



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:14 PM UTC

PDB ID : 2YBV / pdb_00002ybv
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

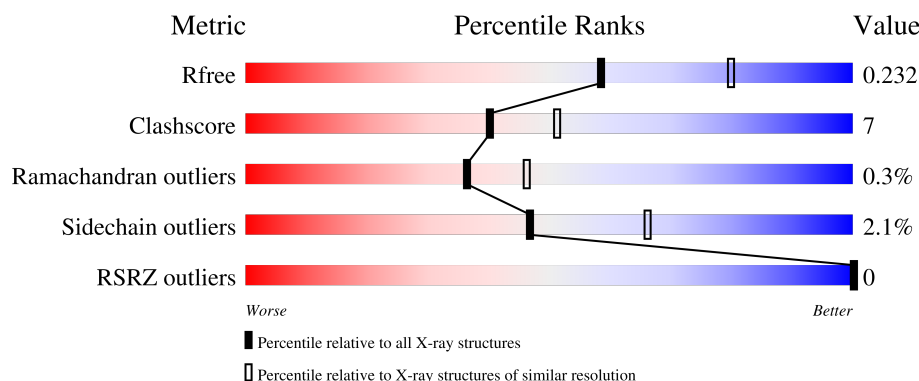
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	 77% 12% • 10%
1	C	475	 77% 12% • 10%
1	E	475	 76% 14% 10%
1	G	475	 78% 11% • 10%
1	I	475	 76% 13% • 10%

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Mol	Chain	Length	Quality of chain
1	K	475	
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	C	N	O	S	0	0	0
			869	557	146	159	7			
2	N	104	Total	C	N	O	S	0	0	0
			869	557	146	159	7			
2	P	104	Total	C	N	O	S	0	0	0
			869	557	146	159	7			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is water.

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

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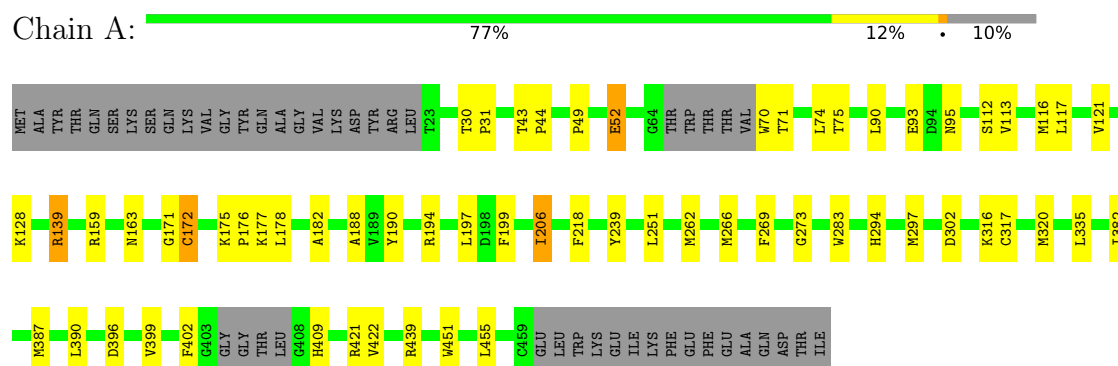
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	112	Total 112	O 112	0	0
4	H	4	Total 4	O 4	0	0
4	I	87	Total 87	O 87	0	0
4	J	16	Total 16	O 16	0	0
4	K	73	Total 73	O 73	0	0
4	L	7	Total 7	O 7	0	0
4	M	77	Total 77	O 77	0	0
4	N	9	Total 9	O 9	0	0
4	O	80	Total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

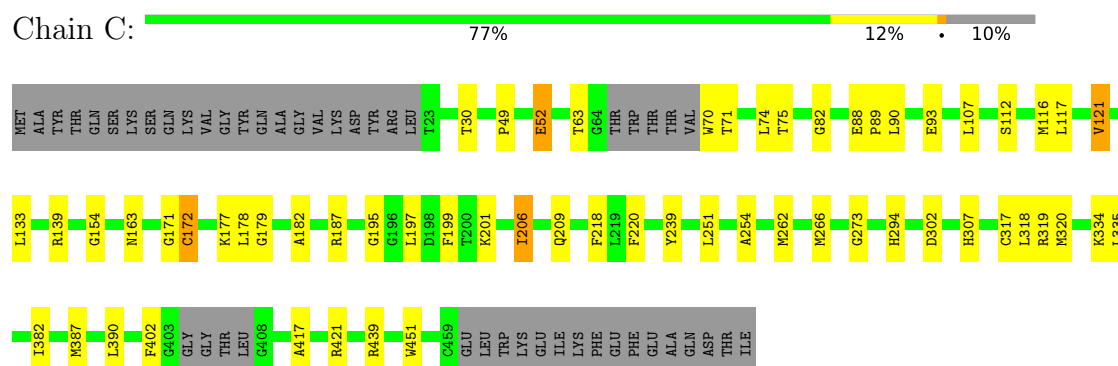
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

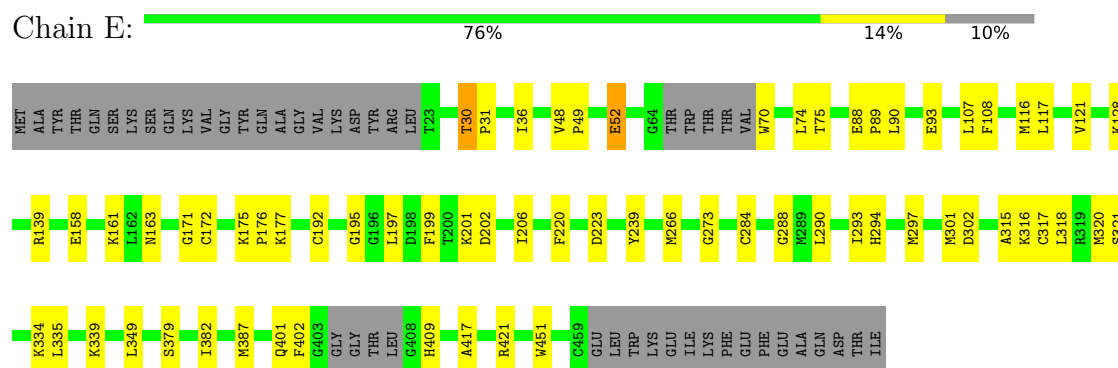
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

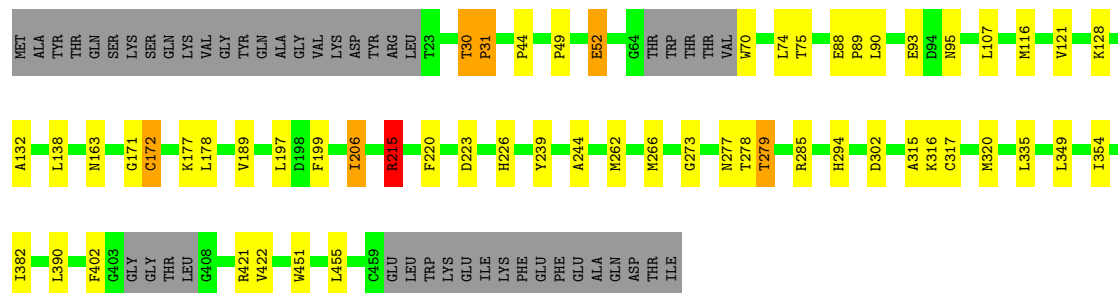


• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



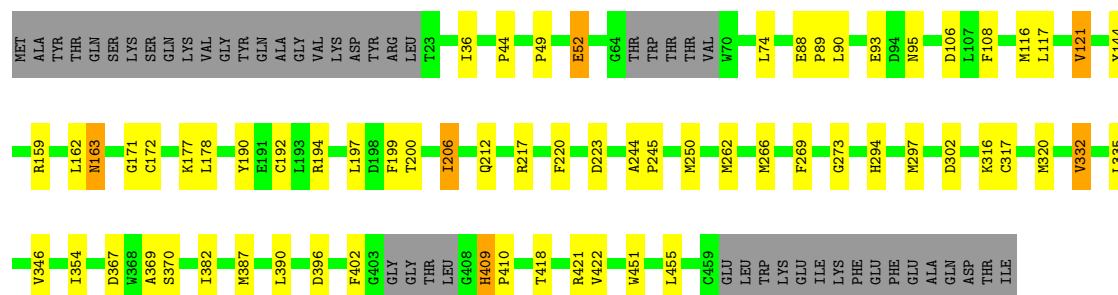
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain G:  78% 11% 10%



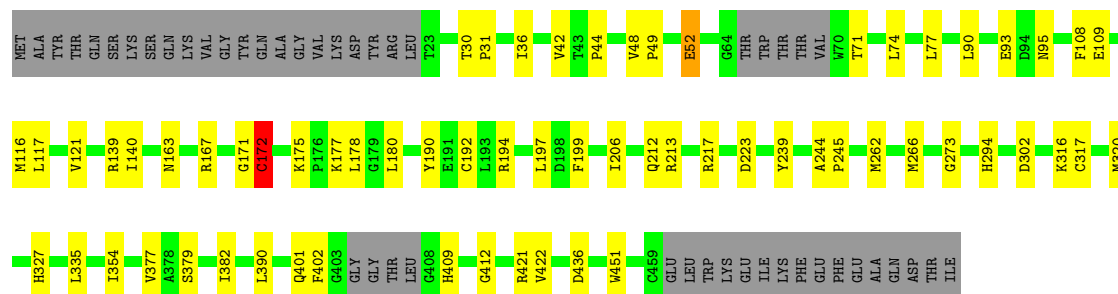
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain I:  76% 13% 10%



- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

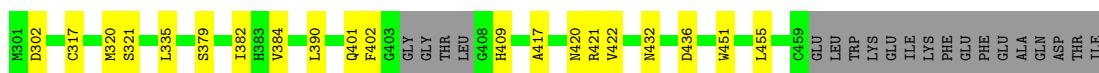
Chain K:  76% 13% 10%



- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

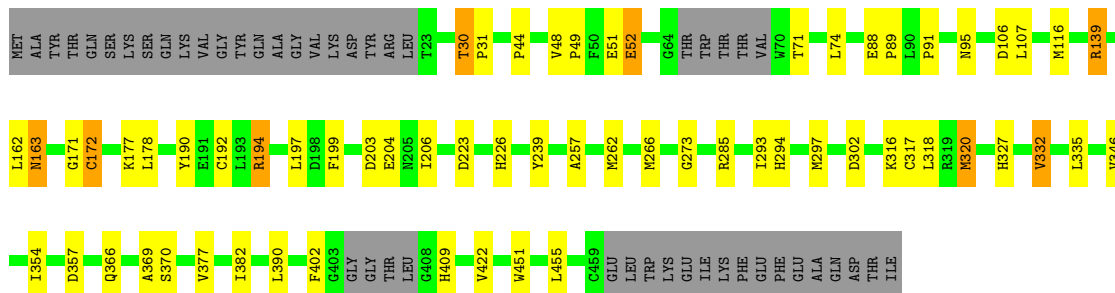
Chain M:  75% 14% 10%





• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain O: 77% 12% 10%



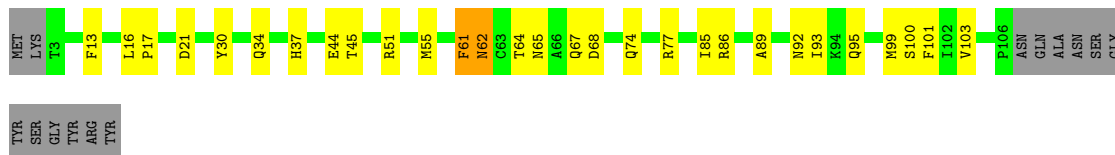
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT

Chain B: 74% 11% 12%



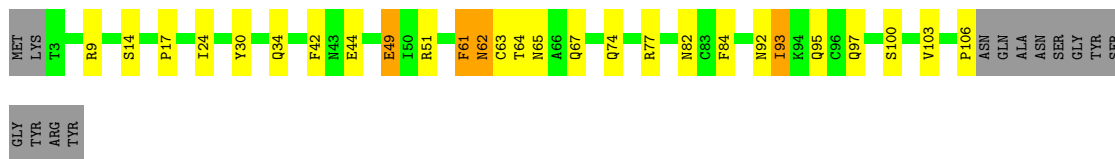
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT

Chain D: 64% 23% 12%



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT

Chain F: 65% 19% 12%



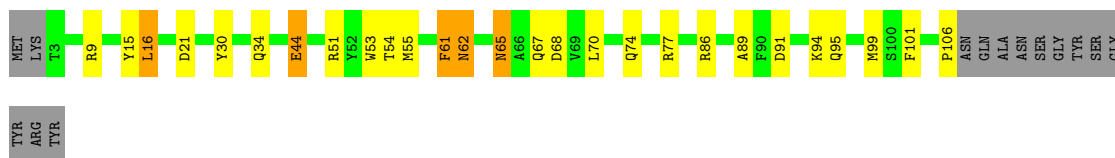
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT

Chain H: 71% 16% 12%



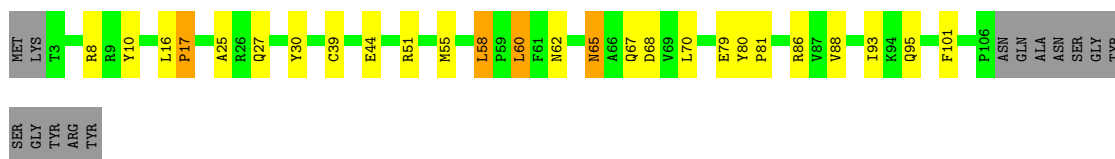
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT

Chain J:  65% 19% • 12%



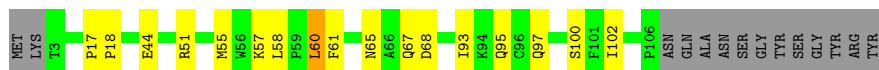
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT

Chain L:  66% 19% • 12%



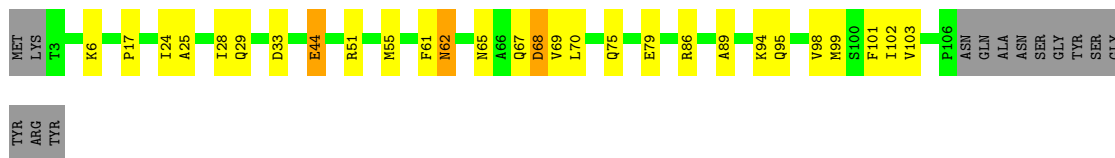
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT

Chain N:  74% 14% • 12%



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT

Chain P:  64% 21% • 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.48Å 163.47Å 163.54Å 90.00° 108.96° 90.00°	Depositor
Resolution (Å)	39.84 – 2.30 39.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.84-2.30) 100.0 (39.84-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.196 , 0.232 0.196 , 0.232	Depositor DCC
R_{free} test set	12993 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	11.8	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 13.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34583	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.31	10/3427 (0.3%)	1.16	12/4642 (0.3%)
1	C	1.31	6/3427 (0.2%)	1.14	9/4642 (0.2%)
1	E	1.30	6/3427 (0.2%)	1.16	10/4642 (0.2%)
1	G	1.32	7/3427 (0.2%)	1.15	9/4642 (0.2%)
1	I	1.27	5/3427 (0.1%)	1.17	10/4642 (0.2%)
1	K	1.29	6/3427 (0.2%)	1.16	7/4642 (0.2%)
1	M	1.29	8/3427 (0.2%)	1.13	11/4642 (0.2%)
1	O	1.29	6/3427 (0.2%)	1.13	7/4642 (0.2%)
2	B	1.09	1/893 (0.1%)	1.11	4/1215 (0.3%)
2	D	1.07	1/893 (0.1%)	1.09	2/1215 (0.2%)
2	F	1.10	0/893	1.15	3/1215 (0.2%)
2	H	1.11	2/893 (0.2%)	1.07	1/1215 (0.1%)
2	J	1.12	0/893	1.10	2/1215 (0.2%)
2	L	1.06	0/893	1.16	6/1215 (0.5%)
2	N	1.01	1/893 (0.1%)	1.07	4/1215 (0.3%)
2	P	1.08	1/893 (0.1%)	1.07	1/1215 (0.1%)
All	All	1.25	60/34560 (0.2%)	1.14	98/46856 (0.2%)

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

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

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	ARG	CZ-NH2	-8.94	1.21	1.33
1	I	421	ARG	CZ-NH2	-8.73	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	ARG	CZ-NH1	-8.13	1.21	1.32
1	E	139	ARG	CZ-NH2	-8.05	1.23	1.33
1	G	421	ARG	CZ-NH2	-7.87	1.23	1.33
1	M	421	ARG	CZ-NH2	-7.08	1.24	1.33
1	E	139	ARG	CZ-NH1	-6.79	1.23	1.32
1	K	140	ILE	N-CA	6.55	1.51	1.46
2	H	17	PRO	CA-C	6.45	1.55	1.51
1	K	48	VAL	N-CA	6.34	1.51	1.46
1	M	218	PHE	CE2-CZ	-6.33	1.19	1.38
1	M	218	PHE	CG-CD2	-6.23	1.25	1.38
1	G	421	ARG	CZ-NH1	-6.11	1.24	1.32
1	A	218	PHE	CG-CD2	-6.09	1.26	1.38
1	K	213	ARG	C-O	6.04	1.31	1.23
2	N	102	ILE	CA-CB	5.98	1.60	1.54
1	C	218	PHE	CG-CD2	-5.93	1.26	1.38
1	G	278	THR	C-O	-5.92	1.17	1.24
1	A	421	ARG	CZ-NH2	-5.91	1.25	1.33
1	A	283	TRP	C-O	-5.89	1.17	1.24
2	B	102	ILE	CA-CB	5.84	1.60	1.54
1	O	366	GLN	C-O	-5.71	1.17	1.24
1	E	284	CYS	CA-C	5.64	1.60	1.52
2	P	102	ILE	CA-CB	5.61	1.60	1.54
1	O	346	VAL	CA-CB	-5.59	1.47	1.54
1	O	320	MET	C-O	-5.57	1.17	1.24
1	E	421	ARG	CZ-NH1	-5.56	1.25	1.32
1	G	138	LEU	C-O	5.54	1.30	1.23
1	M	254	ALA	CA-CB	5.54	1.61	1.53
1	K	172	CYS	CB-SG	5.53	1.99	1.81
1	M	126	GLY	C-O	-5.50	1.19	1.24
1	M	218	PHE	CE1-CZ	-5.48	1.22	1.38
1	G	132	ALA	C-O	5.44	1.30	1.23
2	D	16	LEU	C-N	5.41	1.39	1.33
1	I	367	ASP	C-O	-5.33	1.17	1.24
1	C	421	ARG	CZ-NH1	-5.32	1.25	1.32
1	K	109	GLU	C-O	-5.32	1.17	1.23
1	I	421	ARG	CZ-NH1	-5.32	1.25	1.32
1	E	290	LEU	N-CA	5.24	1.52	1.46
1	M	38	ALA	CA-C	5.20	1.58	1.52
1	A	188	ALA	CA-CB	-5.19	1.45	1.53
1	K	42	VAL	CA-C	5.17	1.58	1.52
1	A	182	ALA	C-O	-5.15	1.18	1.24
1	I	346	VAL	CA-CB	-5.14	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	187	ARG	N-CA	5.14	1.52	1.46
1	A	399	VAL	CA-CB	5.12	1.60	1.54
1	A	218	PHE	CE2-CZ	-5.12	1.23	1.38
1	C	254	ALA	CA-CB	5.11	1.61	1.53
1	A	113	VAL	N-CA	-5.09	1.40	1.46
1	G	31	PRO	C-O	-5.09	1.18	1.23
1	M	298	HIS	C-O	-5.09	1.18	1.24
1	C	182	ALA	C-O	-5.08	1.18	1.24
1	O	257	ALA	CA-C	5.07	1.59	1.52
1	I	250	MET	CA-C	5.07	1.59	1.52
1	C	218	PHE	CE1-CZ	-5.06	1.23	1.38
1	O	194	ARG	C-O	-5.05	1.17	1.24
1	E	158	GLU	CA-C	5.04	1.59	1.52
1	O	357	ASP	N-CA	5.03	1.52	1.46
1	G	279	THR	C-O	-5.03	1.18	1.24
2	H	16	LEU	C-N	5.01	1.38	1.33

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	215	ARG	CD-NE-CZ	10.71	139.39	124.40
1	A	139	ARG	NH1-CZ-NH2	-10.54	105.60	119.30
1	E	139	ARG	NH1-CZ-NH2	-10.41	105.77	119.30
1	I	421	ARG	NH1-CZ-NH2	-9.91	106.41	119.30
1	E	139	ARG	NE-CZ-NH2	9.53	127.77	119.20
1	A	139	ARG	NE-CZ-NH2	8.91	127.22	119.20
1	G	215	ARG	NE-CZ-NH1	8.35	129.85	121.50
1	M	421	ARG	NH1-CZ-NH2	-8.10	108.77	119.30
2	N	61	PHE	N-CA-C	7.84	120.97	111.40
2	L	80	TYR	CA-C-N	-7.53	112.41	120.47
2	L	80	TYR	C-N-CA	-7.53	112.41	120.47
2	F	61	PHE	N-CA-C	7.32	121.45	112.23
2	N	58	LEU	CA-C-N	-7.14	112.64	119.85
2	N	58	LEU	C-N-CA	-7.14	112.64	119.85
1	I	421	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	G	421	ARG	NH1-CZ-NH2	-6.97	110.24	119.30
1	G	128	LYS	N-CA-C	6.71	119.43	111.71
1	I	421	ARG	NE-CZ-NH1	6.59	128.09	121.50
2	H	61	PHE	N-CA-C	6.57	119.77	111.69
1	K	139	ARG	NE-CZ-NH2	6.53	125.08	119.20
2	D	61	PHE	N-CA-C	6.50	120.91	112.92
2	B	61	PHE	N-CA-C	6.43	120.83	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	61	PHE	N-CA-C	6.42	121.37	112.45
2	B	65	ASN	N-CA-C	6.29	119.02	108.02
1	E	421	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	G	215	ARG	NE-CZ-NH2	-6.06	113.75	119.20
1	A	421	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	E	421	ARG	NH1-CZ-NH2	-6.03	111.46	119.30
2	B	57	LYS	CB-CA-C	-5.97	109.70	116.63
1	C	139	ARG	CA-C-N	-5.96	118.30	122.59
1	C	139	ARG	C-N-CA	-5.96	118.30	122.59
1	E	321	SER	N-CA-C	-5.95	104.72	111.14
1	A	128	LYS	N-CA-C	5.90	118.66	111.82
2	N	57	LYS	CB-CA-C	-5.87	109.82	116.63
1	K	421	ARG	NH1-CZ-NH2	-5.83	111.72	119.30
1	A	112	SER	N-CA-C	5.81	119.06	107.62
1	C	421	ARG	NE-CZ-NH2	5.81	124.43	119.20
2	F	92	ASN	N-CA-C	5.81	117.69	111.36
1	E	48	VAL	CA-C-N	-5.80	114.63	120.31
1	E	48	VAL	C-N-CA	-5.80	114.63	120.31
1	M	421	ARG	NE-CZ-NH1	5.79	127.28	121.50
2	L	17	PRO	O-C-N	5.75	123.85	121.15
1	K	421	ARG	NE-CZ-NH2	5.73	124.36	119.20
1	M	139	ARG	NE-CZ-NH2	5.70	124.33	119.20
2	J	61	PHE	N-CA-C	5.68	119.83	113.02
1	A	139	ARG	NE-CZ-NH1	5.67	127.17	121.50
2	L	44	GLU	N-CA-C	5.67	117.46	111.28
1	A	421	ARG	NH1-CZ-NH2	-5.66	111.94	119.30
1	K	409	HIS	CA-C-N	5.66	125.77	119.32
1	K	409	HIS	C-N-CA	5.66	125.77	119.32
1	O	409	HIS	CA-C-N	5.65	125.33	119.05
1	O	409	HIS	C-N-CA	5.65	125.33	119.05
1	C	121	VAL	N-CA-C	5.65	117.60	112.29
2	F	64	THR	N-CA-C	-5.58	106.43	113.18
1	I	121	VAL	CB-CA-C	-5.57	104.77	111.85
2	J	65	ASN	N-CA-C	5.53	117.40	108.34
2	D	92	ASN	N-CA-C	5.52	117.38	111.36
1	C	112	SER	N-CA-C	5.45	118.36	107.62
2	L	16	LEU	CA-C-N	-5.41	115.76	119.66
2	L	16	LEU	C-N-CA	-5.41	115.76	119.66
1	G	421	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	I	106	ASP	N-CA-C	5.39	118.95	112.38
1	E	409	HIS	CA-C-N	5.37	125.44	119.32
1	E	409	HIS	C-N-CA	5.37	125.44	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	189	VAL	N-CA-C	-5.37	105.48	110.53
1	I	144	TYR	N-CA-C	-5.32	105.06	112.45
1	M	421	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	A	43	THR	CA-C-N	-5.25	114.83	120.03
1	A	43	THR	C-N-CA	-5.25	114.83	120.03
1	O	332	VAL	N-CA-C	5.25	116.46	109.37
1	M	321	SER	N-CA-C	-5.24	105.48	111.14
1	A	409	HIS	CA-C-N	5.23	124.86	119.05
1	A	409	HIS	C-N-CA	5.23	124.86	119.05
1	C	154	GLY	N-CA-C	-5.23	106.00	112.33
1	I	269	PHE	N-CA-C	5.22	117.71	111.71
1	I	409	HIS	CA-C-N	5.21	125.26	119.32
1	I	409	HIS	C-N-CA	5.21	125.26	119.32
1	I	332	VAL	N-CA-C	5.21	116.12	109.30
1	O	48	VAL	CA-C-N	-5.20	114.60	119.85
1	O	48	VAL	C-N-CA	-5.20	114.60	119.85
2	B	69	VAL	N-CA-C	-5.19	105.78	110.82
1	M	218	PHE	CD1-CG-CD2	-5.19	110.81	118.60
1	O	139	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	G	244	ALA	N-CA-C	5.16	114.07	108.14
1	C	139	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	K	167	ARG	CA-C-N	5.15	125.08	119.78
1	K	167	ARG	C-N-CA	5.15	125.08	119.78
1	E	128	LYS	N-CA-C	5.13	117.77	111.82
1	M	229	GLN	N-CA-C	-5.13	105.77	112.23
1	M	409	HIS	CA-C-N	5.10	125.14	119.32
1	M	409	HIS	C-N-CA	5.10	125.14	119.32
1	M	45	GLN	N-CA-C	-5.09	103.05	110.08
1	A	269	PHE	N-CA-C	5.09	117.56	111.71
1	M	48	VAL	CA-C-O	5.08	122.15	119.15
1	O	106	ASP	N-CA-C	5.05	118.94	112.87
1	C	319	ARG	N-CA-C	-5.05	105.90	111.71
1	G	277	ASN	N-CA-C	5.05	116.47	111.07
1	C	82	GLY	N-CA-C	-5.00	105.92	112.82

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	40	2
1	C	3348	0	3273	45	2
1	E	3348	0	3273	49	0
1	G	3348	0	3273	41	0
1	I	3348	0	3273	48	0
1	K	3348	0	3273	47	0
1	M	3348	0	3273	50	0
1	O	3348	0	3273	47	0
2	B	869	0	836	12	0
2	D	869	0	836	24	0
2	F	869	0	836	19	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	15	0
2	P	869	0	836	23	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	442	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 7.

All (442) 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:M:317:CYS:HA	1:M:320:MET:HE3	1.41	1.02
1:I:317:CYS:HA	1:I:320:MET:HE3	1.42	1.00
1:K:317:CYS:HA	1:K:320:MET:HE3	1.43	1.00
1:O:177:LYS:O	1:O:206:ILE:HD11	1.63	0.99
1:O:317:CYS:HA	1:O:320:MET:HE3	1.43	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: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:C:317:CYS:HA	1:C:320:MET:HE3	1.49	0.91
1:K:223:ASP:OD2	2:L:51:ARG:HD2	1.71	0.90
2:D:65:ASN:HD21	2:D:67:GLN:HB3	1.38	0.88
1:E:317:CYS:HA	1:E:320:MET:HE3	1.55	0.88
1:K:177:LYS:O	1:K:206:ILE:HD11	1.75	0.87
1:G:317:CYS:HA	1:G:320:MET:HE3	1.57	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
2:N:95:GLN:O	2:N:95:GLN:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HE3	1.61	0.82
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: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:C:116:MET:HE1	1:C:320:MET:HE1	1.64	0.77
1:C:177:LYS:O	1:C:206:ILE:HD11	1.84	0.77
1:A:116:MET:HE1	1:A:320:MET:HE1	1.66	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:HD12	2:L:60:LEU:H	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:116:MET:HE1	1:M:320:MET:HE1	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
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:E:116:MET:HE1	1:E:320:MET:HE1	1.73	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:95:GLN:O	2:L:95:GLN:HG3	1.93	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
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:G:116:MET:HE1	1:G:320:MET:HE1	1.80	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:G:262:MET:HE2	1:G:262:MET:HA	1.79	0.62
1:G:317:CYS:HA	1:G:320:MET:CE	2.26	0.62
1:A:262:MET:HA	1:A:262:MET:HE2	1.80	0.62
1:E:74:LEU:O	2:N:95:GLN:NE2	2.32	0.62
1:I:382:ILE:HG22	1:I:402:PHE:HE2	1.65	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:O:302:ASP:C	1:O:302:ASP:OD1	2.44	0.61
1:M:382:ILE:CG2	1:M:402:PHE:CE1	2.85	0.60
1:O:116:MET:HE1	1:O:320:MET:HE1	1.84	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:E:302:ASP:C	1:E:302:ASP:OD1	2.46	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
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:HD12	2:L:60:LEU:N	2.16	0.58
1:O:172:CYS:HB3	1:O:197:LEU:CD1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:44:GLU:H	2:N:44:GLU:CD	2.12	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
2:D:95:GLN:O	2:D:95:GLN:HG3	2.04	0.56
1:G:285:ARG:NH2	4:G:2045:HOH:O	2.36	0.56
1:I:116:MET:HE1	1:I:320:MET:HE1	1.87	0.56
1:K:116:MET:HE1	1:K:320:MET:HE1	1.87	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
2:J:61:PHE:O	2:J:62:ASN:HB3	2.05	0.55
1:K:302:ASP:OD1	1:K:302:ASP:C	2.50	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: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
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
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
2:N:60:LEU:HD12	2:N:60:LEU:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:97:GLN:HE21	2:N:100:SER:HB2	1.74	0.53
1:C:302:ASP:C	1:C:302:ASP:OD1	2.48	0.53
2:L:65:ASN:HD21	2:L:67:GLN:HB3	1.73	0.53
1:A:302:ASP:OD1	1:A:302:ASP:C	2.49	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:C:266:MET:HE3	1:C:294:HIS:HB2	1.91	0.52
1:G:451:TRP:CZ2	2:H:17:PRO:HD3	2.43	0.52
1:K:266:MET:HE3	1:K:294:HIS:HB2	1.91	0.52
1:C:262:MET:HA	1:C:262:MET:HE2	1.90	0.52
1:C:273:GLY:HA3	1:K:273:GLY:HA3	1.92	0.52
1:G:70:TRP:CH2	2:P:55:MET:HE1	2.44	0.52
2:P:44:GLU:H	2:P:44:GLU:CD	2.17	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
1:C:117:LEU:O	1:C:121:VAL:HG22	2.10	0.52
1:I:302:ASP:OD1	1:I:302:ASP:C	2.50	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:O:262:MET:HA	1:O:262:MET:HE2	1.92	0.52
1:E:70:TRP:CH2	2:N:55:MET:HE1	2.45	0.51
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:266:MET:HE3	1:A:294:HIS:HB2	1.92	0.51
1:G:171:GLY:HA2	1:G:199:PHE:O	2.10	0.51
1:I:266:MET:HE3	1:I:294:HIS:HB2	1.93	0.51
1:O:172:CYS:HB3	1:O:197:LEU:HD13	1.90	0.51
1:E:451:TRP:CZ2	2:F:17:PRO:HD3	2.45	0.51
1:K:262:MET:HE2	1:K:262:MET:HA	1.93	0.51
1:A:75:THR:HG22	2:J:95:GLN:NE2	2.26	0.51
1:C:318:LEU:HD13	1:C:318:LEU:C	2.35	0.51
1:M:436:ASP:OD1	1:M:436:ASP:C	2.54	0.51
1:A:121:VAL:HG23	1:I:297:MET:HG3	1.92	0.51
1:M:36:ILE:HD12	1:M:108:PHE:CE2	2.46	0.51
1:G:107:LEU:HD22	1:O:178:LEU:HD13	1.92	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
1:A:273:GLY:HA3	1:I:273:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:ASN:ND2	2:D:67:GLN:HB3	2.18	0.50
2:P:25:ALA:HB2	2:P:70:LEU:HD22	1.94	0.50
2:F:49:GLU:N	2:F:49:GLU:CD	2.70	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
2:H:74:GLN:HG2	2:H:77:ARG:NH2	2.26	0.50
1:K:316:LYS:C	1:K:320:MET:HE2	2.36	0.50
1:I:451:TRP:CZ2	2:P:17:PRO:HD3	2.47	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:G:273:GLY:HA3	1:O:273:GLY:HA3	1.93	0.49
2:B:26:ARG:HG3	2:B:26:ARG:HH11	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:O:318:LEU:HD13	1:O:318:LEU:C	2.37	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
2:F:49:GLU:CD	2:F:49:GLU:H	2.21	0.48
1:I:262:MET:HE2	1:I:262:MET:HA	1.94	0.48
1:O:91:PRO:HG3	4:O:2018:HOH:O	2.13	0.48
1:E:266:MET:HE3	1:E:294:HIS:HB2	1.93	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:O	2:N:95:GLN:CG	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
1:K:382:ILE:CG2	1:K:390:LEU:HD11	2.44	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:70:TRP:CH2	2:L:55:MET:HE1	2.49	0.48
1:C:239:TYR:HB3	1:C:266:MET:HB2	1.96	0.48
2:D:55:MET:HE1	1:M:70:TRP:CH2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:74:LEU:O	2:L:95:GLN:NE2	2.47	0.47
1:A:316:LYS:C	1:A:320:MET:HE2	2.40	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
1:E:387:MET:HE1	1:E:402:PHE:CZ	2.50	0.47
1:M:239:TYR:HB3	1:M:266:MET:HB2	1.96	0.47
1:M:302:ASP:OD1	1:M:302:ASP:C	2.58	0.47
1:O:139:ARG:HD2	1:O:139:ARG:C	2.40	0.47
1:O:171:GLY:HA2	1:O:199:PHE:O	2.15	0.47
2:P:65:ASN:O	2:P:68:ASP:OD1	2.33	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:J:44:GLU:CD	2:J:44:GLU:H	2.23	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
2:F:24:ILE:HG12	2:F:103:VAL:HG12	1.98	0.46
1:G:302:ASP:C	1:G:302:ASP:OD1	2.59	0.46
1:M:422:VAL:HG23	1:M:455:LEU:HD22	1.97	0.46
1:A:387:MET:HE1	1:A:402:PHE:CZ	2.50	0.46
1:I:52:GLU:H	1:I:52:GLU:HG2	1.57	0.46
1:K:354:ILE:N	1:K:354:ILE:HD12	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
1:E:318:LEU:HD13	1:E:318:LEU:C	2.40	0.46
1:O:316:LYS:C	1:O:320:MET:HE2	2.41	0.46
2:B:9:ARG:NH1	2:B:15:TYR:HA	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:316:LYS:C	1:I:320:MET:HE2	2.41	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:H	2:L:60:LEU:CD1	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: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
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:K:52:GLU:H	1:K:52:GLU:HG2	1.56	0.45
1:A:297:MET:HG3	1:I:121:VAL:HG23	1.99	0.45
2:D:61:PHE:O	2:D:62:ASN:CB	2.65	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
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
1:E:75:THR:CG2	1:M:180:LEU:HD23	2.46	0.44
2:J:74:GLN:HG2	2:J:77:ARG:NH2	2.32	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
1:M:262:MET:HA	1:M:262:MET:HE2	2.00	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:K:436:ASP:OD1	1:K:436:ASP:C	2.60	0.44
2:P:94:LYS:O	2:P:95:GLN:C	2.61	0.44
1:A:70:TRP:CH2	2:J:55:MET:HE1	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:266:MET:HE3	1:G:294:HIS:HB2	1.99	0.44
1:G:354:ILE:HD12	1:G:354:ILE:N	2.32	0.44
1:A:30:THR:HA	1:A:31:PRO:HD3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:139:ARG:HD2	1:M:139:ARG:C	2.43	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
1:C:387:MET:HE1	1:C:402:PHE:CZ	2.53	0.43
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
1:O:266:MET:HE3	1:O:294:HIS:HB2	1.99	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:62:ASN:N	2:P:62:ASN:OD1	2.50	0.43
2:P:86:ARG:HA	2:P:103:VAL:HG22	2.01	0.43
1:A:190:TYR:CZ	1:A:194:ARG:HD3	2.53	0.43
1:O:318:LEU:HD13	1:O:318:LEU:O	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
2:F:44:GLU:CD	2:F:44:GLU:H	2.26	0.43
1:O:382:ILE:HG21	1:O:390:LEU:HD11	2.00	0.43
1:E:316:LYS:C	1:E:320:MET:HE2	2.44	0.43
1:I:49:PRO:CD	1:I:52:GLU:HG3	2.31	0.43
1:A:175:LYS:HA	1:A:176:PRO:C	2.44	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:266:MET:HE3	1:M:294:HIS:HB2	1.99	0.43
1:M:90:LEU:HB3	1:M:93:GLU:HG3	2.00	0.43
1:M:242:VAL:O	1:M:243:THR:C	2.60	0.43
1:C:107:LEU:HD22	1:K:178:LEU:HD13	2.01	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:117:LEU:O	1:K:121:VAL:HG22	2.18	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:HD23	1:A:251:LEU:HA	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: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
1:G:74:LEU:C	2:P:95:GLN:HE22	2.27	0.42
1:I:354:ILE:N	1:I:354:ILE:HD12	2.34	0.42
1:I:418:THR:O	1:I:422:VAL:HG13	2.20	0.42
1:E:301:MET:HG2	1:M:300:VAL:HG12	2.01	0.42
1:A:117:LEU:O	1:A:121:VAL:HG22	2.19	0.42
2:B:102:ILE:HA	2:B:102:ILE:HD12	1.76	0.42
2:F:42:PHE:HA	2:F:84:PHE:O	2.19	0.42
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
1:C:251:LEU:HD23	1:C:251:LEU:HA	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:G:316:LYS:C	1:G:320:MET:HE2	2.45	0.42
2:D:44:GLU:H	2:D:44:GLU:CD	2.28	0.41
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:HG3	2:D:51:ARG:NH1	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:MET:HG3	1:M:121:VAL:HG23	2.01	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:HD12	1:O:354:ILE:N	2.36	0.41
1:M:382:ILE:HG23	1:M:390:LEU:HD11	2.02	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:A:139:ARG:C	1:A:139:ARG:HD2	2.45	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
1:M:117:LEU:O	1:M:118:THR:C	2.62	0.41
2:P:86:ARG:HB2	2:P:101:PHE:O	2.21	0.41
2:D:51:ARG:HD2	1:E:223:ASP:CG	2.42	0.41
1:E:175:LYS:HA	1:E:176:PRO:C	2.46	0.41
1:G:88:GLU:HA	1:G:89:PRO:HD2	1.86	0.41
1:I:409:HIS:HA	1:I:410:PRO:HD3	1.95	0.41
2:J:21:ASP:HB3	2:J:70:LEU:HD21	2.03	0.41
2:J:30:TYR:O	2:J:34:GLN:HG2	2.21	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:HD12	2:N:60:LEU:N	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:E:121:VAL:HG23	1:M:297:MET: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: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:I:387:MET:HE1	1:I:402:PHE:CZ	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:ILE:HD12	1:E:108:PHE:CE2	2.56	0.40
1:O:52:GLU:H	1:O:52:GLU:HG2	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 [i](#)

5.3.1 Protein backbone [i](#)

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%)	43	55
1	O	422/475 (89%)	411 (97%)	11 (3%)	0	100	100
2	B	102/118 (86%)	95 (93%)	4 (4%)	3 (3%)	3	2
2	D	102/118 (86%)	95 (93%)	4 (4%)	3 (3%)	3	2
2	F	102/118 (86%)	92 (90%)	8 (8%)	2 (2%)	6	5
2	H	102/118 (86%)	96 (94%)	5 (5%)	1 (1%)	12	15
2	J	102/118 (86%)	94 (92%)	7 (7%)	1 (1%)	12	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	102/118 (86%)	92 (90%)	8 (8%)	2 (2%)	6	5
2	N	102/118 (86%)	92 (90%)	9 (9%)	1 (1%)	12	15
2	P	102/118 (86%)	92 (90%)	10 (10%)	0	100	100
All	All	4192/4744 (88%)	4040 (96%)	138 (3%)	14 (0%)	36	46

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
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%)	340 (98%)	6 (2%)	53	72
1	C	346/386 (90%)	338 (98%)	8 (2%)	44	63
1	E	346/386 (90%)	340 (98%)	6 (2%)	53	72
1	G	346/386 (90%)	339 (98%)	7 (2%)	48	67
1	I	346/386 (90%)	340 (98%)	6 (2%)	53	72
1	K	346/386 (90%)	339 (98%)	7 (2%)	48	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	346/386 (90%)	340 (98%)	6 (2%)	53	72
1	O	346/386 (90%)	338 (98%)	8 (2%)	44	63
2	B	97/108 (90%)	95 (98%)	2 (2%)	47	66
2	D	97/108 (90%)	94 (97%)	3 (3%)	35	52
2	F	97/108 (90%)	94 (97%)	3 (3%)	35	52
2	H	97/108 (90%)	96 (99%)	1 (1%)	68	82
2	J	97/108 (90%)	93 (96%)	4 (4%)	27	41
2	L	97/108 (90%)	93 (96%)	4 (4%)	27	41
2	N	97/108 (90%)	95 (98%)	2 (2%)	47	66
2	P	97/108 (90%)	94 (97%)	3 (3%)	35	52
All	All	3544/3952 (90%)	3468 (98%)	76 (2%)	47	66

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	71	THR
1	A	163	ASN
1	A	172	CYS
1	A	206	ILE
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	206	ILE
1	C	209	GLN
1	C	334	LYS
1	C	335	LEU
2	D	45	THR
2	D	64	THR
2	D	68	ASP
1	E	30	THR
1	E	52	GLU
1	E	163	ASN
1	E	192	CYS

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Mol	Chain	Res	Type
1	E	334	LYS
1	E	335	LEU
2	F	49	GLU
2	F	63	CYS
2	F	93	ILE
1	G	30	THR
1	G	52	GLU
1	G	163	ASN
1	G	172	CYS
1	G	206	ILE
1	G	279	THR
1	G	335	LEU
2	H	45	THR
1	I	52	GLU
1	I	163	ASN
1	I	192	CYS
1	I	206	ILE
1	I	332	VAL
1	I	335	LEU
2	J	16	LEU
2	J	44	GLU
2	J	68	ASP
2	J	106	PRO
1	K	52	GLU
1	K	71	THR
1	K	163	ASN
1	K	172	CYS
1	K	192	CYS
1	K	335	LEU
1	K	422	VAL
2	L	58	LEU
2	L	60	LEU
2	L	65	ASN
2	L	68	ASP
1	M	52	GLU
1	M	71	THR
1	M	163	ASN
1	M	172	CYS
1	M	192	CYS
1	M	335	LEU
2	N	60	LEU
2	N	68	ASP

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Mol	Chain	Res	Type
1	O	30	THR
1	O	52	GLU
1	O	71	THR
1	O	163	ASN
1	O	172	CYS
1	O	192	CYS
1	O	332	VAL
1	O	335	LEU
2	P	44	GLU
2	P	62	ASN
2	P	68	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	205	ASN
1	A	226	HIS
1	A	401	GLN
2	B	65	ASN
2	B	67	GLN
1	C	156	GLN
1	C	226	HIS
2	D	37	HIS
2	D	62	ASN
2	D	65	ASN
1	E	156	GLN
2	F	65	ASN
2	F	67	GLN
2	F	71	ASN
1	G	401	GLN
2	H	37	HIS
2	H	65	ASN
1	I	156	GLN
2	J	29	GLN
2	J	65	ASN
2	J	97	GLN
1	K	156	GLN
1	K	226	HIS
1	K	429	GLN
2	L	37	HIS
2	L	71	ASN

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Mol	Chain	Res	Type
2	L	75	GLN
2	N	29	GLN
2	N	65	ASN
2	N	97	GLN
1	O	156	GLN
1	O	429	GLN
2	P	37	HIS
2	P	65	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	428/475 (90%)	-1.62	0 100 100	2, 11, 39, 53	0
1	C	428/475 (90%)	-1.61	0 100 100	2, 11, 39, 53	0
1	E	428/475 (90%)	-1.63	0 100 100	2, 11, 39, 53	0
1	G	428/475 (90%)	-1.61	0 100 100	2, 11, 38, 53	0
1	I	428/475 (90%)	-1.60	0 100 100	2, 11, 39, 53	0
1	K	428/475 (90%)	-1.60	0 100 100	2, 11, 39, 53	0
1	M	428/475 (90%)	-1.61	0 100 100	2, 11, 39, 53	0
1	O	428/475 (90%)	-1.60	0 100 100	2, 11, 39, 53	0
2	B	104/118 (88%)	-1.32	0 100 100	19, 33, 52, 64	0
2	D	104/118 (88%)	-1.35	0 100 100	17, 32, 48, 59	0
2	F	104/118 (88%)	-1.44	0 100 100	15, 27, 44, 57	0
2	H	104/118 (88%)	-1.41	0 100 100	16, 28, 51, 62	0
2	J	104/118 (88%)	-1.37	0 100 100	15, 30, 47, 59	0
2	L	104/118 (88%)	-1.33	0 100 100	17, 32, 52, 63	0
2	N	104/118 (88%)	-1.34	0 100 100	18, 33, 53, 62	0
2	P	104/118 (88%)	-1.35	0 100 100	15, 31, 52, 63	0
All	All	4256/4744 (89%)	-1.56	0 100 100	2, 14, 42, 64	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	1460	1/1	0.99	0.05	36,36,36,36	0
3	CL	A	1461	1/1	0.99	0.04	33,33,33,33	0
3	CL	C	1460	1/1	0.99	0.08	38,38,38,38	0
3	CL	C	1461	1/1	0.99	0.04	36,36,36,36	0
3	CL	E	1460	1/1	0.99	0.06	34,34,34,34	0
3	CL	G	1460	1/1	0.99	0.06	33,33,33,33	0
3	CL	G	1461	1/1	0.99	0.04	30,30,30,30	0
3	CL	I	1460	1/1	0.99	0.04	28,28,28,28	0
3	CL	I	1461	1/1	0.99	0.05	34,34,34,34	0
3	CL	K	1460	1/1	0.99	0.05	27,27,27,27	0
3	CL	K	1461	1/1	0.99	0.07	31,31,31,31	0
3	CL	M	1461	1/1	0.99	0.06	34,34,34,34	0
3	CL	O	1460	1/1	0.99	0.05	32,32,32,32	0
3	CL	O	1461	1/1	0.99	0.06	35,35,35,35	0
3	CL	M	1460	1/1	1.00	0.05	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.