



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:41 PM UTC

PDB ID : 5ERB / pdb_00005erb
Title : Ketosynthase from module 5 of the bacillaene synthase from *Bacillus amyloliquefaciens* FZB42
Authors : Wagner, D.T.; Gay, D.C.; Keatinge-Clay, A.T.; Meinke, J.
Deposited on : 2015-11-13
Resolution : 4.20 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

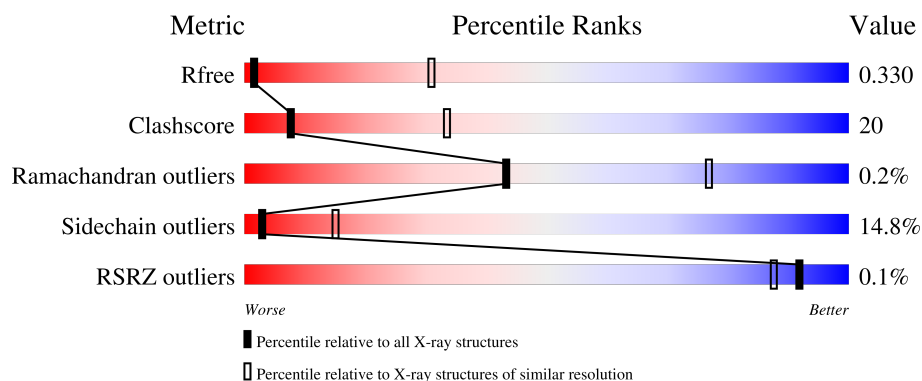
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	640	
1	B	640	
1	C	640	
1	D	640	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18315 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 Polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	0	0
			4543	2859	790	873	21			
1	B	593	Total	C	N	O	S	0	0	0
			4618	2907	798	892	21			
1	C	586	Total	C	N	O	S	0	0	0
			4562	2872	792	878	20			
1	D	590	Total	C	N	O	S	0	0	0
			4592	2886	797	888	21			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q1RS72
A	-18	GLY	-	expression tag	UNP Q1RS72
A	-17	SER	-	expression tag	UNP Q1RS72
A	-16	SER	-	expression tag	UNP Q1RS72
A	-15	HIS	-	expression tag	UNP Q1RS72
A	-14	HIS	-	expression tag	UNP Q1RS72
A	-13	HIS	-	expression tag	UNP Q1RS72
A	-12	HIS	-	expression tag	UNP Q1RS72
A	-11	HIS	-	expression tag	UNP Q1RS72
A	-10	HIS	-	expression tag	UNP Q1RS72
A	-9	SER	-	expression tag	UNP Q1RS72
A	-8	SER	-	expression tag	UNP Q1RS72
A	-7	GLY	-	expression tag	UNP Q1RS72
A	-6	LEU	-	expression tag	UNP Q1RS72
A	-5	VAL	-	expression tag	UNP Q1RS72
A	-4	PRO	-	expression tag	UNP Q1RS72
A	-3	ARG	-	expression tag	UNP Q1RS72
A	-2	GLY	-	expression tag	UNP Q1RS72
A	-1	SER	-	expression tag	UNP Q1RS72
A	0	SER	-	expression tag	UNP Q1RS72
B	-19	MET	-	initiating methionine	UNP Q1RS72

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q1RS72
B	-17	SER	-	expression tag	UNP Q1RS72
B	-16	SER	-	expression tag	UNP Q1RS72
B	-15	HIS	-	expression tag	UNP Q1RS72
B	-14	HIS	-	expression tag	UNP Q1RS72
B	-13	HIS	-	expression tag	UNP Q1RS72
B	-12	HIS	-	expression tag	UNP Q1RS72
B	-11	HIS	-	expression tag	UNP Q1RS72
B	-10	HIS	-	expression tag	UNP Q1RS72
B	-9	SER	-	expression tag	UNP Q1RS72
B	-8	SER	-	expression tag	UNP Q1RS72
B	-7	GLY	-	expression tag	UNP Q1RS72
B	-6	LEU	-	expression tag	UNP Q1RS72
B	-5	VAL	-	expression tag	UNP Q1RS72
B	-4	PRO	-	expression tag	UNP Q1RS72
B	-3	ARG	-	expression tag	UNP Q1RS72
B	-2	GLY	-	expression tag	UNP Q1RS72
B	-1	SER	-	expression tag	UNP Q1RS72
B	0	SER	-	expression tag	UNP Q1RS72
C	-19	MET	-	initiating methionine	UNP Q1RS72
C	-18	GLY	-	expression tag	UNP Q1RS72
C	-17	SER	-	expression tag	UNP Q1RS72
C	-16	SER	-	expression tag	UNP Q1RS72
C	-15	HIS	-	expression tag	UNP Q1RS72
C	-14	HIS	-	expression tag	UNP Q1RS72
C	-13	HIS	-	expression tag	UNP Q1RS72
C	-12	HIS	-	expression tag	UNP Q1RS72
C	-11	HIS	-	expression tag	UNP Q1RS72
C	-10	HIS	-	expression tag	UNP Q1RS72
C	-9	SER	-	expression tag	UNP Q1RS72
C	-8	SER	-	expression tag	UNP Q1RS72
C	-7	GLY	-	expression tag	UNP Q1RS72
C	-6	LEU	-	expression tag	UNP Q1RS72
C	-5	VAL	-	expression tag	UNP Q1RS72
C	-4	PRO	-	expression tag	UNP Q1RS72
C	-3	ARG	-	expression tag	UNP Q1RS72
C	-2	GLY	-	expression tag	UNP Q1RS72
C	-1	SER	-	expression tag	UNP Q1RS72
C	0	SER	-	expression tag	UNP Q1RS72
D	-19	MET	-	initiating methionine	UNP Q1RS72
D	-18	GLY	-	expression tag	UNP Q1RS72
D	-17	SER	-	expression tag	UNP Q1RS72

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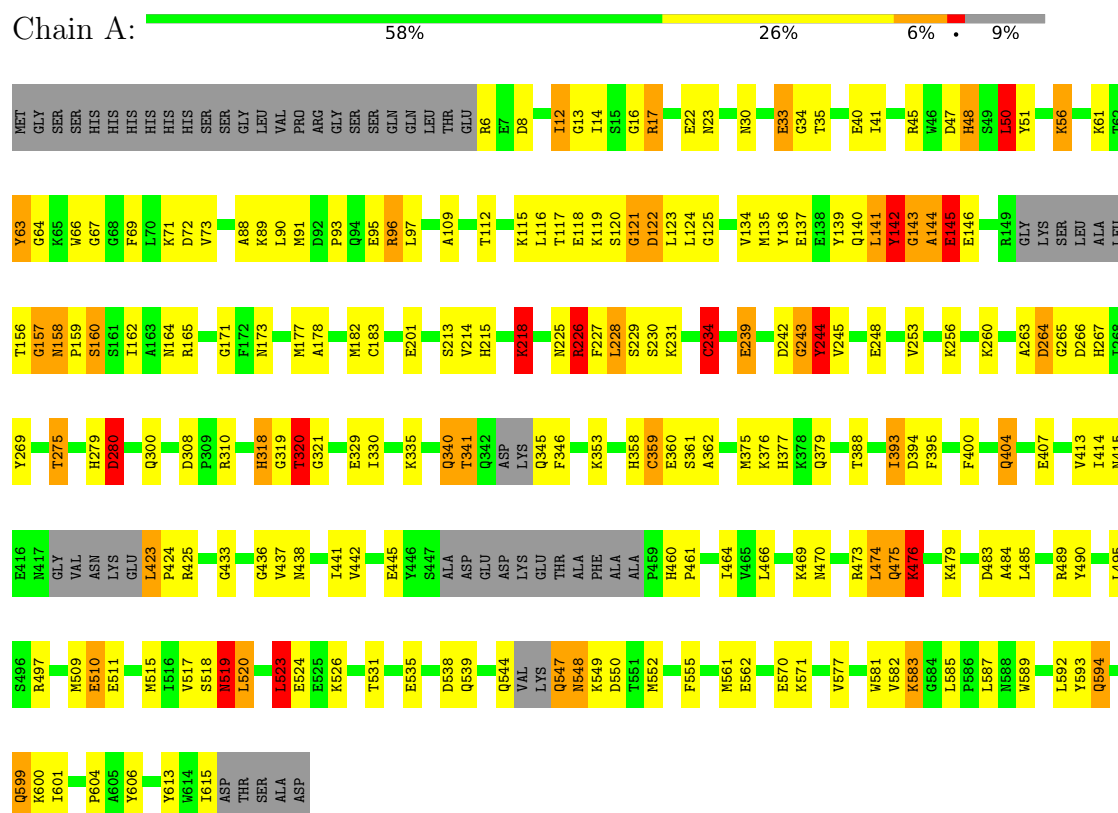
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q1RS72
D	-15	HIS	-	expression tag	UNP Q1RS72
D	-14	HIS	-	expression tag	UNP Q1RS72
D	-13	HIS	-	expression tag	UNP Q1RS72
D	-12	HIS	-	expression tag	UNP Q1RS72
D	-11	HIS	-	expression tag	UNP Q1RS72
D	-10	HIS	-	expression tag	UNP Q1RS72
D	-9	SER	-	expression tag	UNP Q1RS72
D	-8	SER	-	expression tag	UNP Q1RS72
D	-7	GLY	-	expression tag	UNP Q1RS72
D	-6	LEU	-	expression tag	UNP Q1RS72
D	-5	VAL	-	expression tag	UNP Q1RS72
D	-4	PRO	-	expression tag	UNP Q1RS72
D	-3	ARG	-	expression tag	UNP Q1RS72
D	-2	GLY	-	expression tag	UNP Q1RS72
D	-1	SER	-	expression tag	UNP Q1RS72
D	0	SER	-	expression tag	UNP Q1RS72

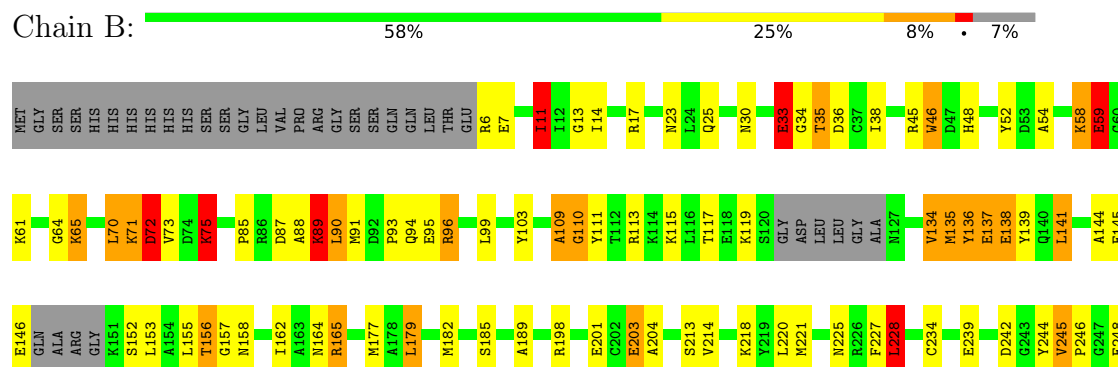
3 Residue-property plots

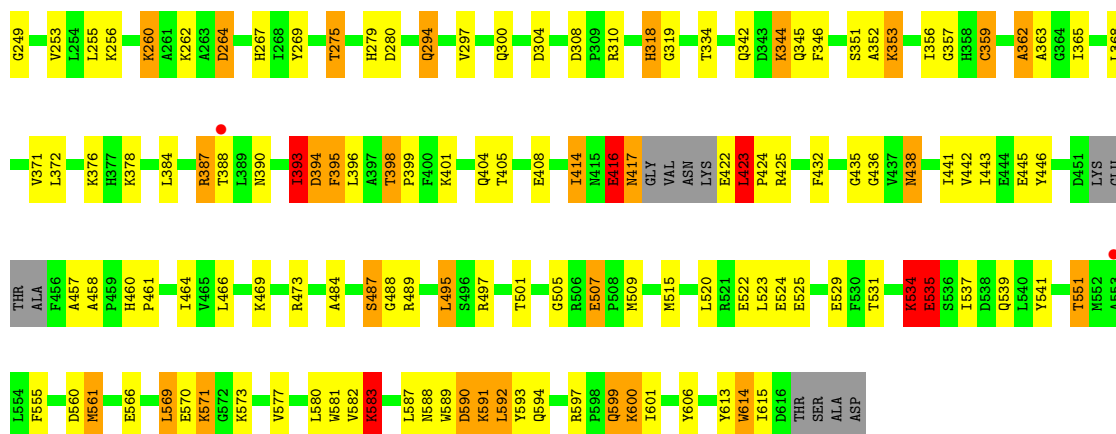
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Polyketide synthase



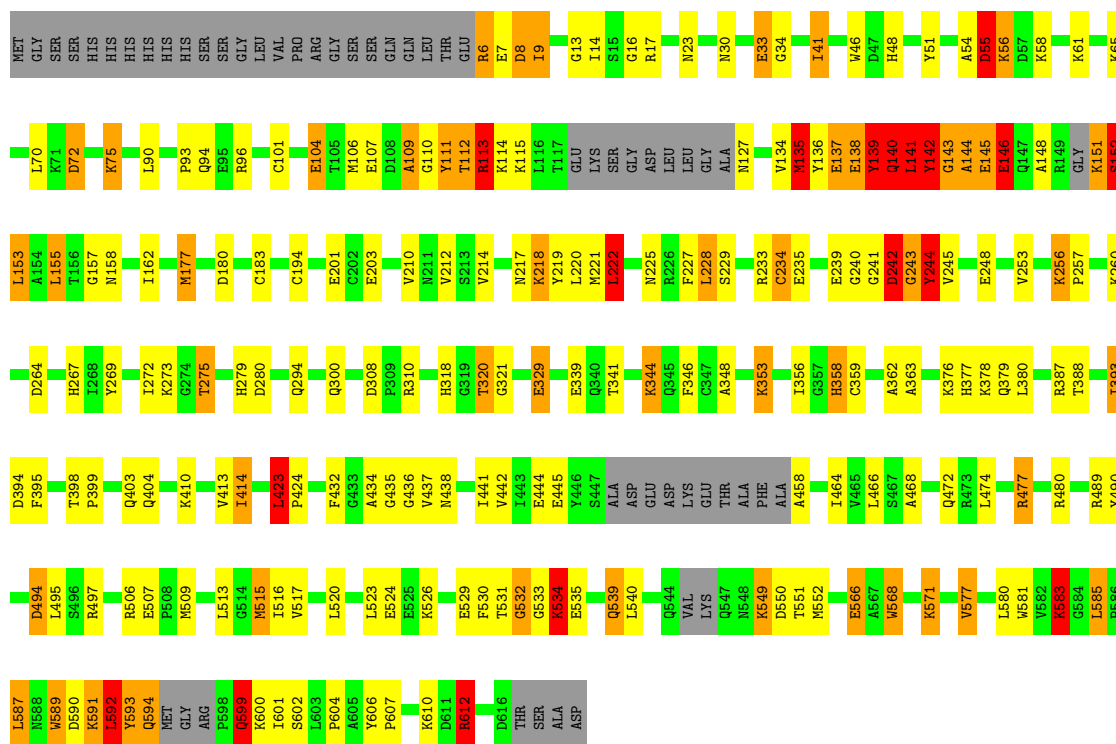
• Molecule 1: Polyketide synthase





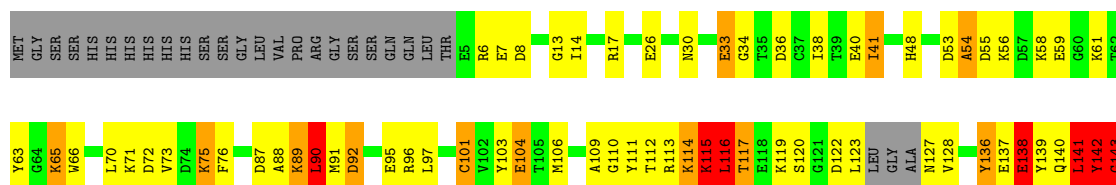
• Molecule 1: Polyketide synthase

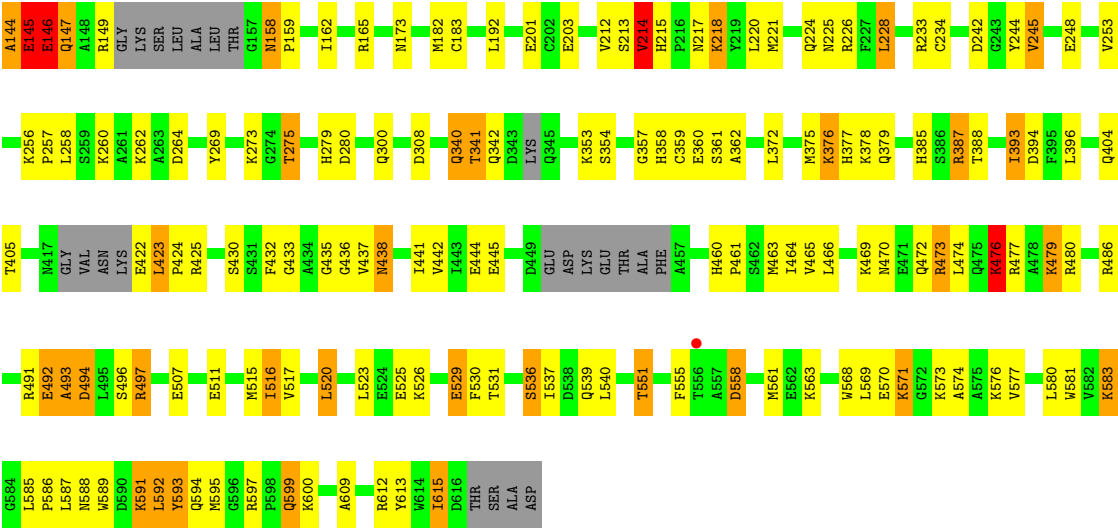
Chain C: 58% 23% 8% 8%



• Molecule 1: Polyketide synthase

Chain D: 57% 26% 7% 8%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.76Å 319.13Å 103.47Å 90.00° 110.26° 90.00°	Depositor
Resolution (Å)	97.07 – 4.20 97.07 – 4.20	Depositor EDS
% Data completeness (in resolution range)	79.9 (97.07-4.20) 78.8 (97.07-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 4.14Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.288 , 0.341 0.281 , 0.330	Depositor DCC
R_{free} test set	1279 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	168.6	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 600.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.115 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18315	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.86	5/4632 (0.1%)	1.53	80/6245 (1.3%)
1	B	0.87	12/4709 (0.3%)	1.72	91/6351 (1.4%)
1	C	0.86	10/4651 (0.2%)	1.73	104/6272 (1.7%)
1	D	0.87	8/4681 (0.2%)	1.60	85/6312 (1.3%)
All	All	0.86	35/18673 (0.2%)	1.65	360/25180 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	3
1	C	0	7
1	D	0	2
All	All	0	20

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	152	SER	C-N	-7.73	1.22	1.33
1	A	121	GLY	C-N	-7.69	1.23	1.33
1	D	143	GLY	C-N	-7.63	1.23	1.33
1	B	393	ILE	CA-CB	7.26	1.64	1.53
1	B	488	GLY	C-N	6.99	1.43	1.33
1	C	434	ALA	C-N	6.96	1.38	1.33
1	C	549	LYS	CA-CB	6.92	1.62	1.53
1	D	117	THR	C-N	-6.84	1.24	1.33
1	B	393	ILE	CA-C	6.51	1.58	1.52
1	B	394	ASP	CA-CB	6.44	1.61	1.53
1	B	59	GLU	C-N	-6.39	1.24	1.33
1	D	359	CYS	C-N	-6.33	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	435	GLY	C-N	-6.30	1.24	1.33
1	A	156	THR	C-N	-6.25	1.24	1.33
1	B	34	GLY	C-N	-6.05	1.25	1.33
1	C	111	TYR	C-N	5.97	1.42	1.33
1	C	240	GLY	C-N	-5.82	1.25	1.33
1	A	226	ARG	CA-CB	5.77	1.60	1.52
1	D	479	LYS	CA-CB	5.75	1.62	1.53
1	B	70	LEU	C-N	5.75	1.41	1.33
1	B	64	GLY	C-N	5.64	1.41	1.33
1	B	435	GLY	C-N	-5.61	1.25	1.33
1	C	225	ASN	C-N	-5.53	1.25	1.33
1	A	225	ASN	C-N	-5.46	1.26	1.33
1	C	242	ASP	C-N	-5.43	1.24	1.33
1	C	139	TYR	C-N	-5.37	1.26	1.33
1	C	435	GLY	C-N	-5.33	1.25	1.33
1	B	225	ASN	C-N	-5.31	1.26	1.33
1	C	414	ILE	C-N	-5.31	1.25	1.33
1	D	361	SER	C-N	-5.26	1.25	1.33
1	B	90	LEU	C-N	-5.22	1.27	1.33
1	D	115	LYS	C-N	-5.20	1.25	1.33
1	B	416	GLU	CA-CB	5.03	1.59	1.53
1	D	113	ARG	C-N	5.03	1.40	1.33
1	A	549	LYS	CA-C	5.02	1.59	1.52

All (360) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	ALA	N-CA-C	41.87	156.92	111.28
1	C	142	TYR	CA-C-N	27.64	150.75	121.45
1	C	142	TYR	C-N-CA	27.64	150.75	121.45
1	D	89	LYS	N-CA-C	-26.83	73.32	110.35
1	A	583	LYS	N-CA-C	-26.17	71.79	110.52
1	B	590	ASP	N-CA-C	-25.27	72.05	109.96
1	D	583	LYS	N-CA-C	-25.14	73.31	110.52
1	D	493	ALA	N-CA-C	-25.09	79.55	110.41
1	C	583	LYS	N-CA-C	-23.41	73.10	110.32
1	A	474	LEU	N-CA-C	22.23	137.28	111.71
1	B	591	LYS	N-CA-C	-22.18	77.69	109.18
1	A	50	LEU	N-CA-C	-22.15	75.74	109.41
1	C	152	SER	N-CA-C	22.10	157.87	110.80
1	B	614	TRP	N-CA-C	22.09	135.05	110.97
1	B	487	SER	N-CA-C	-19.27	77.47	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	583	LYS	N-CA-C	-18.50	80.90	110.32
1	D	54	ALA	N-CA-C	-18.46	87.30	110.19
1	B	613	TYR	N-CA-C	18.21	138.61	112.94
1	C	264	ASP	N-CA-C	-18.13	80.13	108.96
1	D	264	ASP	N-CA-C	-18.07	80.22	108.96
1	C	144	ALA	CA-C-N	-17.76	91.88	122.07
1	C	144	ALA	C-N-CA	-17.76	91.88	122.07
1	A	51	TYR	N-CA-CB	-17.39	83.08	109.69
1	C	140	GLN	N-CA-C	-17.05	92.15	113.97
1	A	33	GLU	N-CA-C	-16.82	81.83	109.24
1	D	144	ALA	N-CA-C	-16.57	89.86	111.24
1	D	142	TYR	N-CA-CB	-16.19	86.92	110.56
1	B	590	ASP	CB-CA-C	16.19	135.79	109.89
1	D	54	ALA	CB-CA-C	16.11	147.22	111.30
1	C	532	GLY	N-CA-C	-16.09	75.05	113.18
1	C	139	TYR	N-CA-C	-15.96	74.00	107.67
1	D	214	VAL	N-CA-CB	-15.67	90.44	111.90
1	C	142	TYR	N-CA-C	-15.54	78.85	107.75
1	B	393	ILE	CB-CA-C	15.45	130.53	113.22
1	B	34	GLY	N-CA-C	-15.45	92.21	112.14
1	C	152	SER	N-CA-CB	-15.35	84.55	110.49
1	C	33	GLU	N-CA-C	-15.02	84.25	108.73
1	A	51	TYR	N-CA-C	14.93	132.34	110.10
1	B	33	GLU	N-CA-C	-14.86	84.50	108.73
1	B	145	GLU	N-CA-C	-14.79	84.79	108.90
1	B	144	ALA	CB-CA-C	-14.65	86.46	110.79
1	C	394	ASP	N-CA-C	-14.37	85.30	108.73
1	D	33	GLU	N-CA-C	-14.29	85.44	108.73
1	A	359	CYS	N-CA-C	-14.22	90.19	110.24
1	C	143	GLY	N-CA-C	-14.20	87.12	112.54
1	C	114	LYS	N-CA-C	13.39	127.17	111.11
1	C	241	GLY	N-CA-C	-13.37	81.50	113.18
1	B	614	TRP	N-CA-CB	-13.21	90.62	109.91
1	B	146	GLU	N-CA-CB	-12.82	88.70	110.50
1	D	143	GLY	N-CA-C	-12.57	83.38	113.18
1	C	146	GLU	N-CA-C	-12.39	88.55	109.24
1	A	394	ASP	N-CA-C	-12.22	87.31	108.20
1	C	142	TYR	O-C-N	-11.98	108.13	122.87
1	A	145	GLU	N-CA-C	-11.91	98.23	113.72
1	B	35	THR	N-CA-C	-11.88	91.27	108.96
1	B	111	TYR	N-CA-C	-11.85	92.63	109.69
1	A	393	ILE	CB-CA-C	-11.74	100.07	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ALA	N-CA-C	-11.71	96.05	113.61
1	D	585	LEU	N-CA-C	-11.52	94.41	110.31
1	D	114	LYS	N-CA-C	-11.50	92.71	109.96
1	C	243	GLY	N-CA-C	11.39	129.94	112.51
1	C	242	ASP	N-CA-C	-11.33	92.55	107.73
1	A	594	GLN	N-CA-C	-11.29	96.20	110.19
1	D	116	LEU	N-CA-C	11.27	126.83	113.20
1	C	244	TYR	CA-CB-CG	-11.07	93.97	113.90
1	A	475	GLN	N-CA-CB	-11.06	95.50	111.54
1	D	226	ARG	N-CA-CB	10.99	126.75	110.49
1	A	143	GLY	N-CA-C	-10.96	87.21	113.18
1	C	55	ASP	N-CA-C	-10.94	94.81	110.24
1	B	65	LYS	N-CA-C	10.78	128.15	112.94
1	B	489	ARG	N-CA-CB	-10.61	94.39	110.20
1	A	242	ASP	N-CA-C	-10.60	88.22	110.80
1	B	591	LYS	CB-CA-C	10.53	133.23	111.11
1	C	592	LEU	CB-CA-C	-10.46	95.51	110.06
1	B	363	ALA	CB-CA-C	-10.33	92.02	109.38
1	C	55	ASP	CB-CA-C	10.30	126.28	109.70
1	A	124	LEU	N-CA-C	10.24	125.30	110.24
1	C	138	GLU	N-CA-C	10.00	132.09	110.80
1	B	33	GLU	CB-CA-C	-9.97	94.05	110.19
1	D	90	LEU	N-CA-CB	9.88	127.06	112.13
1	D	115	LYS	N-CA-C	-9.88	95.11	108.74
1	D	56	LYS	N-CA-C	-9.82	93.40	109.40
1	A	318	HIS	CB-CA-C	-9.71	95.46	111.68
1	B	488	GLY	N-CA-C	-9.71	97.44	111.03
1	C	585	LEU	N-CA-C	-9.58	95.85	110.32
1	B	59	GLU	N-CA-C	-9.57	97.99	110.33
1	C	435	GLY	N-CA-C	-9.56	92.66	111.31
1	D	142	TYR	CB-CA-C	-9.51	94.48	110.56
1	A	437	VAL	N-CA-C	-9.50	95.25	108.27
1	C	112	THR	N-CA-C	9.40	130.82	110.80
1	A	361	SER	CB-CA-C	-9.38	94.31	110.17
1	D	435	GLY	N-CA-C	-9.28	98.04	111.03
1	C	242	ASP	O-C-N	-9.25	112.02	122.75
1	D	494	ASP	N-CA-C	9.22	124.19	111.74
1	D	117	THR	CB-CA-C	-9.11	94.77	110.17
1	D	34	GLY	N-CA-C	-9.06	96.83	110.97
1	C	535	GLU	N-CA-CB	9.04	125.71	110.71
1	C	593	TYR	N-CA-C	9.03	124.15	112.41
1	D	214	VAL	N-CA-C	9.01	119.69	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	144	ALA	N-CA-C	-8.99	96.75	109.69
1	B	138	GLU	N-CA-C	8.93	124.28	113.12
1	A	225	ASN	N-CA-C	-8.91	94.21	108.73
1	A	264	ASP	N-CA-C	-8.87	90.37	107.57
1	B	435	GLY	N-CA-C	-8.87	94.02	111.31
1	A	318	HIS	N-CA-C	-8.83	90.45	107.57
1	D	361	SER	CB-CA-C	-8.79	95.41	110.09
1	C	414	ILE	CB-CA-C	8.78	123.34	112.45
1	C	393	ILE	CB-CA-C	-8.73	103.44	113.22
1	C	593	TYR	N-CA-CB	-8.72	96.81	111.20
1	B	35	THR	N-CA-CB	8.68	125.28	111.56
1	B	109	ALA	CB-CA-C	-8.65	94.35	110.36
1	B	71	LYS	CB-CA-C	-8.63	96.57	110.81
1	B	394	ASP	N-CA-C	-8.61	91.74	107.75
1	C	113	ARG	CB-CA-C	8.59	124.52	109.75
1	B	359	CYS	N-CA-C	-8.56	94.62	108.41
1	A	73	VAL	N-CA-C	8.51	119.29	110.36
1	B	145	GLU	N-CA-CB	-8.49	96.42	110.68
1	C	111	TYR	N-CA-C	8.45	125.50	107.67
1	D	585	LEU	CB-CA-C	8.41	120.36	108.68
1	A	280	ASP	N-CA-C	-8.33	96.51	109.76
1	C	240	GLY	N-CA-C	-8.32	93.47	113.18
1	B	227	PHE	N-CA-C	-8.31	102.73	113.12
1	A	63	TYR	N-CA-C	-8.21	93.37	108.24
1	B	464	ILE	N-CA-C	-8.20	95.30	107.51
1	C	550	ASP	N-CA-C	-8.20	102.51	114.39
1	A	34	GLY	N-CA-C	-8.19	96.74	111.15
1	B	534	LYS	N-CA-C	8.19	122.16	109.96
1	C	600	LYS	N-CA-C	8.08	121.50	110.35
1	D	594	GLN	N-CA-C	-8.07	97.20	109.79
1	D	592	LEU	N-CA-C	-8.04	102.52	111.28
1	B	393	ILE	O-C-N	-8.02	115.22	121.96
1	C	601	ILE	CB-CA-C	8.00	122.58	110.91
1	C	395	PHE	N-CA-C	-7.99	101.72	112.26
1	D	359	CYS	N-CA-C	-7.92	97.95	109.59
1	A	474	LEU	CB-CA-C	-7.89	96.04	110.63
1	C	393	ILE	O-C-N	-7.89	115.33	121.96
1	B	145	GLU	CB-CA-C	-7.88	95.29	109.71
1	B	146	GLU	N-CA-C	7.86	133.01	111.00
1	D	138	GLU	N-CA-C	7.83	123.32	112.04
1	A	121	GLY	O-C-N	-7.75	112.62	122.70
1	D	537	ILE	CB-CA-C	7.72	123.95	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	61	LYS	N-CA-C	-7.70	96.60	108.76
1	C	141	LEU	N-CA-C	7.67	122.76	113.41
1	A	50	LEU	CB-CA-C	-7.66	95.13	110.30
1	C	109	ALA	CB-CA-C	-7.63	95.61	110.11
1	D	496	SER	CB-CA-C	-7.63	96.28	110.01
1	B	551	THR	N-CA-C	-7.62	104.51	113.88
1	A	245	VAL	N-CA-CB	-7.60	100.58	111.21
1	B	264	ASP	N-CA-C	-7.55	93.70	107.75
1	D	117	THR	N-CA-C	7.55	123.42	113.30
1	B	65	LYS	N-CA-CB	-7.54	98.54	110.98
1	C	363	ALA	CB-CA-C	-7.53	96.42	109.07
1	A	121	GLY	N-CA-C	-7.50	95.41	113.18
1	C	115	LYS	CB-CA-C	7.47	122.68	111.17
1	C	145	GLU	N-CA-C	-7.46	96.69	108.63
1	D	33	GLU	CB-CA-C	-7.46	98.10	110.19
1	D	476	LYS	N-CA-C	7.45	122.65	112.90
1	B	156	THR	CB-CA-C	-7.39	100.06	111.66
1	C	139	TYR	CB-CA-C	-7.36	101.28	111.95
1	A	395	PHE	CB-CA-C	7.28	123.39	112.03
1	B	110	GLY	N-CA-C	7.26	124.08	113.48
1	A	320	THR	N-CA-C	-7.25	102.56	111.40
1	C	244	TYR	N-CA-C	7.22	120.75	110.14
1	D	213	SER	N-CA-C	7.22	121.99	107.41
1	C	140	GLN	CB-CA-C	7.13	121.05	109.07
1	C	599	GLN	N-CA-C	-7.11	98.22	108.60
1	B	435	GLY	O-C-N	-7.08	118.11	123.35
1	C	592	LEU	N-CA-C	7.07	120.91	110.30
1	B	89	LYS	N-CA-C	-7.05	103.02	111.69
1	C	532	GLY	CA-C-N	7.01	129.21	122.27
1	C	532	GLY	C-N-CA	7.01	129.21	122.27
1	D	612	ARG	N-CA-C	7.01	120.18	108.20
1	C	612	ARG	N-CA-C	6.99	120.14	108.20
1	B	488	GLY	O-C-N	6.95	128.89	122.77
1	B	87	ASP	CB-CA-C	-6.94	98.02	110.37
1	C	152	SER	O-C-N	-6.91	113.40	122.59
1	D	147	GLN	N-CA-CB	6.90	123.04	110.76
1	B	416	GLU	N-CA-C	-6.89	98.00	108.67
1	D	116	LEU	N-CA-CB	-6.88	99.27	110.42
1	A	594	GLN	CA-C-O	-6.86	114.81	122.01
1	B	11	ILE	CB-CA-C	6.82	120.92	110.96
1	A	495	LEU	CB-CA-C	-6.81	98.03	110.63
1	D	122	ASP	CB-CA-C	6.80	119.96	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	ILE	CA-CB-CG1	6.79	121.94	110.40
1	B	89	LYS	CB-CA-C	6.76	123.08	110.70
1	C	33	GLU	CB-CA-C	-6.76	99.24	110.19
1	C	539	GLN	N-CA-C	-6.75	103.63	112.41
1	A	394	ASP	CB-CA-C	6.75	121.58	110.78
1	B	318	HIS	N-CA-C	-6.74	96.83	108.56
1	A	243	GLY	N-CA-C	6.72	123.59	112.30
1	B	35	THR	CB-CA-C	6.72	126.33	111.09
1	A	158	ASN	N-CA-CB	6.71	122.32	110.37
1	C	539	GLN	CB-CA-C	-6.69	100.18	111.02
1	C	435	GLY	O-C-N	-6.69	118.40	123.35
1	D	595	MET	CB-CA-C	-6.67	97.14	110.42
1	B	464	ILE	CB-CA-C	6.67	120.65	111.31
1	D	143	GLY	O-C-N	-6.66	114.04	122.70
1	D	393	ILE	CB-CA-C	-6.64	100.41	111.29
1	B	318	HIS	O-C-N	-6.63	114.57	122.46
1	C	227	PHE	N-CA-C	-6.63	105.49	113.97
1	A	239	GLU	N-CA-CB	6.60	120.03	110.20
1	D	55	ASP	N-CA-C	-6.59	100.13	109.96
1	C	495	LEU	N-CA-C	6.59	120.42	112.38
1	D	360	GLU	N-CA-C	-6.58	104.03	111.14
1	B	36	ASP	N-CA-C	-6.57	96.52	108.02
1	D	551	THR	N-CA-C	-6.53	105.85	113.88
1	A	475	GLN	N-CA-C	-6.51	102.57	111.56
1	D	144	ALA	N-CA-CB	-6.51	100.50	110.07
1	C	72	ASP	N-CA-C	6.50	120.79	112.86
1	B	70	LEU	O-C-N	6.50	130.37	123.03
1	B	395	PHE	CB-CA-C	-6.50	99.19	110.17
1	C	568	TRP	CB-CA-C	-6.49	99.81	110.85
1	D	387	ARG	N-CA-C	6.49	120.30	112.38
1	A	225	ASN	CB-CA-C	6.48	120.68	110.19
1	B	61	LYS	N-CA-C	-6.46	99.38	109.72
1	D	595	MET	N-CA-CB	-6.46	99.57	110.49
1	D	122	ASP	N-CA-C	-6.46	100.34	109.96
1	B	72	ASP	N-CA-C	6.43	119.06	111.02
1	A	319	GLY	N-CA-C	-6.43	97.95	113.18
1	D	404	GLN	N-CA-C	6.42	117.94	111.07
1	A	35	THR	N-CA-CB	6.38	121.30	110.71
1	B	119	LYS	N-CA-C	6.35	117.89	110.97
1	A	362	ALA	N-CA-C	-6.35	104.85	112.59
1	B	352	ALA	N-CA-C	-6.34	104.59	112.90
1	D	497	ARG	N-CA-C	-6.33	105.21	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	365	ILE	N-CA-C	-6.32	104.88	111.58
1	C	225	ASN	N-CA-C	-6.32	98.91	108.96
1	C	585	LEU	CB-CA-C	6.30	117.39	108.76
1	D	437	VAL	N-CA-C	-6.30	98.97	108.17
1	D	394	ASP	N-CA-C	-6.29	96.05	107.75
1	B	394	ASP	N-CA-CB	6.28	120.76	110.39
1	C	110	GLY	N-CA-C	6.24	124.51	114.90
1	C	111	TYR	N-CA-CB	-6.22	101.50	111.58
1	D	435	GLY	O-C-N	-6.22	117.30	122.77
1	A	227	PHE	N-CA-C	-6.21	106.02	113.97
1	A	244	TYR	N-CA-C	6.20	119.65	109.85
1	D	104	GLU	N-CA-CB	6.18	119.30	110.16
1	D	147	GLN	N-CA-C	-6.17	100.67	108.45
1	D	225	ASN	N-CA-C	-6.17	99.16	108.96
1	A	280	ASP	N-CA-CB	6.16	119.50	109.95
1	D	592	LEU	CB-CA-C	6.13	120.96	110.79
1	B	535	GLU	N-CA-C	6.11	118.65	108.13
1	B	203	GLU	CA-CB-CG	6.10	126.31	114.10
1	D	123	LEU	N-CA-CB	6.10	120.88	110.50
1	C	222	LEU	CA-CB-CG	6.10	137.65	116.30
1	D	359	CYS	CB-CA-C	6.09	119.39	110.26
1	D	341	THR	CB-CA-C	6.08	120.65	110.43
1	A	473	ARG	CB-CG-CD	6.07	125.26	111.30
1	C	344	LYS	N-CA-C	6.06	119.51	111.75
1	C	534	LYS	CA-C-N	-6.06	111.35	121.89
1	C	534	LYS	C-N-CA	-6.06	111.35	121.89
1	C	34	GLY	N-CA-C	-6.04	98.86	113.18
1	A	519	ASN	N-CA-C	6.04	119.39	109.85
1	A	340	GLN	N-CA-C	6.04	123.14	114.39
1	C	242	ASP	N-CA-CB	6.03	120.57	111.35
1	A	48	HIS	N-CA-C	-6.01	103.90	111.11
1	A	122	ASP	N-CA-C	-6.00	98.01	110.80
1	D	362	ALA	N-CA-C	-5.98	103.44	111.87
1	A	234	CYS	CB-CA-C	5.97	120.33	110.78
1	A	615	ILE	CB-CG1-CD1	5.97	126.34	113.80
1	A	214	VAL	N-CA-C	5.96	118.92	112.96
1	A	90	LEU	N-CA-C	5.93	118.93	110.68
1	C	177	MET	N-CA-C	5.93	117.86	108.79
1	B	177	MET	N-CA-C	5.92	117.85	108.79
1	B	593	TYR	N-CA-C	-5.92	103.52	111.87
1	D	387	ARG	CB-CA-C	-5.89	97.89	110.32
1	B	225	ASN	N-CA-C	-5.88	99.61	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	MET	N-CA-C	5.88	117.79	108.79
1	C	240	GLY	O-C-N	-5.88	115.06	122.70
1	D	56	LYS	N-CA-CB	5.86	121.02	110.83
1	D	115	LYS	CB-CA-C	-5.86	98.00	111.95
1	D	146	GLU	CB-CA-C	5.81	121.71	109.79
1	C	222	LEU	N-CA-CB	-5.79	101.37	110.06
1	C	494	ASP	N-CA-CB	-5.77	101.69	110.92
1	D	340	GLN	N-CA-C	5.75	122.28	113.19
1	A	510	GLU	CB-CG-CD	5.74	122.35	112.60
1	A	495	LEU	N-CA-C	5.73	118.30	111.71
1	B	242	ASP	N-CA-C	5.73	120.55	112.93
1	C	550	ASP	CB-CA-C	5.73	118.66	109.27
1	D	464	ILE	N-CA-C	-5.71	98.19	106.88
1	A	437	VAL	N-CA-CB	5.71	121.68	111.63
1	A	263	ALA	N-CA-C	5.71	117.18	111.07
1	B	71	LYS	N-CA-C	5.70	117.59	108.41
1	A	64	GLY	N-CA-C	-5.70	99.67	113.18
1	C	395	PHE	N-CA-CB	5.70	120.52	111.17
1	C	135	MET	N-CA-C	5.68	119.42	111.30
1	B	218	LYS	CB-CG-CD	5.67	124.35	111.30
1	C	153	LEU	N-CA-CB	-5.67	100.90	110.49
1	D	59	GLU	N-CA-CB	-5.64	102.62	110.29
1	C	280	ASP	N-CA-C	5.61	119.21	112.93
1	B	416	GLU	N-CA-CB	5.56	118.84	109.94
1	A	245	VAL	N-CA-C	5.56	120.90	108.88
1	B	228	LEU	N-CA-C	5.55	117.69	110.53
1	B	54	ALA	N-CA-C	-5.55	101.76	110.36
1	C	144	ALA	CA-C-O	-5.54	114.90	121.60
1	A	56	LYS	N-CA-C	5.53	118.87	111.24
1	D	280	ASP	N-CA-C	5.52	119.11	112.93
1	A	476	LYS	N-CA-C	-5.51	104.10	112.04
1	A	404	GLN	N-CA-C	5.49	117.34	111.36
1	B	571	LYS	CB-CA-C	5.46	119.96	110.79
1	D	245	VAL	N-CA-CB	-5.44	103.60	111.21
1	B	245	VAL	CB-CA-C	5.42	121.23	111.36
1	C	113	ARG	N-CA-C	-5.42	105.33	113.89
1	C	214	VAL	N-CA-C	5.41	120.58	109.34
1	A	89	LYS	CB-CA-C	5.40	119.44	110.81
1	C	437	VAL	N-CA-C	-5.37	100.39	108.12
1	B	89	LYS	N-CA-CB	5.36	118.19	110.20
1	B	136	TYR	N-CA-CB	5.36	117.96	109.71
1	A	266	ASP	N-CA-CB	5.35	121.47	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	GLY	N-CA-C	-5.34	100.51	113.18
1	A	218	LYS	CA-CB-CG	5.34	124.78	114.10
1	C	6	ARG	CB-CG-CD	5.34	123.58	111.30
1	D	242	ASP	N-CA-C	5.33	120.02	112.93
1	B	507	GLU	N-CA-CB	5.33	118.44	110.02
1	C	144	ALA	O-C-N	-5.31	115.27	122.81
1	C	221	MET	CA-C-N	5.31	127.65	120.38
1	C	221	MET	C-N-CA	5.31	127.65	120.38
1	A	144	ALA	CB-CA-C	-5.30	100.76	109.99
1	B	582	VAL	O-C-N	5.29	127.21	121.87
1	C	532	GLY	O-C-N	5.27	129.55	122.70
1	D	55	ASP	N-CA-CB	-5.27	101.19	109.51
1	D	145	GLU	N-CA-C	5.26	121.46	112.99
1	A	226	ARG	CB-CG-CD	5.25	123.37	111.30
1	A	464	ILE	N-CA-C	-5.24	98.91	106.88
1	B	423	LEU	N-CA-C	-5.24	103.17	109.72
1	D	404	GLN	N-CA-CB	-5.24	102.41	110.01
1	D	120	SER	N-CA-C	5.23	116.98	111.28
1	C	245	VAL	N-CA-CB	-5.20	103.93	111.21
1	C	9	ILE	N-CA-CB	5.20	118.32	111.25
1	C	112	THR	N-CA-CB	-5.19	101.72	110.49
1	D	615	ILE	N-CA-C	5.18	117.96	109.78
1	C	398	THR	N-CA-C	-5.17	103.66	110.39
1	D	136	TYR	N-CA-C	5.16	117.84	107.41
1	B	458	ALA	N-CA-C	-5.15	102.66	110.39
1	D	539	GLN	N-CA-C	5.15	119.19	113.01
1	B	495	LEU	N-CA-C	5.15	117.56	111.33
1	D	593	TYR	N-CA-CB	-5.14	102.21	110.39
1	D	465	VAL	N-CA-C	-5.14	101.08	108.89
1	C	423	LEU	N-CA-C	-5.13	103.31	109.72
1	A	335	LYS	CA-CB-CG	5.10	124.30	114.10
1	B	75	LYS	N-CA-C	5.10	118.07	110.52
1	B	600	LYS	N-CA-C	5.09	116.50	110.19
1	C	589	TRP	CB-CA-C	-5.09	100.44	110.11
1	A	613	TYR	CB-CA-C	5.09	119.71	109.38
1	C	242	ASP	CA-C-N	5.09	128.23	121.01
1	C	242	ASP	C-N-CA	5.09	128.23	121.01
1	D	613	TYR	N-CA-CB	-5.08	102.51	110.69
1	A	119	LYS	CB-CA-C	-5.08	99.46	109.67
1	A	473	ARG	CB-CA-C	-5.08	100.87	110.01
1	B	59	GLU	O-C-N	-5.06	116.71	122.68
1	C	58	LYS	N-CA-C	5.05	117.04	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	LEU	CB-CG-CD1	5.04	125.82	110.70
1	D	141	LEU	N-CA-C	5.04	119.14	112.89
1	B	58	LYS	N-CA-C	5.03	117.02	110.43
1	B	362	ALA	N-CA-C	-5.03	102.07	109.62
1	B	90	LEU	O-C-N	-5.03	116.30	122.68
1	A	600	LYS	N-CA-C	5.02	116.41	110.19
1	A	213	SER	N-CA-C	5.02	117.54	107.41
1	C	358	HIS	N-CA-C	-5.01	102.22	109.59
1	A	160	SER	CB-CA-C	-5.01	99.98	109.95

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	GLY	Mainchain
1	A	157	GLY	Mainchain
1	A	244	TYR	Mainchain
1	A	475	GLN	Peptide
1	A	518	SER	Peptide
1	A	519	ASN	Peptide
1	A	592	LEU	Peptide
1	A	72	ASP	Peptide
1	B	137	GLU	Peptide
1	B	457	ALA	Peptide
1	B	72	ASP	Peptide
1	C	139	TYR	Mainchain
1	C	142	TYR	Mainchain,Peptide
1	C	152	SER	Mainchain
1	C	242	ASP	Mainchain
1	C	244	TYR	Sidechain
1	C	534	LYS	Mainchain
1	D	137	GLU	Peptide
1	D	143	GLY	Mainchain

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	4543	0	4470	158	0
1	B	4618	0	4540	154	1
1	C	4562	0	4491	265	0
1	D	4592	0	4505	211	1
All	All	18315	0	18006	730	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (730) 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:A:141:LEU:HD21	1:A:215:HIS:CE1	1.26	1.63
1:D:142:TYR:CE2	1:D:615:ILE:HG12	1.29	1.56
1:D:142:TYR:CE2	1:D:615:ILE:CG1	1.77	1.56
1:C:135:MET:CG	1:D:159:PRO:HD2	1.18	1.52
1:C:458:ALA:N	1:C:594:GLN:HB3	1.30	1.46
1:C:458:ALA:HA	1:C:594:GLN:CG	1.51	1.40
1:A:141:LEU:HD23	1:A:215:HIS:CG	1.57	1.40
1:C:135:MET:CG	1:D:159:PRO:CD	1.97	1.38
1:C:458:ALA:CB	1:C:594:GLN:OE1	1.71	1.37
1:C:458:ALA:CA	1:C:594:GLN:HG2	1.55	1.35
1:C:135:MET:HG3	1:D:159:PRO:CD	1.52	1.34
1:D:117:THR:HG21	1:D:127:ASN:N	1.43	1.33
1:C:151:LYS:HZ2	1:D:224:GLN:NE2	1.28	1.32
1:A:141:LEU:CD2	1:A:215:HIS:CE1	2.16	1.29
1:C:458:ALA:N	1:C:594:GLN:CB	1.97	1.28
1:C:135:MET:SD	1:D:159:PRO:CD	2.16	1.27
1:C:135:MET:HB2	1:C:180:ASP:OD2	1.25	1.26
1:C:137:GLU:HG2	1:D:136:TYR:CE2	1.68	1.26
1:A:141:LEU:HD23	1:A:215:HIS:CD2	1.70	1.26
1:A:141:LEU:CD2	1:A:215:HIS:CG	2.19	1.23
1:A:136:TYR:OH	1:A:360:GLU:OE2	1.54	1.23
1:C:135:MET:HE1	1:D:158:ASN:ND2	1.52	1.23
1:A:143:GLY:HA3	1:A:146:GLU:CG	1.67	1.22
1:C:93:PRO:HD2	1:C:138:GLU:OE1	1.05	1.21
1:D:141:LEU:HD21	1:D:215:HIS:NE2	1.56	1.21
1:D:142:TYR:CD2	1:D:615:ILE:HG13	1.75	1.21
1:C:55:ASP:O	1:C:56:LYS:HD2	1.39	1.20
1:B:484:ALA:O	1:B:487:SER:O	1.60	1.19
1:C:135:MET:SD	1:D:159:PRO:HD2	1.79	1.19
1:C:497:ARG:CD	1:C:599:GLN:HE22	1.57	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:TYR:HD2	1:A:142:TYR:CE2	1.62	1.16
1:A:141:LEU:CD2	1:A:215:HIS:ND1	2.09	1.16
1:D:142:TYR:CE2	1:D:615:ILE:HG13	1.57	1.16
1:A:143:GLY:CA	1:A:146:GLU:HG2	1.74	1.15
1:D:340:GLN:O	1:D:341:THR:HG23	1.43	1.15
1:C:497:ARG:CG	1:C:599:GLN:HE22	1.60	1.14
1:C:589:TRP:O	1:C:592:LEU:CD2	1.94	1.14
1:A:141:LEU:HD21	1:A:215:HIS:NE2	1.62	1.13
1:A:141:LEU:CD2	1:A:215:HIS:CD2	2.30	1.13
1:A:16:GLY:O	1:A:17:ARG:NH1	1.82	1.12
1:C:529:GLU:O	1:C:532:GLY:O	1.64	1.11
1:B:310:ARG:HA	1:B:346:PHE:HZ	1.08	1.10
1:A:16:GLY:O	1:A:17:ARG:CZ	1.99	1.10
1:A:144:ALA:HB1	1:B:141:LEU:HD11	1.25	1.10
1:C:137:GLU:CG	1:D:136:TYR:CE2	2.35	1.10
1:C:497:ARG:CD	1:C:599:GLN:NE2	2.15	1.09
1:C:137:GLU:HG2	1:D:136:TYR:CD2	1.88	1.08
1:A:144:ALA:CB	1:B:141:LEU:HD11	1.83	1.07
1:C:93:PRO:CD	1:C:138:GLU:OE1	2.01	1.07
1:C:135:MET:HE1	1:D:158:ASN:HD22	1.05	1.07
1:A:141:LEU:HD21	1:A:215:HIS:ND1	1.66	1.07
1:B:534:LYS:O	1:B:534:LYS:NZ	1.86	1.07
1:A:139:TYR:CD2	1:A:142:TYR:CE2	2.42	1.06
1:D:141:LEU:HD21	1:D:215:HIS:CD2	1.90	1.06
1:C:458:ALA:CA	1:C:594:GLN:CG	2.22	1.06
1:D:136:TYR:OH	1:D:140:GLN:OE1	1.72	1.05
1:C:151:LYS:NZ	1:D:224:GLN:NE2	2.04	1.05
1:C:458:ALA:HB2	1:C:594:GLN:OE1	0.88	1.05
1:C:93:PRO:HD2	1:C:138:GLU:CD	1.82	1.04
1:C:497:ARG:HD2	1:C:599:GLN:OE1	1.57	1.04
1:A:139:TYR:CD2	1:A:142:TYR:HE2	1.73	1.03
1:B:529:GLU:OE1	1:B:535:GLU:CD	2.02	1.02
1:C:151:LYS:NZ	1:D:224:GLN:HE21	1.56	1.02
1:C:135:MET:CB	1:C:180:ASP:OD2	2.08	1.01
1:A:393:ILE:O	1:A:393:ILE:HG13	1.61	1.00
1:C:497:ARG:HD2	1:C:599:GLN:CD	1.87	0.99
1:C:589:TRP:O	1:C:592:LEU:HD21	1.61	0.99
1:B:310:ARG:HA	1:B:346:PHE:CZ	1.97	0.99
1:C:137:GLU:CD	1:D:136:TYR:CE2	2.41	0.99
1:C:136:TYR:CE1	1:C:218:LYS:HD2	1.98	0.99
1:D:117:THR:CG2	1:D:127:ASN:N	2.25	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LYS:O	1:B:356:ILE:O	1.80	0.98
1:C:497:ARG:HG2	1:C:599:GLN:HE22	1.25	0.97
1:C:135:MET:CE	1:D:158:ASN:HD22	1.77	0.96
1:C:151:LYS:NZ	1:D:221:MET:HA	1.81	0.96
1:C:458:ALA:HB2	1:C:594:GLN:CD	1.90	0.96
1:A:218:LYS:NZ	1:A:360:GLU:OE1	1.99	0.95
1:C:497:ARG:NE	1:C:599:GLN:NE2	2.15	0.95
1:C:9:ILE:HD11	1:C:194:CYS:SG	2.07	0.95
1:C:219:TYR:HA	1:C:222:LEU:HD13	1.45	0.94
1:D:142:TYR:CD2	1:D:615:ILE:CG1	2.43	0.94
1:D:117:THR:HG22	1:D:127:ASN:HB3	1.49	0.93
1:C:497:ARG:NE	1:C:599:GLN:HE22	1.65	0.93
1:C:137:GLU:OE1	1:D:140:GLN:OE1	1.87	0.93
1:A:393:ILE:O	1:A:393:ILE:CG1	2.15	0.92
1:C:144:ALA:O	1:C:146:GLU:N	2.01	0.92
1:B:30:ASN:O	1:B:33:GLU:O	1.88	0.92
1:A:310:ARG:HD3	1:A:341:THR:HG21	1.50	0.92
1:D:115:LYS:NZ	1:D:117:THR:HG23	1.85	0.91
1:C:497:ARG:CG	1:C:599:GLN:NE2	2.30	0.91
1:B:110:GLY:HA3	1:B:600:LYS:HE2	1.53	0.90
1:D:114:LYS:HG3	1:D:114:LYS:O	1.71	0.90
1:D:115:LYS:HE2	1:D:128:VAL:CG2	2.02	0.89
1:D:393:ILE:HG13	1:D:393:ILE:O	1.70	0.89
1:D:141:LEU:CD2	1:D:215:HIS:NE2	2.35	0.89
1:D:581:TRP:O	1:D:583:LYS:O	1.90	0.89
1:A:581:TRP:O	1:A:583:LYS:O	1.90	0.89
1:C:137:GLU:OE1	1:D:140:GLN:CD	2.16	0.89
1:D:393:ILE:O	1:D:393:ILE:CG1	2.20	0.89
1:C:151:LYS:HZ1	1:D:221:MET:HA	1.36	0.88
1:D:279:HIS:CD2	1:D:436:GLY:O	2.26	0.88
1:D:116:LEU:H	1:D:116:LEU:HD23	1.39	0.88
1:C:135:MET:HB2	1:C:180:ASP:CG	1.99	0.88
1:A:141:LEU:CD2	1:A:215:HIS:NE2	2.27	0.88
1:C:474:LEU:HD22	1:C:477:ARG:CZ	2.02	0.88
1:D:141:LEU:HD13	1:D:142:TYR:N	1.90	0.87
1:A:520:LEU:O	1:A:523:LEU:HD12	1.74	0.86
1:A:140:GLN:C	1:A:142:TYR:H	1.81	0.86
1:A:30:ASN:O	1:A:33:GLU:O	1.93	0.86
1:A:228:LEU:HD22	1:A:244:TYR:O	1.75	0.85
1:C:135:MET:HE1	1:D:158:ASN:CG	1.90	0.85
1:C:151:LYS:HG3	1:C:152:SER:H	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:TYR:O	1:A:143:GLY:C	2.17	0.85
1:C:279:HIS:CD2	1:C:436:GLY:O	2.28	0.85
1:D:142:TYR:HE2	1:D:615:ILE:CG1	1.39	0.85
1:A:519:ASN:OD1	1:A:520:LEU:C	2.21	0.84
1:D:581:TRP:C	1:D:583:LYS:O	2.19	0.84
1:A:581:TRP:C	1:A:583:LYS:O	2.20	0.84
1:C:497:ARG:HG2	1:C:599:GLN:NE2	1.91	0.84
1:C:153:LEU:HD11	1:D:221:MET:HG3	1.58	0.84
1:B:45:ARG:NH2	1:B:213:SER:O	2.09	0.84
1:C:30:ASN:O	1:C:33:GLU:O	1.96	0.84
1:C:136:TYR:CD1	1:C:218:LYS:HD2	2.13	0.83
1:D:256:LYS:HE2	1:D:260:LYS:HB2	1.60	0.83
1:C:135:MET:SD	1:D:159:PRO:HD3	2.16	0.83
1:D:115:LYS:HE2	1:D:128:VAL:HG23	1.59	0.83
1:A:40:GLU:OE2	1:A:48:HIS:HE1	1.61	0.83
1:A:310:ARG:HD3	1:A:341:THR:CG2	2.09	0.83
1:C:592:LEU:H	1:C:592:LEU:HD23	1.43	0.82
1:C:135:MET:CG	1:D:159:PRO:HD3	2.06	0.82
1:C:393:ILE:O	1:C:393:ILE:HG13	1.77	0.82
1:B:93:PRO:HG2	1:B:139:TYR:OH	1.80	0.82
1:D:233:ARG:NH2	1:D:354:SER:O	2.12	0.82
1:B:592:LEU:CD2	1:B:594:GLN:H	1.91	0.82
1:D:568:TRP:O	1:D:571:LYS:HE2	1.79	0.82
1:C:151:LYS:HZ1	1:D:221:MET:CA	1.92	0.82
1:B:359:CYS:HB2	1:B:362:ALA:O	1.79	0.82
1:A:144:ALA:CB	1:B:141:LEU:CD1	2.58	0.81
1:C:294:GLN:OE1	1:C:329:GLU:OE1	1.99	0.80
1:C:139:TYR:HB3	1:C:142:TYR:O	1.80	0.80
1:A:279:HIS:CD2	1:A:436:GLY:O	2.35	0.80
1:A:279:HIS:ND1	1:A:280:ASP:O	2.15	0.80
1:C:581:TRP:O	1:C:583:LYS:O	1.99	0.79
1:C:393:ILE:O	1:C:393:ILE:CG1	2.30	0.79
1:C:497:ARG:CD	1:C:599:GLN:CD	2.51	0.79
1:B:581:TRP:O	1:B:583:LYS:O	2.01	0.79
1:C:140:GLN:OE1	1:C:151:LYS:O	2.00	0.79
1:D:340:GLN:O	1:D:341:THR:CG2	2.30	0.79
1:C:581:TRP:C	1:C:583:LYS:O	2.25	0.78
1:B:588:ASN:O	1:B:590:ASP:O	2.01	0.78
1:D:30:ASN:O	1:D:33:GLU:O	2.00	0.78
1:C:9:ILE:CD1	1:C:194:CYS:SG	2.72	0.77
1:C:529:GLU:C	1:C:532:GLY:O	2.28	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ASN:OD1	1:A:520:LEU:O	2.03	0.76
1:C:612:ARG:O	1:C:612:ARG:HG2	1.86	0.76
1:B:460:HIS:CG	1:B:461:PRO:HD3	2.20	0.76
1:C:135:MET:HG3	1:D:159:PRO:HD2	0.76	0.76
1:A:143:GLY:HA3	1:A:146:GLU:HG2	0.81	0.76
1:C:135:MET:HG3	1:D:159:PRO:CG	2.16	0.76
1:C:589:TRP:O	1:C:592:LEU:HD22	1.86	0.76
1:D:273:LYS:HE3	1:D:444:GLU:HB2	1.69	0.75
1:B:398:THR:HG22	1:B:399:PRO:HD2	1.68	0.75
1:C:137:GLU:HG2	1:D:136:TYR:HE2	1.47	0.75
1:B:156:THR:HG23	1:B:156:THR:O	1.87	0.75
1:C:152:SER:O	1:C:157:GLY:N	2.20	0.75
1:D:115:LYS:HZ3	1:D:117:THR:HG23	1.50	0.75
1:A:517:VAL:HB	1:A:519:ASN:HD22	1.51	0.74
1:A:218:LYS:CE	1:A:360:GLU:OE1	2.35	0.74
1:C:136:TYR:CE1	1:C:218:LYS:CD	2.69	0.74
1:C:592:LEU:HD23	1:C:592:LEU:N	2.03	0.74
1:D:73:VAL:O	1:D:96:ARG:NH2	2.20	0.74
1:B:345:GLN:HG2	1:B:401:LYS:HD2	1.68	0.74
1:B:560:ASP:OD1	1:B:561:MET:N	2.20	0.74
1:D:372:LEU:O	1:D:375:MET:HG3	1.86	0.74
1:A:88:ALA:HA	1:A:91:MET:HE3	1.69	0.74
1:C:329:GLU:OE1	1:C:329:GLU:HA	1.87	0.73
1:A:140:GLN:C	1:A:142:TYR:N	2.46	0.73
1:B:346:PHE:HD2	1:B:399:PRO:HB3	1.54	0.73
1:C:273:LYS:HE3	1:C:444:GLU:HB2	1.69	0.73
1:B:581:TRP:C	1:B:583:LYS:O	2.32	0.73
1:B:70:LEU:HG	1:B:248:GLU:OE2	1.88	0.73
1:C:134:VAL:HG21	1:C:210:VAL:O	1.89	0.73
1:C:497:ARG:CD	1:C:599:GLN:OE1	2.34	0.72
1:C:140:GLN:HA	1:C:140:GLN:NE2	2.03	0.72
1:A:523:LEU:HD13	1:A:524:GLU:H	1.53	0.72
1:C:228:LEU:HD22	1:C:244:TYR:O	1.88	0.72
1:D:88:ALA:C	1:D:89:LYS:O	2.04	0.72
1:A:485:LEU:HD13	1:A:523:LEU:HD23	1.72	0.72
1:C:138:GLU:HG2	1:C:139:TYR:CD2	2.25	0.71
1:D:76:PHE:CD1	1:D:96:ARG:HG3	2.24	0.71
1:C:151:LYS:NZ	1:D:221:MET:CA	2.50	0.71
1:C:458:ALA:CB	1:C:594:GLN:CD	2.56	0.70
1:D:591:LYS:HE3	1:D:591:LYS:N	2.06	0.70
1:A:91:MET:HG3	1:A:96:ARG:HH12	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ALA:HB1	1:B:141:LEU:CD1	2.14	0.70
1:C:581:TRP:HD1	1:C:587:LEU:HD11	1.55	0.70
1:D:117:THR:HG22	1:D:127:ASN:CB	2.20	0.70
1:D:473:ARG:HD2	1:D:473:ARG:N	2.06	0.70
1:C:93:PRO:CD	1:C:138:GLU:CD	2.59	0.70
1:C:137:GLU:CD	1:D:136:TYR:CZ	2.69	0.70
1:B:555:PHE:HA	1:B:561:MET:SD	2.31	0.70
1:C:75:LYS:HD3	1:C:610:LYS:HA	1.73	0.70
1:C:458:ALA:CA	1:C:594:GLN:CB	2.61	0.70
1:C:566:GLU:OE2	1:C:591:LYS:NZ	2.25	0.70
1:C:581:TRP:CD1	1:C:587:LEU:HD11	2.27	0.69
1:C:318:HIS:CE1	1:C:320:THR:HG22	2.27	0.69
1:D:141:LEU:CD2	1:D:215:HIS:CD2	2.74	0.69
1:C:144:ALA:HB3	1:C:146:GLU:OE1	1.92	0.69
1:A:173:ASN:OD1	1:B:279:HIS:O	2.11	0.69
1:B:110:GLY:CA	1:B:600:LYS:HE2	2.22	0.69
1:C:359:CYS:HB2	1:C:362:ALA:O	1.93	0.69
1:D:116:LEU:HD23	1:D:116:LEU:N	2.06	0.69
1:A:139:TYR:CE2	1:A:142:TYR:HE2	2.10	0.69
1:D:115:LYS:HZ1	1:D:117:THR:HG23	1.55	0.69
1:B:460:HIS:CD2	1:B:461:PRO:HD3	2.28	0.69
1:D:492:GLU:C	1:D:493:ALA:O	2.18	0.68
1:B:346:PHE:HD2	1:B:399:PRO:CB	2.05	0.68
1:A:142:TYR:O	1:A:144:ALA:N	2.26	0.68
1:C:235:GLU:H	1:C:244:TYR:HE1	1.42	0.68
1:A:318:HIS:O	1:A:329:GLU:OE1	2.11	0.67
1:B:505:GLY:HA3	1:B:600:LYS:HZ3	1.60	0.67
1:D:141:LEU:HD13	1:D:141:LEU:C	2.19	0.67
1:B:589:TRP:HA	1:B:591:LYS:HG3	1.76	0.67
1:C:244:TYR:N	1:C:244:TYR:CD2	2.61	0.67
1:A:340:GLN:HG3	1:A:340:GLN:O	1.93	0.67
1:A:445:GLU:OE1	1:A:445:GLU:N	2.27	0.67
1:B:91:MET:HE3	1:B:96:ARG:HE	1.60	0.67
1:B:359:CYS:CB	1:B:362:ALA:O	2.43	0.67
1:A:122:ASP:O	1:A:123:LEU:HG	1.95	0.66
1:B:505:GLY:HA3	1:B:600:LYS:NZ	2.10	0.66
1:B:6:ARG:CZ	1:B:304:ASP:O	2.44	0.66
1:C:229:SER:HB2	1:C:243:GLY:O	1.95	0.66
1:D:53:ASP:CG	1:D:54:ALA:O	2.38	0.66
1:C:497:ARG:HE	1:C:599:GLN:NE2	1.94	0.66
1:D:110:GLY:O	1:D:600:LYS:HE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:LYS:CE	1:D:260:LYS:HB2	2.26	0.65
1:D:142:TYR:HE2	1:D:615:ILE:HG12	0.57	0.65
1:A:523:LEU:HD13	1:A:524:GLU:N	2.11	0.65
1:C:256:LYS:HD3	1:C:257:PRO:HD2	1.77	0.65
1:D:141:LEU:O	1:D:141:LEU:HD22	1.96	0.65
1:D:228:LEU:HD22	1:D:244:TYR:O	1.95	0.65
1:B:135:MET:HE1	1:B:182:MET:O	1.97	0.65
1:B:592:LEU:HD22	1:B:594:GLN:H	1.59	0.65
1:C:244:TYR:CE2	1:C:321:GLY:C	2.75	0.65
1:B:228:LEU:HD22	1:B:244:TYR:O	1.97	0.65
1:C:474:LEU:HD22	1:C:477:ARG:NH2	2.11	0.65
1:C:497:ARG:HE	1:C:599:GLN:HE22	1.45	0.65
1:D:119:LYS:HE2	1:D:173:ASN:CG	2.21	0.65
1:C:137:GLU:CG	1:D:136:TYR:CD2	2.70	0.64
1:C:530:PHE:CE1	1:C:540:LEU:HD22	2.31	0.64
1:D:53:ASP:C	1:D:54:ALA:O	2.30	0.64
1:A:93:PRO:HA	1:A:96:ARG:HD2	1.79	0.64
1:A:425:ARG:HB2	1:A:445:GLU:CD	2.21	0.64
1:B:501:THR:HG23	1:B:600:LYS:HE3	1.80	0.64
1:C:54:ALA:O	1:C:55:ASP:C	2.40	0.64
1:C:515:MET:SD	1:C:516:ILE:N	2.69	0.64
1:C:134:VAL:CG2	1:C:210:VAL:O	2.46	0.64
1:D:516:ILE:HD13	1:D:574:ALA:HB1	1.78	0.64
1:B:600:LYS:HG3	1:B:601:ILE:H	1.63	0.63
1:D:114:LYS:O	1:D:114:LYS:CG	2.46	0.63
1:B:529:GLU:OE1	1:B:535:GLU:OE2	2.15	0.63
1:C:16:GLY:O	1:C:17:ARG:HD3	1.98	0.63
1:C:533:GLY:O	1:C:534:LYS:HB2	1.97	0.63
1:A:120:SER:OG	1:A:122:ASP:CG	2.42	0.63
1:A:218:LYS:HE2	1:A:360:GLU:OE1	1.97	0.63
1:B:353:LYS:HD3	1:B:353:LYS:N	2.13	0.63
1:C:148:ALA:O	1:C:151:LYS:HD3	1.98	0.63
1:D:141:LEU:CD2	1:D:215:HIS:CE1	2.82	0.63
1:C:539:GLN:C	1:C:540:LEU:HD12	2.23	0.62
1:A:116:LEU:HD13	1:A:171:GLY:O	1.99	0.62
1:A:375:MET:HG2	1:A:445:GLU:OE2	1.99	0.62
1:C:141:LEU:O	1:C:143:GLY:O	2.17	0.62
1:A:120:SER:OG	1:A:122:ASP:OD1	2.18	0.62
1:A:234:CYS:HA	1:A:244:TYR:CE1	2.35	0.61
1:D:101:CYS:HA	1:D:104:GLU:HG2	1.82	0.61
1:C:136:TYR:CE1	1:C:218:LYS:HG3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:THR:HB	1:D:114:LYS:HG2	1.83	0.61
1:C:153:LEU:HG	1:D:221:MET:SD	2.41	0.61
1:D:143:GLY:O	1:D:144:ALA:C	2.40	0.61
1:D:115:LYS:HE2	1:D:128:VAL:HG21	1.81	0.61
1:C:310:ARG:NH1	1:C:341:THR:O	2.34	0.61
1:B:70:LEU:N	1:B:248:GLU:OE1	2.34	0.60
1:C:17:ARG:NE	1:C:101:CYS:SG	2.74	0.60
1:C:592:LEU:CD2	1:C:592:LEU:H	2.12	0.60
1:C:136:TYR:CE2	1:C:218:LYS:NZ	2.62	0.60
1:D:76:PHE:CD1	1:D:96:ARG:CG	2.83	0.60
1:D:142:TYR:CZ	1:D:615:ILE:CG1	2.70	0.60
1:B:103:TYR:OH	1:B:507:GLU:OE2	2.18	0.60
1:C:151:LYS:HG3	1:C:152:SER:N	2.16	0.60
1:D:353:LYS:HD2	1:D:358:HIS:ND1	2.16	0.60
1:D:375:MET:O	1:D:378:LYS:HD2	2.02	0.60
1:C:151:LYS:HZ3	1:D:224:GLN:HE21	1.49	0.60
1:A:63:TYR:HE2	1:A:230:SER:O	1.84	0.60
1:B:529:GLU:HB3	1:B:535:GLU:HG3	1.83	0.60
1:B:11:ILE:HD11	1:B:372:LEU:CD1	2.31	0.59
1:C:458:ALA:CA	1:C:594:GLN:HB3	2.26	0.59
1:C:566:GLU:CD	1:C:591:LYS:NZ	2.61	0.59
1:D:258:LEU:HG	1:D:262:LYS:HE3	1.85	0.59
1:C:606:TYR:HB3	1:C:607:PRO:HD2	1.85	0.59
1:A:139:TYR:O	1:A:142:TYR:CD2	2.54	0.59
1:B:35:THR:O	1:B:384:LEU:HD21	2.03	0.59
1:C:477:ARG:HH22	1:C:513:LEU:HB3	1.68	0.59
1:B:534:LYS:O	1:B:534:LYS:CG	2.50	0.59
1:C:468:ALA:CB	1:C:474:LEU:HD21	2.33	0.59
1:B:592:LEU:CD2	1:B:594:GLN:N	2.66	0.59
1:C:222:LEU:HG	1:C:228:LEU:HG	1.85	0.59
1:C:591:LYS:O	1:C:593:TYR:CD2	2.56	0.59
1:D:430:SER:HB3	1:D:432:PHE:HE1	1.68	0.59
1:B:155:LEU:O	1:B:156:THR:HG22	2.03	0.58
1:C:135:MET:CG	1:C:180:ASP:OD2	2.51	0.58
1:C:9:ILE:HG13	1:C:272:ILE:HB	1.85	0.58
1:C:90:LEU:HB3	1:C:155:LEU:HG	1.86	0.58
1:C:592:LEU:HG	1:C:592:LEU:O	2.03	0.58
1:A:134:VAL:HG11	1:A:162:ILE:HD13	1.86	0.58
1:B:580:LEU:O	1:B:583:LYS:O	2.22	0.58
1:C:477:ARG:NH2	1:C:513:LEU:HB3	2.19	0.58
1:A:244:TYR:CD2	1:A:320:THR:O	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:LYS:HD3	1:B:534:LYS:N	2.17	0.58
1:C:474:LEU:HD22	1:C:477:ARG:NE	2.17	0.58
1:D:95:GLU:CB	1:D:162:ILE:HD13	2.34	0.58
1:A:91:MET:SD	1:A:96:ARG:NH1	2.77	0.58
1:C:138:GLU:OE2	1:C:139:TYR:CE2	2.57	0.58
1:C:137:GLU:CG	1:D:136:TYR:HE2	2.09	0.57
1:C:497:ARG:CG	1:C:599:GLN:CD	2.75	0.57
1:D:87:ASP:C	1:D:89:LYS:O	2.47	0.57
1:C:55:ASP:O	1:C:56:LYS:CD	2.33	0.57
1:A:160:SER:O	1:A:164:ASN:CG	2.48	0.57
1:C:136:TYR:CE1	1:C:218:LYS:CG	2.88	0.57
1:C:141:LEU:O	1:C:141:LEU:HD12	2.05	0.57
1:C:148:ALA:HB3	1:C:151:LYS:HD2	1.86	0.57
1:C:136:TYR:HE1	1:C:218:LYS:HG3	1.68	0.57
1:D:17:ARG:HB3	1:D:70:LEU:HD11	1.87	0.57
1:D:115:LYS:CE	1:D:128:VAL:CG2	2.82	0.57
1:A:91:MET:CG	1:A:96:ARG:HH12	2.17	0.57
1:A:555:PHE:CD2	1:A:585:LEU:HD13	2.39	0.57
1:B:589:TRP:CA	1:B:591:LYS:HG3	2.35	0.56
1:C:494:ASP:OD1	1:C:494:ASP:O	2.23	0.56
1:C:242:ASP:O	1:C:244:TYR:CE2	2.58	0.56
1:C:592:LEU:HD12	1:C:594:GLN:HE22	1.70	0.56
1:A:50:LEU:HD23	1:A:50:LEU:O	2.05	0.56
1:A:139:TYR:CD2	1:A:142:TYR:CD2	2.91	0.56
1:C:70:LEU:HG	1:C:248:GLU:OE1	2.04	0.56
1:C:497:ARG:HG3	1:C:599:GLN:OE1	2.05	0.56
1:C:135:MET:HG2	1:D:159:PRO:CD	2.24	0.56
1:A:93:PRO:HA	1:A:96:ARG:CD	2.35	0.56
1:B:344:LYS:O	1:B:345:GLN:C	2.48	0.56
1:B:529:GLU:OE1	1:B:535:GLU:OE1	2.24	0.56
1:A:135:MET:HE2	1:A:360:GLU:HG2	1.87	0.56
1:A:318:HIS:CD2	1:A:320:THR:HG22	2.41	0.56
1:A:318:HIS:HD2	1:A:320:THR:HG22	1.71	0.56
1:B:534:LYS:O	1:B:534:LYS:HG2	2.05	0.56
1:D:116:LEU:H	1:D:116:LEU:CD2	2.01	0.56
1:D:141:LEU:C	1:D:141:LEU:HD22	2.30	0.56
1:A:17:ARG:NE	1:A:17:ARG:HA	2.21	0.55
1:B:310:ARG:HG3	1:B:346:PHE:CZ	2.40	0.55
1:D:142:TYR:CZ	1:D:615:ILE:HG12	2.20	0.55
1:B:93:PRO:CG	1:B:139:TYR:OH	2.54	0.55
1:D:173:ASN:CG	1:D:173:ASN:O	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:ALA:CA	1:C:594:GLN:CD	2.76	0.55
1:D:145:GLU:OE1	1:D:146:GLU:CD	2.50	0.55
1:D:217:ASN:OD1	1:D:218:LYS:N	2.40	0.55
1:A:244:TYR:CG	1:A:320:THR:O	2.60	0.55
1:A:136:TYR:OH	1:A:360:GLU:CD	2.41	0.55
1:B:580:LEU:HD12	1:B:583:LYS:HE2	1.87	0.55
1:A:135:MET:HB3	1:A:136:TYR:CE2	2.41	0.54
1:A:484:ALA:HB1	1:A:489:ARG:CZ	2.37	0.54
1:C:497:ARG:CG	1:C:599:GLN:OE1	2.55	0.54
1:B:351:SER:OG	1:B:353:LYS:HB2	2.07	0.54
1:D:14:ILE:HG22	1:D:253:VAL:HG12	1.90	0.54
1:A:330:ILE:CG2	1:A:400:PHE:CZ	2.91	0.54
1:D:432:PHE:CD2	1:D:438:ASN:HB3	2.42	0.54
1:B:371:VAL:HG11	1:B:443:ILE:HD12	1.89	0.54
1:C:94:GLN:OE1	1:C:162:ILE:HD11	2.07	0.54
1:C:139:TYR:HD1	1:C:142:TYR:HB2	1.73	0.54
1:C:592:LEU:HD12	1:C:594:GLN:NE2	2.21	0.54
1:B:592:LEU:HD23	1:B:594:GLN:H	1.71	0.54
1:B:279:HIS:CD2	1:B:436:GLY:O	2.61	0.54
1:A:14:ILE:HG22	1:A:253:VAL:HG12	1.90	0.54
1:C:16:GLY:C	1:C:17:ARG:HD3	2.32	0.54
1:B:134:VAL:HG11	1:B:162:ILE:HD13	1.90	0.53
1:C:489:ARG:NH1	1:C:490:TYR:OH	2.41	0.53
1:B:414:ILE:HG12	1:B:422:GLU:N	2.24	0.53
1:C:144:ALA:C	1:C:146:GLU:N	2.60	0.53
1:D:115:LYS:NZ	1:D:117:THR:CG2	2.67	0.53
1:A:63:TYR:CE2	1:A:230:SER:O	2.61	0.53
1:A:137:GLU:OE2	1:A:158:ASN:N	2.42	0.53
1:B:14:ILE:HG22	1:B:253:VAL:HG12	1.90	0.53
1:B:136:TYR:OH	1:B:139:TYR:N	2.41	0.53
1:A:66:TRP:HE3	1:A:67:GLY:N	2.06	0.53
1:C:51:TYR:HA	1:C:61:LYS:HE3	1.91	0.53
1:C:140:GLN:NE2	1:C:140:GLN:CA	2.72	0.53
1:C:152:SER:O	1:C:157:GLY:CA	2.57	0.53
1:D:591:LYS:HE3	1:D:591:LYS:H	1.71	0.53
1:C:234:CYS:HA	1:C:244:TYR:CD1	2.43	0.53
1:A:145:GLU:O	1:A:145:GLU:CD	2.52	0.53
1:A:88:ALA:O	1:A:91:MET:HG2	2.09	0.53
1:C:243:GLY:C	1:C:244:TYR:CD2	2.86	0.53
1:A:48:HIS:C	1:A:48:HIS:CD2	2.87	0.52
1:C:530:PHE:CZ	1:C:540:LEU:HD22	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:HIS:O	1:A:359:CYS:C	2.50	0.52
1:C:590:ASP:C	1:C:592:LEU:HD23	2.34	0.52
1:A:330:ILE:HG23	1:A:400:PHE:CZ	2.44	0.52
1:B:179:LEU:HD21	1:B:189:ALA:HB2	1.90	0.52
1:C:458:ALA:N	1:C:594:GLN:HB2	2.11	0.52
1:A:47:ASP:O	1:A:50:LEU:HD22	2.09	0.52
1:C:111:TYR:O	1:C:111:TYR:CG	2.62	0.52
1:A:244:TYR:CE1	1:A:321:GLY:HA3	2.44	0.52
1:C:153:LEU:HD21	1:D:221:MET:HE3	1.92	0.52
1:C:75:LYS:HD3	1:C:610:LYS:CA	2.40	0.52
1:D:95:GLU:CA	1:D:162:ILE:HD13	2.40	0.52
1:D:116:LEU:HD12	1:D:203:GLU:OE1	2.09	0.52
1:D:593:TYR:N	1:D:593:TYR:CD2	2.77	0.52
1:B:368:LEU:HD13	1:B:443:ILE:HD11	1.91	0.52
1:C:6:ARG:HG3	1:C:7:GLU:OE2	2.10	0.51
1:D:139:TYR:CD1	1:D:139:TYR:C	2.88	0.51
1:A:182:MET:SD	1:B:158:ASN:ND2	2.81	0.51
1:C:458:ALA:HA	1:C:594:GLN:HG2	0.64	0.51
1:C:566:GLU:OE1	1:C:591:LYS:NZ	2.42	0.51
1:D:234:CYS:SG	1:D:245:VAL:HG12	2.51	0.51
1:D:430:SER:HB3	1:D:432:PHE:CE1	2.46	0.51
1:D:492:GLU:HG3	1:D:520:LEU:CD2	2.40	0.51
1:B:592:LEU:HD21	1:B:594:GLN:HA	1.92	0.51
1:C:359:CYS:CB	1:C:362:ALA:O	2.57	0.51
1:C:14:ILE:HG22	1:C:253:VAL:HG12	1.91	0.51
1:B:6:ARG:NH2	1:B:304:ASP:O	2.43	0.51
1:C:138:GLU:OE2	1:C:139:TYR:HE2	1.92	0.51
1:B:255:LEU:O	1:B:256:LYS:HG3	2.09	0.51
1:C:90:LEU:O	1:C:155:LEU:HD12	2.10	0.51
1:D:87:ASP:HA	1:D:90:LEU:HD23	1.92	0.51
1:D:491:ARG:O	1:D:493:ALA:O	2.29	0.51
1:B:234:CYS:SG	1:B:245:VAL:HG12	2.51	0.51
1:C:244:TYR:CZ	1:C:321:GLY:HA3	2.45	0.51
1:B:46:TRP:NE1	1:B:214:VAL:O	2.32	0.51
1:C:414:ILE:HB	1:C:423:LEU:HD12	1.92	0.51
1:C:580:LEU:HD12	1:C:583:LYS:HE2	1.92	0.51
1:C:55:ASP:N	1:C:55:ASP:OD1	2.43	0.51
1:C:203:GLU:O	1:C:256:LYS:HD3	2.11	0.51
1:D:551:THR:HG21	1:D:583:LYS:NZ	2.25	0.51
1:D:96:ARG:HE	1:D:97:LEU:HG	1.76	0.50
1:B:395:PHE:CD1	1:B:395:PHE:C	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ARG:NH2	1:B:445:GLU:HG3	2.27	0.50
1:B:501:THR:HG23	1:B:600:LYS:CE	2.41	0.50
1:C:135:MET:HG3	1:C:180:ASP:OD2	2.11	0.50
1:A:17:ARG:CZ	1:A:23:ASN:HA	2.41	0.50
1:A:158:ASN:OD1	1:A:159:PRO:HD2	2.10	0.50
1:B:438:ASN:OD1	1:B:438:ASN:N	2.44	0.50
1:B:589:TRP:C	1:B:591:LYS:HG3	2.35	0.50
1:A:393:ILE:O	1:A:393:ILE:CD1	2.58	0.50
1:C:139:TYR:CD1	1:C:142:TYR:HB2	2.46	0.50
1:A:544:GLN:HB3	1:A:547:GLN:HB2	1.94	0.50
1:C:93:PRO:CD	1:C:138:GLU:OE2	2.60	0.50
1:C:242:ASP:O	1:C:244:TYR:HE2	1.94	0.50
1:A:140:GLN:O	1:A:142:TYR:N	2.45	0.50
1:A:555:PHE:HD2	1:A:585:LEU:HD13	1.76	0.50
1:D:103:TYR:OH	1:D:507:GLU:HG3	2.11	0.50
1:D:536:SER:HA	1:D:540:LEU:HD21	1.94	0.50
1:A:66:TRP:HE3	1:A:67:GLY:CA	2.25	0.50
1:D:141:LEU:HD23	1:D:215:HIS:CE1	2.47	0.50
1:A:555:PHE:O	1:A:561:MET:SD	2.70	0.49
1:B:497:ARG:HG2	1:B:599:GLN:O	2.12	0.49
1:D:599:GLN:OE1	1:D:600:LYS:O	2.29	0.49
1:A:135:MET:HB3	1:A:136:TYR:CD2	2.47	0.49
1:A:515:MET:HG3	1:A:526:LYS:CD	2.42	0.49
1:B:416:GLU:O	1:B:417:ASN:HB2	2.12	0.49
1:D:573:LYS:HG3	1:D:576:LYS:HD3	1.94	0.49
1:A:310:ARG:O	1:A:345:GLN:HG2	2.12	0.49
1:A:158:ASN:ND2	1:B:182:MET:SD	2.82	0.49
1:A:40:GLU:CD	1:A:48:HIS:HE1	2.19	0.49
1:A:497:ARG:HG2	1:A:599:GLN:O	2.11	0.49
1:B:93:PRO:HG2	1:B:139:TYR:CZ	2.48	0.49
1:B:137:GLU:HB2	1:B:138:GLU:HG3	1.95	0.49
1:C:222:LEU:HG	1:C:228:LEU:CG	2.43	0.49
1:C:566:GLU:CD	1:C:591:LYS:HZ2	2.19	0.49
1:D:95:GLU:HA	1:D:162:ILE:HD13	1.95	0.49
1:D:256:LYS:HD2	1:D:257:PRO:HD2	1.95	0.49
1:A:489:ARG:HH22	1:A:604:PRO:HD3	1.77	0.49
1:C:348:ALA:HB1	1:C:403:GLN:CD	2.38	0.49
1:D:116:LEU:N	1:D:116:LEU:CD2	2.72	0.49
1:D:393:ILE:O	1:D:393:ILE:CD1	2.60	0.49
1:A:414:ILE:O	1:A:414:ILE:HG22	2.13	0.49
1:B:535:GLU:HB3	1:B:537:ILE:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:HIS:HE1	1:C:602:SER:HB2	1.78	0.49
1:B:534:LYS:O	1:B:534:LYS:CD	2.60	0.48
1:B:334:THR:HG23	1:B:398:THR:HG23	1.95	0.48
1:D:588:ASN:CG	1:D:591:LYS:NZ	2.72	0.48
1:C:445:GLU:OE1	1:C:445:GLU:HA	2.13	0.48
1:A:17:ARG:CZ	1:A:17:ARG:HA	2.43	0.48
1:D:95:GLU:HA	1:D:162:ILE:CD1	2.43	0.48
1:D:87:ASP:O	1:D:89:LYS:O	2.31	0.48
1:C:509:MET:HE3	1:C:606:TYR:CZ	2.47	0.48
1:D:474:LEU:HD11	1:D:511:GLU:HB3	1.94	0.48
1:B:509:MET:HE1	1:B:606:TYR:CD2	2.49	0.48
1:C:152:SER:C	1:C:157:GLY:H	2.19	0.48
1:C:177:MET:HE1	1:D:192:LEU:HD11	1.95	0.48
1:C:212:VAL:HA	1:C:248:GLU:HG2	1.95	0.48
1:A:310:ARG:CD	1:A:341:THR:HG21	2.32	0.48
1:A:476:LYS:HA	1:A:479:LYS:HB2	1.96	0.48
1:A:509:MET:HE1	1:A:606:TYR:CD2	2.48	0.48
1:B:368:LEU:CD1	1:B:443:ILE:HD11	2.44	0.48
1:B:539:GLN:HB3	1:B:541:TYR:CE1	2.49	0.48
1:C:112:THR:HG23	1:C:113:ARG:N	2.29	0.48
1:D:445:GLU:OE1	1:D:445:GLU:HA	2.14	0.48
1:D:497:ARG:HG3	1:D:599:GLN:O	2.14	0.48
1:D:75:LYS:NZ	1:D:609:ALA:O	2.38	0.48
1:A:66:TRP:CE3	1:A:67:GLY:N	2.82	0.47
1:A:561:MET:SD	1:A:561:MET:C	2.97	0.47
1:B:11:ILE:HD11	1:B:372:LEU:HD11	1.94	0.47
1:B:38:ILE:HD11	1:B:357:GLY:N	2.29	0.47
1:D:529:GLU:OE1	1:D:530:PHE:N	2.46	0.47
1:A:137:GLU:OE2	1:A:157:GLY:HA2	2.13	0.47
1:B:91:MET:HE3	1:B:96:ARG:NE	2.26	0.47
1:A:116:LEU:HB3	1:A:125:GLY:HA2	1.96	0.47
1:A:474:LEU:HD11	1:A:511:GLU:HB3	1.96	0.47
1:A:489:ARG:NH2	1:A:604:PRO:HD3	2.30	0.47
1:B:134:VAL:HG21	1:B:162:ILE:HD13	1.97	0.47
1:C:568:TRP:CD2	1:C:577:VAL:HG21	2.49	0.47
1:C:107:GLU:OE1	1:C:506:ARG:NH1	2.48	0.47
1:C:137:GLU:CD	1:D:136:TYR:HH	2.22	0.47
1:A:143:GLY:O	1:A:146:GLU:O	2.31	0.47
1:C:229:SER:CB	1:C:243:GLY:O	2.61	0.47
1:C:458:ALA:HA	1:C:594:GLN:CD	2.31	0.47
1:B:99:LEU:HD11	1:B:165:ARG:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:GLU:OE1	1:D:145:GLU:C	2.58	0.47
1:D:183:CYS:HB2	1:D:433:GLY:HA2	1.97	0.47
1:C:219:TYR:O	1:C:222:LEU:HD22	2.15	0.47
1:C:256:LYS:NZ	1:C:260:LYS:HD2	2.30	0.47
1:A:144:ALA:HB2	1:B:141:LEU:CD1	2.41	0.47
1:C:72:ASP:HB2	1:C:75:LYS:HE3	1.96	0.47
1:C:107:GLU:OE2	1:C:606:TYR:CE2	2.68	0.47
1:B:262:LYS:HE3	1:B:446:TYR:CZ	2.50	0.47
1:B:294:GLN:NE2	1:B:432:PHE:CZ	2.83	0.47
1:A:229:SER:HB2	1:A:243:GLY:O	2.15	0.47
1:B:88:ALA:O	1:B:91:MET:HE2	2.14	0.47
1:D:551:THR:HG21	1:D:583:LYS:HZ2	1.79	0.47
1:C:151:LYS:HZ1	1:D:221:MET:N	2.13	0.46
1:B:179:LEU:HD11	1:B:185:SER:O	2.16	0.46
1:C:606:TYR:HB3	1:C:607:PRO:CD	2.45	0.46
1:D:212:VAL:HA	1:D:248:GLU:HG2	1.97	0.46
1:C:244:TYR:CG	1:C:320:THR:O	2.69	0.46
1:D:127:ASN:N	1:D:173:ASN:H	2.13	0.46
1:B:248:GLU:HG3	1:B:249:GLY:N	2.28	0.46
1:B:445:GLU:OE1	1:B:446:TYR:O	2.34	0.46
1:D:515:MET:HG3	1:D:526:LYS:NZ	2.30	0.46
1:A:122:ASP:O	1:A:123:LEU:CG	2.63	0.46
1:B:414:ILE:HD12	1:B:414:ILE:H	1.79	0.46
1:B:587:LEU:HD11	1:B:589:TRP:CD2	2.51	0.46
1:C:234:CYS:HA	1:C:244:TYR:CE1	2.51	0.46
1:D:569:LEU:HD13	1:D:592:LEU:HA	1.96	0.46
1:C:423:LEU:HD23	1:C:424:PRO:HD2	1.98	0.46
1:D:515:MET:SD	1:D:517:VAL:HG13	2.56	0.46
1:A:587:LEU:HD11	1:A:589:TRP:CD2	2.50	0.46
1:B:539:GLN:HB3	1:B:541:TYR:CZ	2.51	0.46
1:D:36:ASP:CG	1:D:233:ARG:NH1	2.73	0.46
1:D:88:ALA:O	1:D:91:MET:HE2	2.16	0.46
1:A:520:LEU:O	1:A:523:LEU:CD1	2.57	0.46
1:B:592:LEU:CD2	1:B:592:LEU:C	2.89	0.45
1:C:135:MET:HB3	1:C:135:MET:HE2	1.67	0.45
1:C:137:GLU:OE1	1:D:140:GLN:CG	2.63	0.45
1:D:555:PHE:CZ	1:D:586:PRO:O	2.69	0.45
1:D:587:LEU:HD11	1:D:589:TRP:CD2	2.52	0.45
1:B:378:LYS:HG2	1:B:425:ARG:NH1	2.31	0.45
1:B:390:ASN:O	1:B:393:ILE:HG23	2.15	0.45
1:C:151:LYS:HZ3	1:D:221:MET:CB	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:MET:CE	1:C:606:TYR:CE2	2.99	0.45
1:D:377:HIS:O	1:D:379:GLN:HG3	2.16	0.45
1:C:348:ALA:HB1	1:C:403:GLN:CG	2.46	0.45
1:D:38:ILE:HG12	1:D:233:ARG:NH1	2.32	0.45
1:B:432:PHE:HD1	1:B:438:ASN:HB3	1.82	0.45
1:C:153:LEU:CD1	1:D:221:MET:HG3	2.37	0.45
1:A:423:LEU:HD23	1:A:424:PRO:HD2	1.99	0.45
1:B:423:LEU:HD23	1:B:424:PRO:HD2	1.98	0.45
1:C:464:ILE:HD11	1:C:517:VAL:HG21	1.98	0.45
1:D:92:ASP:OD1	1:D:92:ASP:N	2.49	0.45
1:C:151:LYS:HZ3	1:D:221:MET:HA	1.77	0.45
1:D:218:LYS:HG2	1:D:221:MET:HE2	1.99	0.45
1:A:183:CYS:HB2	1:A:433:GLY:HA2	1.97	0.45
1:B:152:SER:O	1:B:157:GLY:HA3	2.16	0.45
1:C:137:GLU:OE1	1:D:136:TYR:CE2	2.69	0.45
1:D:493:ALA:O	1:D:494:ASP:OD1	2.35	0.45
1:C:17:ARG:NH2	1:C:104:GLU:OE1	2.50	0.45
1:C:135:MET:HG2	1:C:135:MET:O	2.16	0.45
1:A:116:LEU:CD1	1:A:171:GLY:O	2.65	0.44
1:C:580:LEU:O	1:C:583:LYS:O	2.35	0.44
1:D:101:CYS:HA	1:D:104:GLU:CG	2.47	0.44
1:B:35:THR:O	1:B:384:LEU:CD2	2.65	0.44
1:B:297:VAL:HG21	1:B:438:ASN:HB2	1.97	0.44
1:C:571:LYS:H	1:C:571:LYS:HG2	1.69	0.44
1:D:516:ILE:CD1	1:D:574:ALA:HB1	2.44	0.44
1:C:135:MET:HG2	1:D:159:PRO:HD3	1.95	0.44
1:D:423:LEU:HD23	1:D:424:PRO:HD2	1.98	0.44
1:A:13:GLY:HA3	1:A:109:ALA:HB2	1.99	0.44
1:A:515:MET:SD	1:A:517:VAL:HG13	2.57	0.44
1:B:91:MET:CE	1:B:96:ARG:HE	2.27	0.44
1:A:12:ILE:HD13	1:A:256:LYS:HG2	1.99	0.44
1:A:69:PHE:HA	1:A:248:GLU:OE2	2.18	0.44
1:A:112:THR:O	1:A:115:LYS:HB2	2.18	0.44
1:A:460:HIS:ND1	1:A:461:PRO:O	2.51	0.44
1:C:380:LEU:HD13	1:C:403:GLN:HE22	1.83	0.44
1:D:13:GLY:HA3	1:D:109:ALA:HB2	2.00	0.44
1:A:244:TYR:CE2	1:A:320:THR:O	2.71	0.44
1:C:93:PRO:HG2	1:C:138:GLU:CD	2.43	0.44
1:B:93:PRO:HD2	1:B:139:TYR:CE1	2.52	0.43
1:D:106:MET:HG2	1:D:111:TYR:O	2.17	0.43
1:B:58:LYS:C	1:B:59:GLU:O	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:ALA:CB	1:C:474:LEU:CD2	2.96	0.43
1:D:53:ASP:CB	1:D:54:ALA:O	2.67	0.43
1:D:460:HIS:HB3	1:D:461:PRO:HD3	1.99	0.43
1:B:103:TYR:OH	1:B:507:GLU:CD	2.61	0.43
1:B:535:GLU:HB3	1:B:537:ILE:HD11	2.00	0.43
1:C:13:GLY:HA3	1:C:109:ALA:HB2	1.99	0.43
1:D:117:THR:HG21	1:D:127:ASN:CA	2.38	0.43
1:D:138:GLU:HB3	1:D:214:VAL:HG21	2.00	0.43
1:B:73:VAL:O	1:B:96:ARG:NH1	2.51	0.43
1:B:260:LYS:CE	1:B:264:ASP:HB2	2.48	0.43
1:C:8:ASP:N	1:C:8:ASP:OD1	2.51	0.43
1:A:12:ILE:HD13	1:A:256:LYS:CG	2.49	0.43
1:B:13:GLY:HA3	1:B:109:ALA:HB2	1.99	0.43
1:B:589:TRP:O	1:B:591:LYS:HG3	2.19	0.43
1:C:468:ALA:HB2	1:C:474:LEU:HD21	1.99	0.43
1:C:539:GLN:HB2	1:C:540:LEU:HD12	2.01	0.43
1:D:95:GLU:CA	1:D:162:ILE:CD1	2.97	0.43
1:B:94:GLN:NE2	1:B:134:VAL:HG12	2.34	0.43
1:C:468:ALA:HB3	1:C:474:LEU:HD21	2.00	0.43
1:C:515:MET:HG2	1:C:526:LYS:HD3	2.01	0.43
1:B:589:TRP:O	1:B:590:ASP:C	2.54	0.43
1:C:587:LEU:N	1:C:587:LEU:HD12	2.34	0.43
1:D:115:LYS:HD2	1:D:128:VAL:HG21	2.01	0.43
1:A:415:ASN:ND2	1:C:387:ARG:O	2.51	0.43
1:B:260:LYS:HE3	1:B:264:ASP:HB2	2.00	0.43
1:B:318:HIS:CE1	1:B:432:PHE:O	2.72	0.43
1:B:487:SER:O	1:B:487:SER:OG	2.34	0.43
1:C:127:ASN:OD1	1:C:203:GLU:HG3	2.18	0.43
1:C:585:LEU:HG	1:C:587:LEU:HG	2.00	0.43
1:D:476:LYS:HG2	1:D:479:LYS:HE3	2.01	0.42
1:D:615:ILE:N	1:D:615:ILE:HD13	2.33	0.42
1:D:38:ILE:HD11	1:D:357:GLY:N	2.34	0.42
1:A:264:ASP:O	1:A:265:GLY:C	2.61	0.42
1:B:204:ALA:HB2	1:B:256:LYS:CG	2.49	0.42
1:C:41:ILE:HG12	1:C:65:LYS:O	2.19	0.42
1:C:158:ASN:ND2	1:D:182:MET:SD	2.83	0.42
1:D:14:ILE:HG12	1:D:269:TYR:CE2	2.54	0.42
1:D:233:ARG:HE	1:D:385:HIS:CD2	2.37	0.42
1:D:571:LYS:H	1:D:571:LYS:HG3	1.71	0.42
1:A:358:HIS:C	1:A:359:CYS:O	2.56	0.42
1:B:139:TYR:OH	1:B:614:TRP:CH2	2.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:GLU:CB	1:B:537:ILE:HD12	2.49	0.42
1:C:14:ILE:HG12	1:C:269:TYR:CE2	2.55	0.42
1:D:588:ASN:CG	1:D:591:LYS:HZ3	2.27	0.42
1:A:582:VAL:C	1:A:583:LYS:O	2.40	0.42
1:D:393:ILE:O	1:D:393:ILE:HD12	2.20	0.42
1:A:14:ILE:HG12	1:A:269:TYR:CE2	2.55	0.42
1:C:140:GLN:CD	1:C:151:LYS:O	2.62	0.42
1:D:115:LYS:CE	1:D:128:VAL:HG21	2.47	0.42
1:A:66:TRP:CE3	1:A:67:GLY:CA	3.01	0.42
1:A:490:TYR:CE2	1:A:601:ILE:HD11	2.54	0.42
1:C:318:HIS:CE1	1:C:432:PHE:O	2.72	0.42
1:C:526:LYS:CG	1:C:540:LEU:HD21	2.49	0.42
1:D:117:THR:CG2	1:D:127:ASN:CA	2.96	0.42
1:A:226:ARG:O	1:A:226:ARG:HG2	2.20	0.42
1:B:52:TYR:HA	1:B:65:LYS:HE3	2.02	0.42
1:C:346:PHE:CD2	1:C:399:PRO:O	2.73	0.42
1:D:90:LEU:CG	1:D:90:LEU:O	2.67	0.42
1:D:117:THR:CG2	1:D:127:ASN:HB3	2.35	0.42
1:D:526:LYS:O	1:D:529:GLU:OE1	2.38	0.42
1:B:346:PHE:HD2	1:B:399:PRO:HB2	1.82	0.42
1:B:535:GLU:HB2	1:B:537:ILE:HD12	2.02	0.42
1:C:183:CYS:SG	1:C:358:HIS:NE2	2.85	0.42
1:D:41:ILE:HG12	1:D:65:LYS:O	2.19	0.42
1:D:65:LYS:HB3	1:D:66:TRP:CE3	2.55	0.42
1:D:599:GLN:HG2	1:D:600:LYS:N	2.34	0.42
1:B:432:PHE:CD1	1:B:438:ASN:HB3	2.55	0.41
1:C:9:ILE:HD13	1:C:194:CYS:SG	2.58	0.41
1:D:143:GLY:O	1:D:144:ALA:O	2.38	0.41
1:B:11:ILE:CD1	1:B:372:LEU:HD11	2.50	0.41
1:B:535:GLU:CB	1:B:537:ILE:CD1	2.97	0.41
1:C:70:LEU:HG	1:C:248:GLU:CD	2.45	0.41
1:B:592:LEU:HD23	1:B:594:GLN:N	2.34	0.41
1:B:398:THR:CG2	1:B:399:PRO:HD2	2.46	0.41
1:B:566:GLU:HA	1:B:569:LEU:HD23	2.02	0.41
1:C:275:THR:HG22	1:C:441:ILE:HD12	2.03	0.41
1:C:599:GLN:NE2	1:C:599:GLN:C	2.78	0.41
1:D:76:PHE:CD1	1:D:96:ARG:HG2	2.55	0.41
1:A:275:THR:HG22	1:A:441:ILE:HD12	2.02	0.41
1:A:593:TYR:C	1:A:594:GLN:O	2.55	0.41
1:C:353:LYS:HD3	1:C:358:HIS:CD2	2.55	0.41
1:C:506:ARG:NH2	1:C:604:PRO:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:LEU:O	1:D:90:LEU:HG	2.19	0.41
1:B:30:ASN:C	1:B:33:GLU:O	2.62	0.41
1:B:275:THR:HG22	1:B:441:ILE:HD12	2.03	0.41
1:D:600:LYS:HD2	1:D:600:LYS:HA	1.90	0.41
1:A:96:ARG:HG2	1:A:97:LEU:N	2.36	0.41
1:A:561:MET:SD	1:A:562:GLU:HG2	2.61	0.41
1:B:14:ILE:HG12	1:B:269:TYR:CE2	2.55	0.41
1:B:589:TRP:O	1:B:591:LYS:N	2.54	0.41
1:C:137:GLU:OE1	1:D:140:GLN:HG2	2.21	0.41
1:C:377:HIS:O	1:C:379:GLN:HG3	2.20	0.41
1:A:144:ALA:HB2	1:B:141:LEU:HD13	2.03	0.41
1:A:377:HIS:O	1:A:379:GLN:HG3	2.21	0.41
1:C:593:TYR:O	1:C:594:GLN:C	2.62	0.41
1:D:115:LYS:HZ3	1:D:117:THR:CG2	2.25	0.41
1:A:159:PRO:O	1:A:178:ALA:HB2	2.21	0.41
1:C:93:PRO:CG	1:C:138:GLU:CD	2.94	0.41
1:C:151:LYS:NZ	1:D:221:MET:CB	2.84	0.41
1:C:217:ASN:HD22	1:D:140:GLN:HE22	1.68	0.41
1:C:515:MET:SD	1:C:539:GLN:O	2.79	0.41
1:D:36:ASP:OD1	1:D:233:ARG:NH1	2.54	0.41
1:D:375:MET:SD	1:D:376:LYS:N	2.94	0.41
1:C:140:GLN:OE1	1:C:152:SER:HB3	2.21	0.41
1:A:490:TYR:CZ	1:A:601:ILE:HD11	2.56	0.40
1:B:6:ARG:NH1	1:B:304:ASP:O	2.53	0.40
1:B:85:PRO:O	1:B:89:LYS:HG2	2.22	0.40
1:C:93:PRO:CG	1:C:138:GLU:OE2	2.69	0.40
1:C:474:LEU:HD23	1:C:474:LEU:HA	1.79	0.40
1:D:96:ARG:HD2	1:D:97:LEU:N	2.36	0.40
1:B:72:ASP:HB2	1:B:75:LYS:HD3	2.03	0.40
1:A:489:ARG:HD2	1:A:490:TYR:CE2	2.57	0.40
1:A:548:ASN:ND2	1:A:548:ASN:H	2.20	0.40
1:B:342:GLN:HE21	1:B:342:GLN:HB2	1.58	0.40
1:C:353:LYS:HB2	1:C:353:LYS:HE2	1.83	0.40
1:D:72:ASP:HB2	1:D:75:LYS:HD3	2.03	0.40
1:D:183:CYS:SG	1:D:358:HIS:NE2	2.83	0.40
1:D:555:PHE:O	1:D:558:ASP:OD2	2.38	0.40
1:A:183:CYS:SG	1:A:358:HIS:NE2	2.93	0.40
1:B:103:TYR:HH	1:B:507:GLU:CD	2.21	0.40
1:C:136:TYR:CZ	1:C:218:LYS:NZ	2.87	0.40
1:C:356:ILE:HD12	1:C:359:CYS:SG	2.62	0.40
1:D:275:THR:HG22	1:D:441:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLU:CD	1:A:48:HIS:CE1	2.99	0.40
1:B:136:TYR:CD2	1:B:136:TYR:C	2.97	0.40
1:B:294:GLN:HE21	1:B:294:GLN:HB3	1.69	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ARG:O	1:D:405:THR:OG1[2_646]	2.01	0.19

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	572/640 (89%)	529 (92%)	40 (7%)	3 (0%)	24	62
1	B	583/640 (91%)	543 (93%)	38 (6%)	2 (0%)	36	71
1	C	574/640 (90%)	533 (93%)	41 (7%)	0	100	100
1	D	578/640 (90%)	543 (94%)	35 (6%)	0	100	100
All	All	2307/2560 (90%)	2148 (93%)	154 (7%)	5 (0%)	43	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	ASP
1	A	141	LEU
1	A	142	TYR
1	B	113	ARG
1	B	246	PRO

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	479/524 (91%)	416 (87%)	63 (13%)	4	17
1	B	488/524 (93%)	407 (83%)	81 (17%)	2	12
1	C	482/524 (92%)	412 (86%)	70 (14%)	3	15
1	D	484/524 (92%)	412 (85%)	72 (15%)	3	15
All	All	1933/2096 (92%)	1647 (85%)	286 (15%)	3	15

All (286) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	8	ASP
1	A	12	ILE
1	A	17	ARG
1	A	22	GLU
1	A	41	ILE
1	A	45	ARG
1	A	50	LEU
1	A	56	LYS
1	A	61	LYS
1	A	71	LYS
1	A	95	GLU
1	A	96	ARG
1	A	117	THR
1	A	118	GLU
1	A	142	TYR
1	A	145	GLU
1	A	165	ARG
1	A	201	GLU
1	A	218	LYS
1	A	226	ARG
1	A	228	LEU
1	A	231	LYS
1	A	234	CYS

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Mol	Chain	Res	Type
1	A	239	GLU
1	A	244	TYR
1	A	260	LYS
1	A	267	HIS
1	A	275	THR
1	A	280	ASP
1	A	300	GLN
1	A	308	ASP
1	A	320	THR
1	A	341	THR
1	A	346	PHE
1	A	353	LYS
1	A	376	LYS
1	A	388	THR
1	A	404	GLN
1	A	407	GLU
1	A	413	VAL
1	A	423	LEU
1	A	438	ASN
1	A	442	VAL
1	A	466	LEU
1	A	469	LYS
1	A	470	ASN
1	A	476	LYS
1	A	483	ASP
1	A	510	GLU
1	A	520	LEU
1	A	523	LEU
1	A	531	THR
1	A	535	GLU
1	A	539	GLN
1	A	547	GLN
1	A	548	ASN
1	A	550	ASP
1	A	552	MET
1	A	570	GLU
1	A	571	LYS
1	A	577	VAL
1	A	599	GLN
1	B	7	GLU
1	B	11	ILE
1	B	17	ARG

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Mol	Chain	Res	Type
1	B	23	ASN
1	B	25	GLN
1	B	33	GLU
1	B	46	TRP
1	B	48	HIS
1	B	59	GLU
1	B	71	LYS
1	B	75	LYS
1	B	89	LYS
1	B	90	LEU
1	B	95	GLU
1	B	96	ARG
1	B	115	LYS
1	B	117	THR
1	B	134	VAL
1	B	135	MET
1	B	141	LEU
1	B	153	LEU
1	B	164	ASN
1	B	165	ARG
1	B	179	LEU
1	B	198	ARG
1	B	201	GLU
1	B	203	GLU
1	B	220	LEU
1	B	221	MET
1	B	228	LEU
1	B	239	GLU
1	B	260	LYS
1	B	267	HIS
1	B	275	THR
1	B	280	ASP
1	B	294	GLN
1	B	300	GLN
1	B	308	ASP
1	B	344	LYS
1	B	353	LYS
1	B	376	LYS
1	B	387	ARG
1	B	388	THR
1	B	393	ILE
1	B	394	ASP

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Mol	Chain	Res	Type
1	B	396	LEU
1	B	398	THR
1	B	404	GLN
1	B	405	THR
1	B	408	GLU
1	B	414	ILE
1	B	416	GLU
1	B	417	ASN
1	B	423	LEU
1	B	438	ASN
1	B	442	VAL
1	B	466	LEU
1	B	469	LYS
1	B	473	ARG
1	B	495	LEU
1	B	515	MET
1	B	520	LEU
1	B	522	GLU
1	B	523	LEU
1	B	524	GLU
1	B	525	GLU
1	B	531	THR
1	B	534	LYS
1	B	535	GLU
1	B	551	THR
1	B	561	MET
1	B	569	LEU
1	B	570	GLU
1	B	571	LYS
1	B	573	LYS
1	B	577	VAL
1	B	583	LYS
1	B	592	LEU
1	B	597	ARG
1	B	599	GLN
1	B	615	ILE
1	C	8	ASP
1	C	23	ASN
1	C	41	ILE
1	C	46	TRP
1	C	48	HIS
1	C	55	ASP

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Mol	Chain	Res	Type
1	C	56	LYS
1	C	75	LYS
1	C	96	ARG
1	C	104	GLU
1	C	106	MET
1	C	113	ARG
1	C	135	MET
1	C	137	GLU
1	C	140	GLN
1	C	141	LEU
1	C	145	GLU
1	C	146	GLU
1	C	151	LYS
1	C	155	LEU
1	C	201	GLU
1	C	218	LYS
1	C	220	LEU
1	C	222	LEU
1	C	228	LEU
1	C	233	ARG
1	C	234	CYS
1	C	239	GLU
1	C	256	LYS
1	C	275	THR
1	C	300	GLN
1	C	308	ASP
1	C	320	THR
1	C	329	GLU
1	C	339	GLU
1	C	344	LYS
1	C	353	LYS
1	C	376	LYS
1	C	378	LYS
1	C	388	THR
1	C	404	GLN
1	C	410	LYS
1	C	413	VAL
1	C	423	LEU
1	C	438	ASN
1	C	442	VAL
1	C	466	LEU
1	C	472	GLN

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Mol	Chain	Res	Type
1	C	477	ARG
1	C	480	ARG
1	C	507	GLU
1	C	515	MET
1	C	520	LEU
1	C	523	LEU
1	C	524	GLU
1	C	531	THR
1	C	534	LYS
1	C	549	LYS
1	C	551	THR
1	C	552	MET
1	C	566	GLU
1	C	571	LYS
1	C	577	VAL
1	C	583	LYS
1	C	587	LEU
1	C	591	LYS
1	C	592	LEU
1	C	594	GLN
1	C	599	GLN
1	C	612	ARG
1	D	6	ARG
1	D	7	GLU
1	D	8	ASP
1	D	26	GLU
1	D	40	GLU
1	D	41	ILE
1	D	48	HIS
1	D	58	LYS
1	D	63	TYR
1	D	65	LYS
1	D	71	LYS
1	D	75	LYS
1	D	90	LEU
1	D	92	ASP
1	D	101	CYS
1	D	115	LYS
1	D	116	LEU
1	D	138	GLU
1	D	141	LEU
1	D	142	TYR

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Mol	Chain	Res	Type
1	D	145	GLU
1	D	146	GLU
1	D	147	GLN
1	D	149	ARG
1	D	158	ASN
1	D	165	ARG
1	D	201	GLU
1	D	214	VAL
1	D	218	LYS
1	D	220	LEU
1	D	228	LEU
1	D	275	THR
1	D	300	GLN
1	D	308	ASP
1	D	342	GLN
1	D	376	LYS
1	D	387	ARG
1	D	388	THR
1	D	396	LEU
1	D	422	GLU
1	D	423	LEU
1	D	425	ARG
1	D	438	ASN
1	D	442	VAL
1	D	463	MET
1	D	466	LEU
1	D	469	LYS
1	D	470	ASN
1	D	472	GLN
1	D	473	ARG
1	D	476	LYS
1	D	477	ARG
1	D	480	ARG
1	D	486	ARG
1	D	492	GLU
1	D	516	ILE
1	D	520	LEU
1	D	523	LEU
1	D	525	GLU
1	D	529	GLU
1	D	531	THR
1	D	536	SER

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Mol	Chain	Res	Type
1	D	558	ASP
1	D	561	MET
1	D	563	LYS
1	D	570	GLU
1	D	571	LYS
1	D	577	VAL
1	D	580	LEU
1	D	591	LYS
1	D	597	ARG
1	D	599	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	94	GLN
1	A	100	GLN
1	A	173	ASN
1	A	199	ASN
1	A	377	HIS
1	A	472	GLN
1	A	548	ASN
1	B	48	HIS
1	B	94	GLN
1	B	100	GLN
1	B	127	ASN
1	B	191	HIS
1	B	199	ASN
1	B	279	HIS
1	B	318	HIS
1	B	342	GLN
1	B	385	HIS
1	B	404	GLN
1	B	460	HIS
1	B	547	GLN
1	C	100	GLN
1	C	191	HIS
1	C	199	ASN
1	C	217	ASN
1	C	267	HIS
1	C	318	HIS
1	C	377	HIS

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Mol	Chain	Res	Type
1	C	415	ASN
1	C	417	ASN
1	C	599	GLN
1	D	100	GLN
1	D	158	ASN
1	D	164	ASN
1	D	199	ASN
1	D	215	HIS
1	D	224	GLN
1	D	267	HIS
1	D	279	HIS
1	D	292	ASN
1	D	340	GLN
1	D	377	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	584/640 (91%)	-0.54	0 100 100	23, 191, 295, 377	0
1	B	593/640 (92%)	-0.59	2 (0%) 90 80	30, 189, 285, 364	0
1	C	586/640 (91%)	-0.60	0 100 100	23, 193, 285, 402	0
1	D	590/640 (92%)	-0.64	1 (0%) 91 83	23, 191, 285, 399	0
All	All	2353/2560 (91%)	-0.59	3 (0%) 92 87	23, 191, 290, 402	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	THR	2.4
1	B	553	ALA	2.2
1	D	556	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.