O	1460	1/1	0.96	0.14	32,32,32,32	0
3	CL	C	1461	1/1	0.97	0.08	36,36,36,36	0
3	CL	I	1460	1/1	0.97	0.13	28,28,28,28	0
3	CL	K	1460	1/1	0.98	0.14	27,27,27,27	0
3	CL	G	1461	1/1	0.98	0.08	30,30,30,30	0
3	CL	C	1460	1/1	0.98	0.15	38,38,38,38	0
3	CL	E	1460	1/1	0.98	0.11	34,34,34,34	0
3	CL	G	1460	1/1	0.98	0.11	33,33,33,33	0
3	CL	A	1461	1/1	0.98	0.07	33,33,33,33	0
3	CL	M	1460	1/1	0.99	0.13	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.