



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:22 AM UTC

PDB ID : 5A0Z / pdb_00005a0z
Title : STRUCTURE OF CUTC CHOLINE LYASE CHOLINE FREE FORM FROM KLEBSIELLA PNEUMONIAE
Authors : Kalnins, G.; Tars, K.
Deposited on : 2015-04-27
Resolution : 3.00 Å(reported)

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

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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

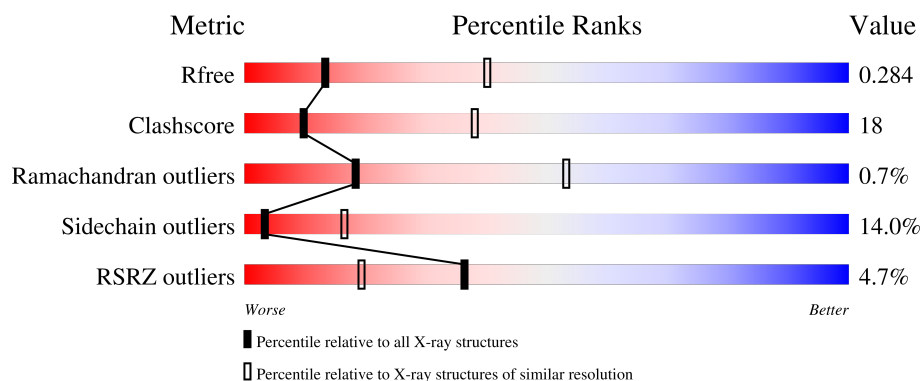
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	792	3% 62% 25% 7% • 5%
1	B	792	2% 63% 24% 6% • 6%
1	C	792	5% 62% 25% 6% • 6%
1	D	792	8% 60% 22% 6% • 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23177 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.

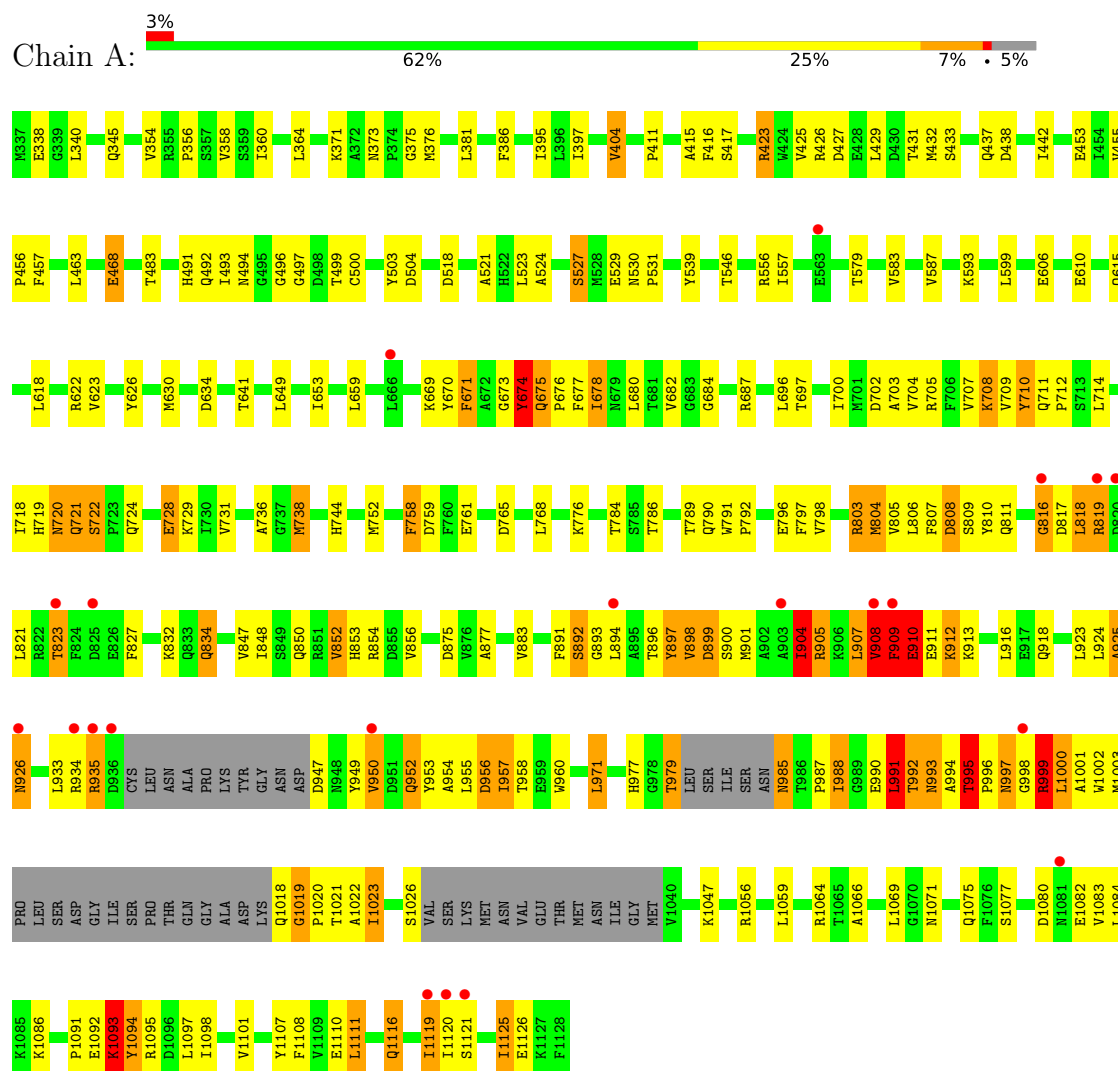
- Molecule 1 is a protein called CHOLINE TRIMETHYLAMINE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	750	Total	C	N	O	S	0	0	0
			5919	3747	1020	1114	38			
1	B	746	Total	C	N	O	S	0	0	0
			5868	3715	1011	1103	39			
1	C	746	Total	C	N	O	S	0	0	0
			5856	3707	1005	1107	37			
1	D	710	Total	C	N	O	S	0	0	0
			5534	3507	947	1046	34			

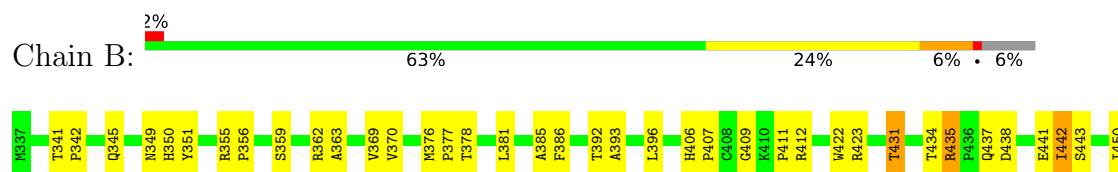
3 Residue-property plots

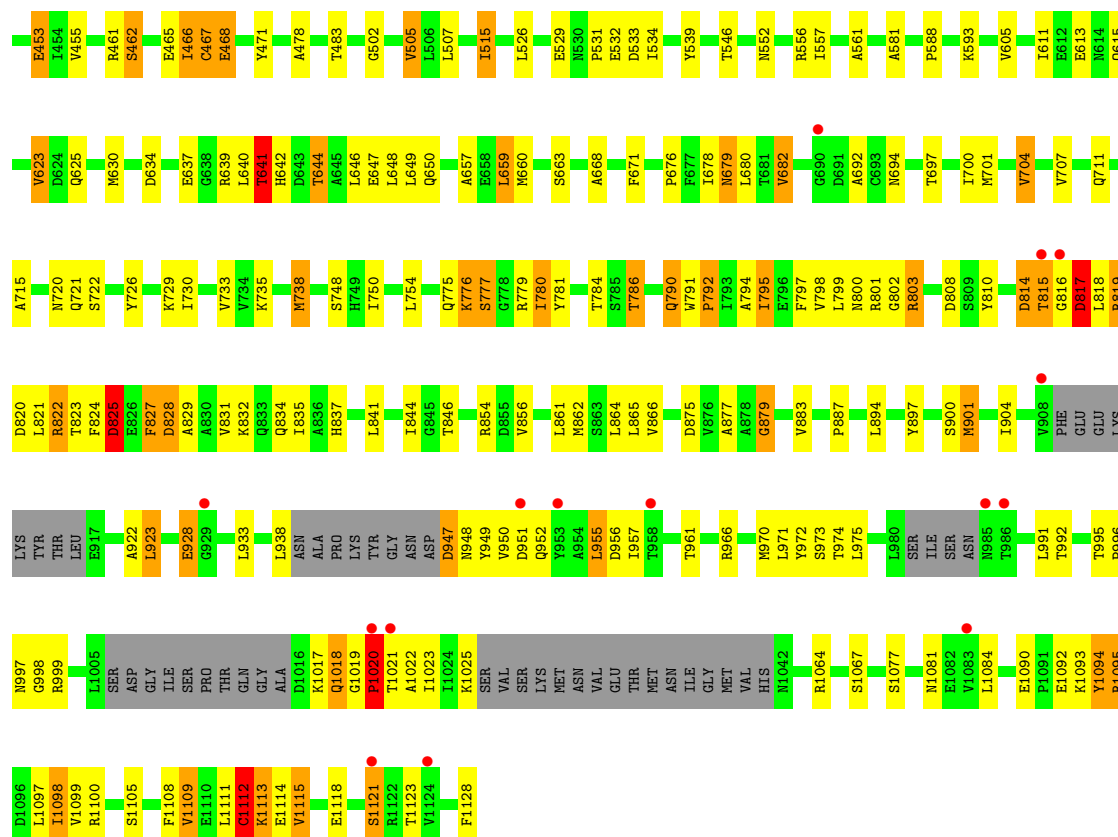
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

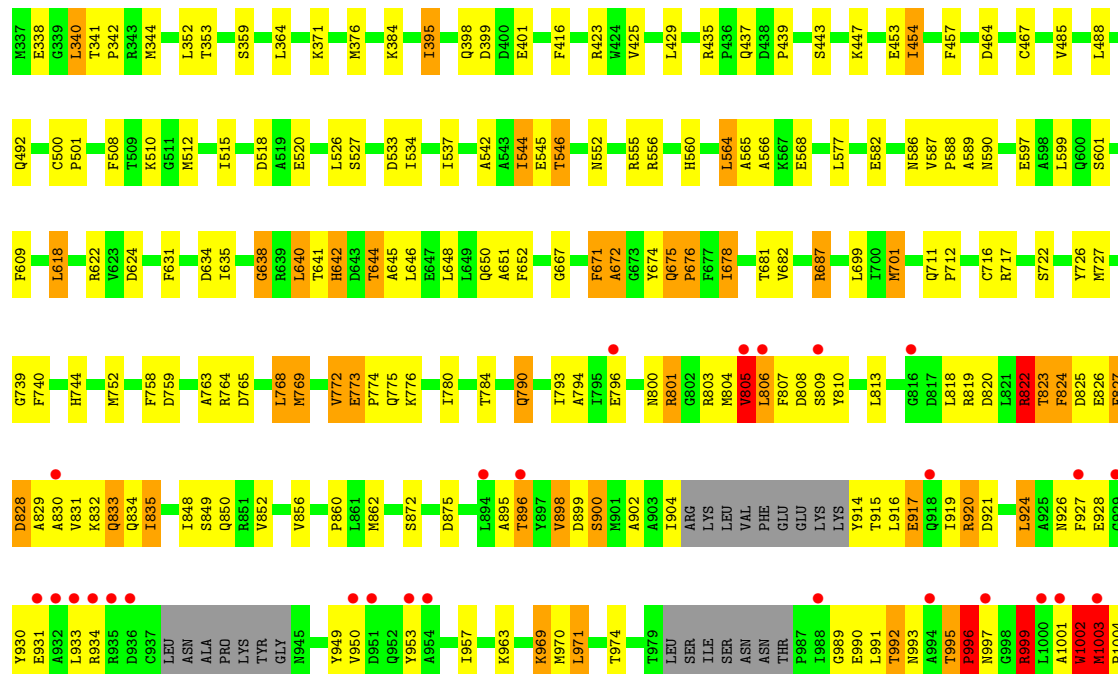


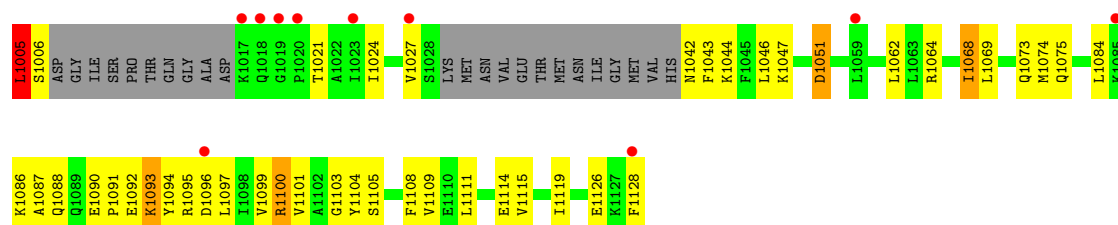
• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE



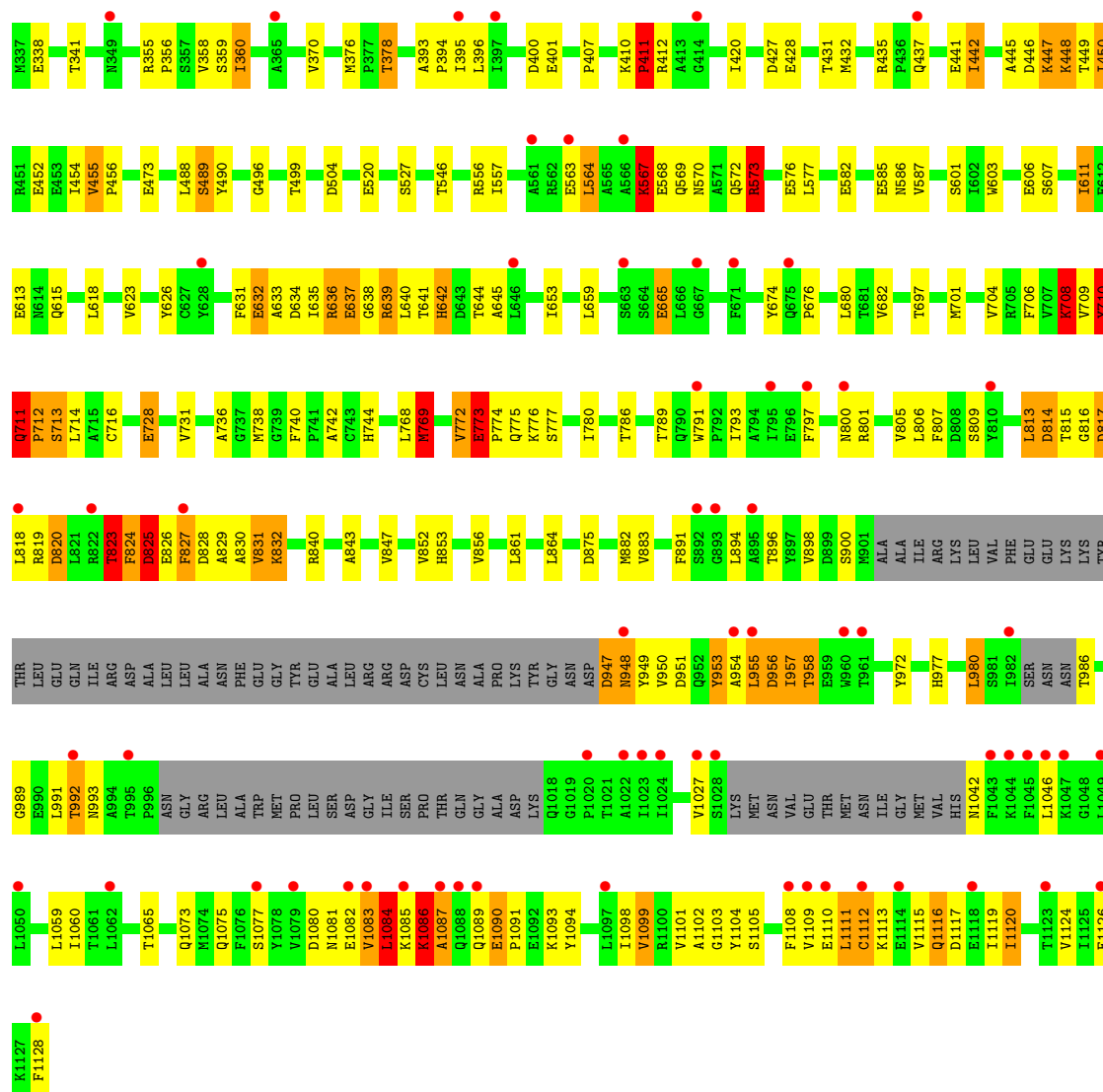


• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE





● Molecule 1: CHOLINE TRIMETHYLAMINE LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.60Å 154.55Å 120.78Å 90.00° 96.85° 90.00°	Depositor
Resolution (Å)	119.92 – 3.00 119.92 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.5 (119.92-3.00) 88.5 (119.92-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.232 , 0.286 0.234 , 0.284	Depositor DCC
R_{free} test set	3342 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	23177	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.09% 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	1.06	13/6041 (0.2%)	1.15	33/8170 (0.4%)
1	B	1.00	9/5987 (0.2%)	1.16	28/8099 (0.3%)
1	C	1.01	8/5977 (0.1%)	1.16	41/8089 (0.5%)
1	D	0.91	8/5649 (0.1%)	1.12	33/7652 (0.4%)
All	All	1.00	38/23654 (0.2%)	1.15	135/32010 (0.4%)

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	5
1	B	0	4
1	C	0	4
1	D	0	2
All	All	0	15

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	675	GLN	C-N	8.90	1.40	1.33
1	A	675	GLN	C-N	8.74	1.40	1.33
1	A	527	SER	C-O	-7.32	1.15	1.23
1	C	1003	MET	C-N	6.86	1.40	1.33
1	A	530	ASN	C-N	6.72	1.41	1.34
1	B	466	ILE	C-O	-6.65	1.16	1.24
1	A	892	SER	CA-C	-6.59	1.44	1.52
1	B	467	CYS	C-O	-6.46	1.16	1.24
1	C	678	ILE	C-O	-6.36	1.17	1.24
1	B	435	ARG	CA-C	-6.19	1.46	1.53
1	B	883	VAL	C-O	-6.05	1.18	1.24
1	B	777	SER	C-O	-5.89	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1019	GLY	C-N	5.87	1.41	1.34
1	A	908	VAL	CA-C	5.87	1.60	1.52
1	A	708	LYS	CA-C	-5.83	1.48	1.53
1	D	773	GLU	C-N	5.82	1.40	1.33
1	C	763	ALA	C-O	-5.76	1.17	1.24
1	A	530	ASN	C-O	-5.70	1.18	1.24
1	C	341	THR	C-N	5.61	1.41	1.34
1	C	773	GLU	C-N	5.60	1.41	1.33
1	B	468	GLU	C-O	-5.55	1.17	1.24
1	B	455	VAL	CA-CB	5.55	1.56	1.54
1	A	492	GLN	C-O	-5.50	1.17	1.24
1	A	722	SER	C-N	5.47	1.40	1.33
1	A	758	PHE	C-O	-5.42	1.17	1.23
1	D	774	PRO	N-CD	5.34	1.55	1.47
1	C	342	PRO	N-CD	5.29	1.55	1.47
1	D	769	MET	CA-C	-5.26	1.46	1.52
1	B	435	ARG	C-N	5.20	1.41	1.34
1	D	716	CYS	CA-C	-5.19	1.46	1.52
1	A	728	GLU	C-O	-5.17	1.18	1.24
1	D	411	PRO	N-CD	5.16	1.54	1.47
1	B	462	SER	C-O	-5.15	1.17	1.23
1	C	774	PRO	N-CD	5.13	1.54	1.47
1	D	712	PRO	N-CD	5.06	1.54	1.47
1	D	711	GLN	C-O	-5.05	1.18	1.24
1	D	410	LYS	C-N	5.03	1.40	1.33
1	A	759	ASP	CA-C	-5.01	1.46	1.53

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1112	CYS	N-CA-C	12.61	119.12	108.78
1	D	454	ILE	N-CA-C	11.50	121.34	110.53
1	B	952	GLN	N-CA-C	9.91	126.32	112.04
1	A	710	TYR	N-CA-C	9.77	121.93	111.28
1	C	822	ARG	N-CA-C	9.06	124.21	111.52
1	A	1093	LYS	N-CA-C	8.97	120.83	111.14
1	A	910	GLU	N-CA-C	-8.69	98.24	110.50
1	D	814	ASP	N-CA-C	8.60	121.88	110.53
1	C	926	ASN	N-CA-C	8.54	123.27	111.74
1	A	493	ILE	N-CA-C	8.43	120.18	112.17
1	D	711	GLN	N-CA-C	-8.34	94.73	108.82
1	C	921	ASP	N-CA-C	8.26	120.36	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	999	ARG	N-CA-C	-8.01	98.62	110.23
1	C	898	VAL	CB-CA-C	-7.97	101.77	111.97
1	D	711	GLN	C-N-CD	7.95	138.08	120.60
1	C	823	THR	N-CA-C	7.89	123.70	107.37
1	C	828	ASP	N-CA-C	-7.80	98.61	110.70
1	B	817	ASP	N-CA-C	7.79	119.41	111.07
1	A	819	ARG	N-CA-C	-7.73	95.69	108.76
1	A	674	TYR	N-CA-C	7.70	119.92	110.91
1	C	995	THR	C-N-CD	7.70	137.53	120.60
1	C	1096	ASP	N-CA-C	7.47	119.42	111.28
1	C	996	PRO	CA-N-CD	-7.46	101.05	111.50
1	D	813	LEU	N-CA-C	7.43	118.08	108.34
1	D	573	ARG	N-CA-C	7.42	119.44	111.36
1	B	431	THR	N-CA-C	7.31	120.30	111.82
1	B	515	ILE	N-CA-C	-7.15	103.81	110.53
1	C	638	GLY	N-CA-C	6.90	124.18	115.21
1	C	758	PHE	CA-C-N	6.87	131.12	120.75
1	C	758	PHE	C-N-CA	6.87	131.12	120.75
1	D	710	TYR	N-CA-C	6.87	118.85	111.36
1	C	1003	MET	CA-C-N	-6.80	111.86	120.23
1	C	1003	MET	C-N-CA	-6.80	111.86	120.23
1	C	805	VAL	N-CA-C	6.78	120.60	112.80
1	A	722	SER	CA-C-N	-6.67	113.11	119.85
1	A	722	SER	C-N-CA	-6.67	113.11	119.85
1	B	1112	CYS	CA-C-O	6.67	121.81	117.94
1	A	897	TYR	N-CA-C	6.65	122.29	114.04
1	C	769	MET	N-CA-C	6.64	120.97	113.01
1	D	1084	LEU	N-CA-C	6.46	122.05	114.04
1	B	1093	LYS	N-CA-C	-6.41	101.46	110.50
1	A	999	ARG	N-CA-C	6.41	120.39	111.74
1	D	824	PHE	N-CA-C	-6.40	104.30	111.28
1	B	844	ILE	N-CA-C	6.34	116.51	110.42
1	A	816	GLY	N-CA-C	6.33	121.57	111.64
1	A	926	ASN	N-CA-C	6.31	120.37	107.69
1	C	676	PRO	CA-N-CD	-6.20	103.33	112.00
1	A	1119	ILE	N-CA-C	-6.15	104.86	110.82
1	A	1019	GLY	CA-C-N	-6.11	112.62	118.97
1	A	1019	GLY	C-N-CA	-6.11	112.62	118.97
1	D	567	LYS	N-CA-C	6.09	118.00	111.36
1	B	461	ARG	N-CA-C	6.08	120.85	113.38
1	A	677	PHE	N-CA-C	6.07	119.93	111.74
1	C	772	VAL	N-CA-C	6.04	118.70	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	844	ILE	CB-CA-C	-5.98	104.32	111.97
1	A	908	VAL	CB-CA-C	5.97	121.08	111.29
1	C	675	GLN	CA-C-N	-5.95	114.16	120.94
1	C	675	GLN	C-N-CA	-5.95	114.16	120.94
1	C	1002	TRP	N-CA-C	-5.93	104.81	111.28
1	A	678	ILE	N-CA-CB	5.91	116.97	110.53
1	D	823	THR	N-CA-C	-5.91	98.06	108.23
1	D	773	GLU	CA-C-N	-5.90	114.53	120.31
1	D	773	GLU	C-N-CA	-5.90	114.53	120.31
1	C	758	PHE	N-CA-C	5.89	118.50	110.55
1	B	378	THR	N-CA-C	5.87	117.55	111.03
1	C	773	GLU	CA-C-N	-5.87	113.89	119.76
1	C	773	GLU	C-N-CA	-5.87	113.89	119.76
1	A	531	PRO	CA-N-CD	-5.83	103.84	112.00
1	A	676	PRO	CA-N-CD	-5.81	103.86	112.00
1	A	684	GLY	N-CA-C	5.78	117.93	112.04
1	D	1083	VAL	N-CA-C	5.74	117.63	112.17
1	B	641	THR	N-CA-C	-5.73	100.64	109.52
1	D	1112	CYS	N-CA-C	5.72	116.61	108.54
1	B	827	PHE	N-CA-C	5.72	127.01	111.00
1	C	831	VAL	N-CA-C	-5.71	104.93	110.42
1	B	1019	GLY	CA-C-N	-5.68	112.75	119.84
1	B	1019	GLY	C-N-CA	-5.68	112.75	119.84
1	D	355	ARG	CA-C-N	5.65	126.91	119.84
1	D	355	ARG	C-N-CA	5.65	126.91	119.84
1	D	455	VAL	CA-C-N	-5.61	113.90	119.56
1	D	455	VAL	C-N-CA	-5.61	113.90	119.56
1	A	496	GLY	N-CA-C	5.59	119.26	112.49
1	C	1096	ASP	CB-CA-C	-5.55	101.57	110.79
1	C	399	ASP	N-CA-C	5.53	119.65	113.01
1	D	410	LYS	CA-C-N	-5.53	114.26	119.90
1	D	410	LYS	C-N-CA	-5.53	114.26	119.90
1	A	953	TYR	CA-C-N	5.53	127.69	120.28
1	A	953	TYR	C-N-CA	5.53	127.69	120.28
1	A	675	GLN	CA-C-N	-5.49	114.39	121.04
1	A	675	GLN	C-N-CA	-5.49	114.39	121.04
1	B	825	ASP	N-CA-C	-5.49	99.10	110.80
1	C	790	GLN	N-CA-C	5.49	116.48	108.14
1	C	644	THR	CB-CA-C	-5.48	101.53	110.85
1	D	1086	LYS	N-CA-C	-5.47	105.31	111.28
1	A	1125	ILE	N-CA-CB	5.42	116.44	110.53
1	C	950	VAL	N-CA-C	-5.41	105.66	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1094	TYR	N-CA-C	5.39	118.67	111.24
1	C	920	ARG	N-CA-C	-5.36	105.34	111.07
1	C	740	PHE	N-CA-C	-5.35	103.19	110.36
1	D	992	THR	N-CA-C	5.35	119.50	111.96
1	A	494	ASN	N-CA-C	5.35	117.81	109.52
1	C	672	ALA	N-CA-C	-5.34	103.84	110.41
1	B	901	MET	N-CA-C	-5.33	106.45	113.12
1	D	827	PHE	N-CA-C	-5.31	105.49	111.28
1	C	1005	LEU	N-CA-C	-5.30	99.65	108.34
1	D	637	GLU	N-CA-C	-5.30	105.52	112.72
1	D	456	PRO	CA-N-CD	-5.29	104.60	112.00
1	C	454	ILE	N-CA-C	5.27	116.09	111.56
1	A	991	LEU	N-CA-C	5.26	119.66	112.88
1	D	378	THR	N-CA-C	5.23	117.73	111.71
1	D	817	ASP	N-CA-C	5.23	116.23	108.60
1	A	898	VAL	N-CA-C	-5.21	105.30	110.62
1	C	996	PRO	N-CA-C	5.20	125.62	112.10
1	B	471	TYR	N-CA-C	-5.19	105.52	111.07
1	A	995	THR	CA-C-N	-5.18	113.37	119.84
1	A	995	THR	C-N-CA	-5.18	113.37	119.84
1	D	772	VAL	N-CA-C	5.17	117.15	112.29
1	B	879	GLY	CA-C-N	5.15	126.58	120.14
1	B	879	GLY	C-N-CA	5.15	126.58	120.14
1	B	453	GLU	N-CA-C	5.15	121.77	110.80
1	C	485	VAL	N-CA-C	-5.15	105.30	110.30
1	B	455	VAL	O-C-N	5.14	123.71	120.42
1	D	1087	ALA	N-CA-C	-5.14	105.80	111.71
1	C	341	THR	CA-C-N	-5.10	113.78	119.19
1	C	341	THR	C-N-CA	-5.10	113.78	119.19
1	D	712	PRO	CA-N-CD	-5.08	104.38	111.50
1	A	904	ILE	N-CA-C	5.07	118.63	112.80
1	B	435	ARG	CA-C-N	-5.07	113.42	119.05
1	B	435	ARG	C-N-CA	-5.07	113.42	119.05
1	B	1121	SER	N-CA-C	5.07	118.72	112.54
1	B	790	GLN	N-CA-C	5.06	115.72	108.74
1	D	587	VAL	N-CA-C	5.06	113.34	109.19
1	D	708	LYS	N-CA-C	5.05	118.70	112.24
1	B	392	THR	CB-CA-C	-5.04	101.96	110.44
1	C	675	GLN	CB-CA-C	-5.01	104.14	109.85

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	891	PHE	Peptide
1	A	909	PHE	Peptide
1	A	925	ALA	Peptide
1	A	950	VAL	Peptide
1	A	992	THR	Peptide
1	B	817	ASP	Peptide
1	B	822	ARG	Peptide
1	B	928	GLU	Peptide
1	B	951	ASP	Peptide
1	C	398	GLN	Peptide
1	C	827	PHE	Peptide
1	C	949	TYR	Peptide
1	C	996	PRO	Peptide
1	D	1101	VAL	Peptide
1	D	825	ASP	Peptide

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	5919	0	5803	182	0
1	B	5868	0	5753	174	0
1	C	5856	0	5720	228	0
1	D	5534	0	5388	224	0
All	All	23177	0	22664	805	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (805) 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:989:GLY:CA	1:C:1005:LEU:CD2	1.78	1.60
1:D:1099:VAL:HG11	1:D:1119:ILE:CG2	1.28	1.58
1:D:949:TYR:O	1:D:953:TYR:CE1	1.69	1.43
1:C:989:GLY:CA	1:C:1005:LEU:HD23	1.43	1.36
1:C:989:GLY:HA3	1:C:1005:LEU:CD2	1.44	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1099:VAL:CG1	1:D:1119:ILE:CG2	2.04	1.35
1:D:573:ARG:NH1	1:D:576:GLU:OE1	1.58	1.32
1:C:819:ARG:CD	1:C:917:GLU:OE2	1.79	1.29
1:C:739:GLY:O	1:C:1100:ARG:NH1	1.65	1.29
1:D:817:ASP:OD2	1:D:819:ARG:HG2	1.29	1.25
1:C:989:GLY:HA2	1:C:1005:LEU:CD2	1.48	1.24
1:D:1116:GLN:O	1:D:1120:ILE:HG13	1.27	1.23
1:A:900:SER:O	1:A:904:ILE:HG23	1.38	1.21
1:D:1116:GLN:O	1:D:1120:ILE:CG1	1.90	1.20
1:C:796:GLU:OE2	1:C:805:VAL:CG2	1.90	1.20
1:D:949:TYR:O	1:D:953:TYR:HE1	0.85	1.19
1:B:794:ALA:O	1:B:798:VAL:HG12	1.47	1.12
1:D:826:GLU:HA	1:D:829:ALA:HB3	1.25	1.12
1:D:1099:VAL:CG1	1:D:1119:ILE:HG21	1.70	1.12
1:A:908:VAL:HB	1:A:909:PHE:HA	1.28	1.11
1:D:641:THR:OG1	1:D:644:THR:OG1	1.68	1.09
1:A:993:ASN:HB3	1:A:994:ALA:HA	1.24	1.09
1:C:819:ARG:HD3	1:C:917:GLU:OE2	0.92	1.09
1:B:423:ARG:NH2	1:B:468:GLU:OE1	1.86	1.08
1:D:1099:VAL:CG1	1:D:1119:ILE:HG23	1.84	1.08
1:B:641:THR:N	1:B:644:THR:OG1	1.87	1.07
1:D:947:ASP:OD1	1:D:949:TYR:N	1.87	1.07
1:C:1092:GLU:N	1:C:1092:GLU:OE1	1.87	1.07
1:C:823:THR:O	1:C:827:PHE:N	1.87	1.07
1:C:898:VAL:HG13	1:C:953:TYR:CD1	1.89	1.07
1:B:1020:PRO:O	1:B:1023:ILE:N	1.88	1.06
1:C:989:GLY:HA2	1:C:1005:LEU:HD21	1.29	1.06
1:A:893:GLY:O	1:A:898:VAL:N	1.87	1.06
1:D:817:ASP:HB3	1:D:820:ASP:OD1	1.56	1.06
1:B:818:LEU:H	1:B:821:LEU:HD22	1.20	1.05
1:B:1112:CYS:SG	1:B:1113:LYS:N	2.23	1.05
1:D:817:ASP:OD2	1:D:819:ARG:CG	2.03	1.05
1:D:640:LEU:HD22	1:D:644:THR:HB	1.39	1.05
1:D:1116:GLN:C	1:D:1120:ILE:HG13	1.81	1.04
1:C:989:GLY:HA3	1:C:1005:LEU:HD22	1.05	1.04
1:D:448:LYS:NZ	1:D:452:GLU:OE2	1.93	0.99
1:C:999:ARG:HH11	1:C:1005:LEU:HD12	1.27	0.99
1:D:826:GLU:CA	1:D:829:ALA:HB3	1.93	0.99
1:C:999:ARG:NH1	1:C:1005:LEU:HA	1.77	0.98
1:D:801:ARG:O	1:D:813:LEU:O	1.81	0.98
1:D:1084:LEU:HD22	1:D:1120:ILE:HG23	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:989:GLY:N	1:C:1005:LEU:HD23	1.78	0.97
1:C:796:GLU:OE2	1:C:805:VAL:HG22	1.65	0.97
1:C:640:LEU:HD13	1:C:645:ALA:HA	1.49	0.95
1:A:954:ALA:O	1:A:958:THR:OG1	1.85	0.95
1:C:896:THR:O	1:C:900:SER:OG	1.84	0.93
1:D:1099:VAL:HG12	1:D:1119:ILE:HG23	1.47	0.93
1:B:637:GLU:OE1	1:B:639:ARG:NH2	2.01	0.93
1:D:1116:GLN:HB3	1:D:1120:ILE:HD11	1.49	0.93
1:D:744:HIS:CG	1:D:768:LEU:HD21	2.03	0.92
1:D:826:GLU:O	1:D:830:ALA:N	2.00	0.92
1:B:828:ASP:O	1:B:831:VAL:N	2.03	0.91
1:D:817:ASP:OD2	1:D:819:ARG:N	2.03	0.91
1:D:704:VAL:HG21	1:D:714:LEU:HD22	1.53	0.91
1:A:893:GLY:HA3	1:A:897:TYR:CB	2.01	0.90
1:A:908:VAL:CB	1:A:909:PHE:HA	2.00	0.90
1:D:1086:LYS:O	1:D:1089:GLN:N	2.05	0.90
1:B:824:PHE:O	1:B:825:ASP:HB2	1.69	0.89
1:D:710:TYR:O	1:D:1105:SER:HB2	1.72	0.89
1:A:905:ARG:HG3	1:A:905:ARG:HH11	1.37	0.89
1:C:818:LEU:HD12	1:C:819:ARG:H	1.36	0.89
1:D:641:THR:HG1	1:D:644:THR:HG1	1.09	0.88
1:C:822:ARG:HA	1:C:822:ARG:NH1	1.88	0.88
1:C:801:ARG:O	1:C:810:TYR:OH	1.90	0.87
1:D:815:THR:HB	1:D:816:GLY:HA2	1.57	0.86
1:B:641:THR:H	1:B:644:THR:HG1	1.17	0.86
1:B:817:ASP:OD1	1:B:820:ASP:HB3	1.76	0.86
1:B:1095:ARG:O	1:B:1109:VAL:HG22	1.75	0.85
1:D:744:HIS:CE1	1:D:768:LEU:CD2	2.60	0.85
1:B:824:PHE:CZ	1:B:827:PHE:HE1	1.95	0.85
1:D:744:HIS:ND1	1:D:768:LEU:HD22	1.92	0.85
1:C:995:THR:OG1	1:C:999:ARG:O	1.94	0.84
1:A:797:PHE:HB3	1:A:834:GLN:HE21	1.43	0.84
1:A:817:ASP:O	1:A:821:LEU:HB2	1.78	0.84
1:A:993:ASN:HB3	1:A:994:ALA:CA	2.07	0.84
1:A:703:ALA:O	1:A:707:VAL:HG12	1.78	0.83
1:C:646:LEU:CD1	1:C:699:LEU:HD22	2.08	0.83
1:C:796:GLU:OE2	1:C:805:VAL:HG23	1.77	0.83
1:A:908:VAL:HG23	1:A:909:PHE:CD1	2.13	0.83
1:D:640:LEU:CD2	1:D:644:THR:HB	2.09	0.83
1:B:817:ASP:HB3	1:B:818:LEU:HA	1.60	0.83
1:B:803:ARG:NH2	1:B:808:ASP:OD1	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:632:GLU:O	1:D:636:ARG:HB2	1.78	0.82
1:A:1093:LYS:N	1:A:1093:LYS:HD2	1.95	0.82
1:A:995:THR:OG1	1:A:998:GLY:HA3	1.80	0.82
1:D:632:GLU:OE1	1:D:636:ARG:NH2	2.12	0.81
1:D:1116:GLN:C	1:D:1120:ILE:CG1	2.47	0.81
1:D:744:HIS:ND1	1:D:768:LEU:CD2	2.43	0.81
1:B:818:LEU:N	1:B:821:LEU:HD22	1.94	0.81
1:A:908:VAL:HB	1:A:909:PHE:CA	2.09	0.81
1:C:999:ARG:NH1	1:C:1005:LEU:HD12	1.94	0.81
1:B:820:ASP:HA	1:B:821:LEU:CB	2.10	0.81
1:D:824:PHE:O	1:D:826:GLU:N	2.14	0.80
1:B:820:ASP:HA	1:B:821:LEU:HB3	1.62	0.80
1:D:826:GLU:C	1:D:829:ALA:H	1.90	0.80
1:D:1084:LEU:HD21	1:D:1120:ILE:HA	1.62	0.80
1:A:818:LEU:O	1:A:819:ARG:NH1	2.15	0.80
1:C:676:PRO:HD2	1:C:711:GLN:NE2	1.97	0.80
1:D:713:SER:OG	1:D:1103:GLY:O	2.00	0.80
1:A:483:THR:OG1	1:A:811:GLN:NE2	2.15	0.79
1:C:1095:ARG:HD2	1:C:1095:ARG:O	1.80	0.79
1:D:815:THR:CB	1:D:816:GLY:HA2	2.13	0.79
1:B:897:TYR:CE1	1:B:957:ILE:HD13	2.18	0.79
1:C:1087:ALA:O	1:C:1091:PRO:HD3	1.83	0.79
1:C:560:HIS:CE1	1:C:564:LEU:HG	2.19	0.78
1:D:1116:GLN:O	1:D:1120:ILE:HG12	1.82	0.78
1:D:1084:LEU:CD2	1:D:1120:ILE:HA	2.13	0.78
1:D:1084:LEU:CD2	1:D:1120:ILE:HG23	2.12	0.78
1:A:790:GLN:NE2	1:A:992:THR:OG1	2.14	0.78
1:C:822:ARG:HH11	1:C:822:ARG:C	1.90	0.78
1:C:989:GLY:CA	1:C:1005:LEU:HD21	1.87	0.77
1:C:1002:TRP:H	1:C:1002:TRP:CD1	1.99	0.77
1:B:437:GLN:OE1	1:B:1112:CYS:HB3	1.84	0.77
1:B:1114:GLU:O	1:B:1118:GLU:N	2.16	0.77
1:A:1066:ALA:HB1	1:A:1071:ASN:HD22	1.49	0.77
1:D:1087:ALA:HB3	1:D:1108:PHE:CE2	2.19	0.77
1:D:1099:VAL:HG11	1:D:1119:ILE:HG21	0.78	0.77
1:D:393:ALA:O	1:D:556:ARG:NH2	2.18	0.77
1:D:953:TYR:O	1:D:956:ASP:HB2	1.85	0.76
1:C:646:LEU:HD13	1:C:699:LEU:HD22	1.65	0.76
1:C:793:ILE:HD11	1:C:804:MET:HG3	1.65	0.76
1:C:819:ARG:HD3	1:C:917:GLU:CD	2.04	0.76
1:D:706:PHE:O	1:D:708:LYS:HD2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:SER:OG	1:B:465:GLU:HG3	1.84	0.76
1:C:796:GLU:CD	1:C:805:VAL:CG2	2.58	0.76
1:D:744:HIS:CG	1:D:768:LEU:CD2	2.67	0.76
1:D:450:ILE:O	1:D:455:VAL:HG23	1.84	0.76
1:D:744:HIS:CD2	1:D:768:LEU:HD21	2.21	0.76
1:A:1084:LEU:CD2	1:A:1097:LEU:HD21	2.16	0.76
1:C:920:ARG:O	1:C:924:LEU:HB2	1.85	0.76
1:A:900:SER:C	1:A:904:ILE:HG23	2.12	0.75
1:C:830:ALA:HA	1:C:833:GLN:OE1	1.86	0.75
1:B:955:LEU:HD23	1:B:956:ASP:N	2.01	0.75
1:D:957:ILE:HD12	1:D:957:ILE:H	1.50	0.75
1:A:1091:PRO:HD2	1:A:1092:GLU:OE1	1.86	0.75
1:B:1113:LYS:HG3	1:B:1114:GLU:N	2.01	0.75
1:C:672:ALA:O	1:C:1104:TYR:OH	2.01	0.75
1:B:897:TYR:CD1	1:B:957:ILE:HD13	2.22	0.75
1:D:1116:GLN:CB	1:D:1120:ILE:HD11	2.16	0.75
1:B:641:THR:O	1:B:644:THR:OG1	2.05	0.75
1:C:796:GLU:OE1	1:C:805:VAL:HG21	1.87	0.75
1:A:731:VAL:HG22	1:A:1059:LEU:HD23	1.69	0.74
1:C:822:ARG:C	1:C:822:ARG:HD3	2.11	0.74
1:C:989:GLY:HA2	1:C:1005:LEU:HD23	1.19	0.74
1:D:634:ASP:O	1:D:640:LEU:N	2.20	0.74
1:A:907:LEU:HD12	1:A:908:VAL:N	2.03	0.74
1:C:800:ASN:C	1:C:801:ARG:HG3	2.12	0.73
1:D:825:ASP:HB3	1:D:829:ALA:HB2	1.71	0.73
1:D:1117:ASP:HA	1:D:1120:ILE:HG13	1.70	0.73
1:D:1084:LEU:HD12	1:D:1084:LEU:H	1.53	0.73
1:D:400:ASP:C	1:D:573:ARG:NH2	2.47	0.72
1:A:375:GLY:HA2	1:B:466:ILE:HG23	1.71	0.72
1:C:1087:ALA:HB2	1:C:1094:TYR:CD2	2.24	0.72
1:A:1084:LEU:HD23	1:A:1097:LEU:HD21	1.72	0.72
1:B:345:GLN:O	1:B:349:ASN:ND2	2.22	0.72
1:C:835:ILE:HD12	1:C:835:ILE:C	2.15	0.72
1:B:795:ILE:HA	1:B:798:VAL:CG1	2.19	0.72
1:C:676:PRO:HD2	1:C:711:GLN:CD	2.15	0.72
1:C:800:ASN:O	1:C:801:ARG:NE	2.23	0.71
1:D:817:ASP:OD2	1:D:819:ARG:CB	2.39	0.70
1:C:769:MET:CB	1:C:775:GLN:HG3	2.20	0.70
1:C:1027:VAL:HG23	1:C:1069:LEU:HD22	1.72	0.70
1:A:905:ARG:HG3	1:A:905:ARG:NH1	2.01	0.70
1:A:904:ILE:HD12	1:A:904:ILE:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:THR:HG23	1:B:864:LEU:HD11	1.73	0.70
1:C:898:VAL:HG13	1:C:953:TYR:CE1	2.25	0.70
1:B:1022:ALA:O	1:B:1025:LYS:HB3	1.92	0.70
1:C:352:LEU:HD22	1:C:1095:ARG:HE	1.56	0.70
1:A:1019:GLY:O	1:A:1023:ILE:HG22	1.91	0.70
1:D:1117:ASP:CA	1:D:1120:ILE:HG13	2.22	0.69
1:D:825:ASP:O	1:D:829:ALA:N	2.25	0.69
1:B:435:ARG:NH2	1:B:438:ASP:O	2.23	0.69
1:D:445:ALA:O	1:D:449:THR:OG1	2.09	0.69
1:D:817:ASP:CG	1:D:819:ARG:HG2	2.13	0.69
1:B:794:ALA:O	1:B:798:VAL:CG1	2.35	0.68
1:C:1002:TRP:O	1:C:1005:LEU:HD13	1.93	0.68
1:C:1003:MET:HG2	1:C:1004:PRO:HD3	1.74	0.68
1:B:634:ASP:HB3	1:B:640:LEU:HD12	1.74	0.68
1:B:676:PRO:HD2	1:B:711:GLN:OE1	1.92	0.68
1:C:999:ARG:HH12	1:C:1005:LEU:HA	1.57	0.68
1:A:1080:ASP:HB3	1:A:1083:VAL:HG23	1.76	0.68
1:B:827:PHE:HA	1:B:829:ALA:N	2.09	0.68
1:C:823:THR:HB	1:C:826:GLU:HB2	1.75	0.68
1:C:1075:GLN:HE22	1:C:1103:GLY:HA2	1.58	0.68
1:A:673:GLY:C	1:A:674:TYR:HD1	2.02	0.68
1:D:828:ASP:C	1:D:832:LYS:HD3	2.17	0.68
1:A:999:ARG:O	1:A:1000:LEU:HB2	1.94	0.68
1:C:793:ILE:HD11	1:C:804:MET:CG	2.24	0.68
1:C:896:THR:HG22	1:C:997:ASN:OD1	1.93	0.68
1:A:893:GLY:C	1:A:898:VAL:H	1.97	0.68
1:C:818:LEU:HD11	1:C:916:LEU:CD1	2.24	0.68
1:C:352:LEU:CD2	1:C:1095:ARG:HE	2.07	0.67
1:B:659:LEU:HD22	1:B:678:ILE:HD11	1.75	0.67
1:C:818:LEU:HD12	1:C:819:ARG:N	2.08	0.67
1:B:786:THR:HG21	1:B:846:THR:HG23	1.77	0.67
1:B:819:ARG:N	1:B:820:ASP:HA	2.09	0.67
1:D:407:PRO:HB3	1:D:611:ILE:HD12	1.75	0.67
1:A:702:ASP:OD1	1:A:729:LYS:NZ	2.24	0.67
1:C:822:ARG:HH11	1:C:823:THR:N	1.92	0.67
1:B:422:TRP:NE1	1:B:465:GLU:OE2	2.27	0.67
1:C:822:ARG:HA	1:C:822:ARG:HH11	1.58	0.67
1:A:483:THR:HB	1:A:804:MET:HE1	1.77	0.67
1:D:1099:VAL:HG11	1:D:1119:ILE:HG22	1.64	0.67
1:A:900:SER:O	1:A:904:ILE:CG2	2.32	0.67
1:D:828:ASP:HA	1:D:832:LYS:CD	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:820:ASP:OD1	1:D:820:ASP:N	2.27	0.66
1:D:1099:VAL:HG21	1:D:1108:PHE:HD1	1.59	0.66
1:A:700:ILE:O	1:A:704:VAL:HG12	1.95	0.66
1:A:670:TYR:CE1	1:A:987:PRO:HG2	2.31	0.66
1:A:721:GLN:HE21	1:A:721:GLN:N	1.94	0.66
1:D:1084:LEU:HA	1:D:1087:ALA:HB2	1.77	0.66
1:D:1117:ASP:HA	1:D:1120:ILE:CG1	2.26	0.65
1:C:995:THR:HA	1:C:996:PRO:C	2.21	0.65
1:D:843:ALA:O	1:D:847:VAL:HG23	1.97	0.65
1:D:826:GLU:C	1:D:830:ALA:H	2.04	0.65
1:D:1084:LEU:HA	1:D:1087:ALA:CB	2.27	0.65
1:C:803:ARG:HA	1:C:809:SER:O	1.97	0.65
1:B:824:PHE:CE2	1:B:827:PHE:CE1	2.86	0.64
1:C:640:LEU:HD13	1:C:645:ALA:CA	2.25	0.64
1:A:491:HIS:O	1:A:853:HIS:HE1	1.81	0.64
1:D:641:THR:OG1	1:D:644:THR:CB	2.45	0.64
1:C:796:GLU:CD	1:C:805:VAL:HG21	2.23	0.64
1:D:828:ASP:HB3	1:D:832:LYS:HZ3	1.62	0.64
1:B:827:PHE:HA	1:B:828:ASP:C	2.22	0.64
1:C:646:LEU:HD12	1:C:699:LEU:HD22	1.79	0.64
1:C:818:LEU:CD1	1:C:819:ARG:H	2.10	0.63
1:C:1003:MET:HG2	1:C:1004:PRO:CD	2.28	0.63
1:B:1020:PRO:HG2	1:B:1021:THR:N	2.14	0.63
1:C:819:ARG:HA	1:C:820:ASP:OD1	1.99	0.63
1:B:623:VAL:HG22	1:B:680:LEU:HD21	1.79	0.63
1:B:795:ILE:HA	1:B:798:VAL:HG12	1.79	0.62
1:B:854:ARG:HA	1:B:877:ALA:HB1	1.79	0.62
1:B:1022:ALA:O	1:B:1025:LYS:N	2.23	0.62
1:A:934:ARG:HD2	1:A:999:ARG:HA	1.82	0.62
1:B:822:ARG:CB	1:B:823:THR:HA	2.29	0.62
1:C:512:MET:HE2	1:C:515:ILE:HD12	1.82	0.62
1:B:1020:PRO:O	1:B:1023:ILE:HG22	2.00	0.62
1:C:1003:MET:CG	1:C:1004:PRO:HD3	2.28	0.62
1:C:1095:ARG:HD2	1:C:1095:ARG:C	2.24	0.62
1:D:826:GLU:HA	1:D:829:ALA:CB	2.16	0.61
1:B:1095:ARG:O	1:B:1109:VAL:CG2	2.46	0.61
1:C:806:LEU:HD13	1:C:991:LEU:HA	1.80	0.61
1:B:824:PHE:CZ	1:B:827:PHE:CE1	2.82	0.61
1:A:899:ASP:OD1	1:A:899:ASP:N	2.32	0.61
1:B:738:MET:O	1:B:1098:ILE:HG22	2.00	0.61
1:D:1083:VAL:O	1:D:1083:VAL:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:573:ARG:HD2	1:D:577:LEU:HG	1.81	0.61
1:D:623:VAL:HG22	1:D:680:LEU:HD21	1.82	0.61
1:D:640:LEU:HD21	1:D:644:THR:CG2	2.31	0.61
1:C:676:PRO:CD	1:C:711:GLN:CD	2.74	0.61
1:C:999:ARG:HH11	1:C:1005:LEU:HA	1.60	0.60
1:C:829:ALA:O	1:C:833:GLN:N	2.31	0.60
1:B:821:LEU:O	1:B:821:LEU:HD23	2.02	0.60
1:D:823:THR:O	1:D:823:THR:HG23	2.00	0.60
1:B:797:PHE:O	1:B:802:GLY:N	2.24	0.60
1:C:1002:TRP:O	1:C:1003:MET:C	2.45	0.60
1:A:682:VAL:CG1	1:A:697:THR:HG23	2.32	0.60
1:C:675:GLN:CG	1:C:1104:TYR:CD2	2.84	0.60
1:C:818:LEU:HD11	1:C:916:LEU:HD12	1.84	0.59
1:A:908:VAL:CG2	1:A:909:PHE:CD1	2.85	0.59
1:D:820:ASP:O	1:D:823:THR:HG22	2.02	0.59
1:C:898:VAL:HG13	1:C:953:TYR:CG	2.36	0.59
1:B:641:THR:O	1:B:644:THR:N	2.35	0.59
1:D:826:GLU:O	1:D:829:ALA:N	2.35	0.59
1:B:776:LYS:HD2	1:B:779:ARG:HD2	1.84	0.59
1:D:736:ALA:HB3	1:D:738:MET:HE2	1.84	0.59
1:C:675:GLN:HG3	1:C:1104:TYR:CD2	2.38	0.59
1:C:806:LEU:HD11	1:C:990:GLU:HB3	1.84	0.59
1:B:738:MET:HG2	1:B:1098:ILE:HG21	1.84	0.58
1:D:744:HIS:CE1	1:D:768:LEU:HD22	2.34	0.58
1:A:992:THR:O	1:A:993:ASN:O	2.22	0.58
1:D:953:TYR:N	1:D:953:TYR:CD1	2.72	0.58
1:A:1091:PRO:CD	1:A:1092:GLU:H	2.16	0.58
1:D:567:LYS:HD2	1:D:567:LYS:N	2.19	0.58
1:D:947:ASP:CG	1:D:949:TYR:H	2.02	0.58
1:C:1002:TRP:CD1	1:C:1002:TRP:N	2.72	0.58
1:A:491:HIS:O	1:A:853:HIS:CE1	2.56	0.58
1:A:1023:ILE:HD13	1:A:1023:ILE:O	2.04	0.58
1:B:900:SER:CB	1:B:997:ASN:CG	2.77	0.58
1:A:371:LYS:HD3	1:A:457:PHE:CE1	2.39	0.57
1:A:847:VAL:HA	1:A:850:GLN:HE21	1.69	0.57
1:D:744:HIS:CE1	1:D:768:LEU:HD23	2.39	0.57
1:B:531:PRO:HA	1:B:534:ILE:HD12	1.86	0.57
1:C:1093:LYS:HB2	1:C:1094:TYR:CE1	2.38	0.57
1:D:607:SER:HA	1:D:659:LEU:HD11	1.86	0.57
1:D:708:LYS:O	1:D:1098:ILE:CD1	2.51	0.57
1:D:1084:LEU:HD12	1:D:1084:LEU:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:ILE:O	1:A:991:LEU:CD2	2.53	0.57
1:C:997:ASN:ND2	1:C:999:ARG:H	2.02	0.57
1:D:1087:ALA:HB3	1:D:1108:PHE:HE2	1.68	0.57
1:A:728:GLU:OE2	1:A:1056:ARG:NE	2.37	0.57
1:A:819:ARG:NH1	1:A:819:ARG:HA	2.20	0.57
1:A:1094:TYR:CD1	1:A:1094:TYR:N	2.72	0.57
1:A:674:TYR:N	1:A:674:TYR:CD1	2.73	0.57
1:A:708:LYS:HG3	1:A:738:MET:HE2	1.87	0.57
1:D:1099:VAL:HG21	1:D:1108:PHE:CD1	2.39	0.57
1:D:1116:GLN:C	1:D:1120:ILE:CD1	2.77	0.57
1:A:708:LYS:HG2	1:A:738:MET:HG2	1.87	0.56
1:A:924:LEU:N	1:A:926:ASN:OD1	2.39	0.56
1:C:930:TYR:CD2	1:C:933:LEU:HB2	2.41	0.56
1:D:712:PRO:O	1:D:740:PHE:CZ	2.59	0.56
1:C:804:MET:O	1:C:808:ASP:N	2.35	0.56
1:C:928:GLU:OE1	1:C:928:GLU:N	2.33	0.56
1:D:1075:GLN:OE1	1:D:1102:ALA:HA	2.06	0.56
1:C:671:PHE:N	1:C:671:PHE:CD1	2.73	0.56
1:C:1003:MET:HG2	1:C:1004:PRO:N	2.20	0.56
1:B:947:ASP:O	1:B:950:VAL:N	2.39	0.56
1:B:995:THR:O	1:B:997:ASN:N	2.34	0.56
1:D:815:THR:CB	1:D:816:GLY:CA	2.84	0.56
1:D:1117:ASP:N	1:D:1120:ILE:HG13	2.20	0.56
1:A:720:ASN:N	1:A:720:ASN:OD1	2.39	0.56
1:B:824:PHE:CE2	1:B:827:PHE:HE1	2.23	0.56
1:D:411:PRO:O	1:D:412:ARG:HB2	2.05	0.55
1:D:708:LYS:O	1:D:1098:ILE:HD12	2.07	0.55
1:A:904:ILE:HD12	1:A:904:ILE:C	2.30	0.55
1:A:354:VAL:HG11	1:A:411:PRO:HB2	1.88	0.55
1:A:356:PRO:HG2	1:A:674:TYR:CE2	2.42	0.55
1:B:1025:LYS:O	1:B:1025:LYS:HG2	2.06	0.55
1:C:1003:MET:HB3	1:C:1004:PRO:CD	2.36	0.55
1:A:579:THR:O	1:A:583:VAL:HG23	2.06	0.55
1:B:507:LEU:HD11	1:B:588:PRO:HB2	1.89	0.55
1:B:641:THR:N	1:B:644:THR:HG1	1.89	0.55
1:B:817:ASP:CB	1:B:818:LEU:HA	2.25	0.55
1:C:642:HIS:C	1:C:642:HIS:CD2	2.85	0.55
1:D:828:ASP:O	1:D:832:LYS:HD3	2.06	0.55
1:B:819:ARG:C	1:B:819:ARG:HD2	2.32	0.55
1:B:1020:PRO:HG2	1:B:1021:THR:H	1.70	0.55
1:C:676:PRO:HD3	1:C:711:GLN:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:819:ARG:CG	1:C:917:GLU:OE2	2.53	0.55
1:D:640:LEU:CD2	1:D:644:THR:CB	2.83	0.55
1:A:796:GLU:OE1	1:A:992:THR:O	2.25	0.55
1:C:646:LEU:HD13	1:C:699:LEU:CD2	2.33	0.55
1:D:603:TRP:CH2	1:D:659:LEU:HD13	2.42	0.55
1:D:950:VAL:HG13	1:D:951:ASP:N	2.22	0.55
1:A:687:ARG:NH2	1:A:761:GLU:OE1	2.39	0.55
1:A:1101:VAL:HG22	1:A:1111:LEU:HD21	1.90	0.55
1:B:897:TYR:CD1	1:B:957:ILE:CD1	2.90	0.55
1:A:758:PHE:CE1	1:A:883:VAL:HG21	2.42	0.54
1:C:1084:LEU:HD23	1:C:1097:LEU:HD21	1.88	0.54
1:D:637:GLU:O	1:D:639:ARG:HG2	2.06	0.54
1:D:642:HIS:C	1:D:642:HIS:CD2	2.85	0.54
1:B:561:ALA:HB3	1:B:581:ALA:HB2	1.89	0.54
1:B:1113:LYS:HG3	1:B:1114:GLU:H	1.71	0.54
1:C:1094:TYR:N	1:C:1094:TYR:CD1	2.73	0.54
1:D:631:PHE:CE1	1:D:635:ILE:HG13	2.42	0.54
1:C:824:PHE:CD1	1:C:824:PHE:C	2.86	0.54
1:B:822:ARG:CB	1:B:823:THR:CA	2.85	0.54
1:C:371:LYS:HD3	1:C:457:PHE:CD1	2.42	0.54
1:C:818:LEU:HD11	1:C:916:LEU:HD13	1.89	0.54
1:B:801:ARG:HD3	1:B:814:ASP:OD1	2.08	0.54
1:D:947:ASP:OD1	1:D:950:VAL:N	2.41	0.54
1:A:893:GLY:HA3	1:A:897:TYR:CA	2.37	0.54
1:A:907:LEU:H	1:A:908:VAL:HG22	1.73	0.54
1:B:801:ARG:NH2	1:B:818:LEU:O	2.40	0.54
1:C:898:VAL:CG1	1:C:953:TYR:CD1	2.79	0.54
1:C:1093:LYS:C	1:C:1094:TYR:CD1	2.85	0.54
1:A:832:LYS:HG2	1:A:960:TRP:CZ2	2.43	0.54
1:B:369:VAL:HG21	1:B:385:ALA:HA	1.90	0.54
1:C:717:ARG:NH2	1:C:764:ARG:O	2.41	0.54
1:A:675:GLN:OE1	1:A:711:GLN:OE1	2.27	0.53
1:D:953:TYR:H	1:D:953:TYR:HD1	1.55	0.53
1:B:634:ASP:CB	1:B:640:LEU:HD12	2.38	0.53
1:C:1003:MET:CG	1:C:1004:PRO:CD	2.86	0.53
1:C:1003:MET:CB	1:C:1004:PRO:CD	2.86	0.53
1:D:697:THR:HG22	1:D:701:MET:HE2	1.89	0.53
1:C:641:THR:O	1:C:644:THR:OG1	2.24	0.53
1:D:400:ASP:C	1:D:573:ARG:HH22	2.13	0.53
1:D:1116:GLN:C	1:D:1120:ILE:HD11	2.34	0.53
1:A:1091:PRO:HD2	1:A:1092:GLU:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:822:ARG:HH11	1:C:822:ARG:CA	2.20	0.53
1:D:828:ASP:HB3	1:D:832:LYS:NZ	2.22	0.53
1:C:631:PHE:CZ	1:C:635:ILE:HG13	2.44	0.53
1:C:1046:LEU:HD22	1:C:1126:GLU:CG	2.39	0.53
1:D:828:ASP:HA	1:D:832:LYS:HD3	1.89	0.53
1:A:673:GLY:C	1:A:674:TYR:CD1	2.85	0.53
1:D:896:THR:O	1:D:900:SER:OG	2.21	0.53
1:C:902:ALA:C	1:C:904:ILE:H	2.17	0.53
1:D:824:PHE:C	1:D:826:GLU:H	2.17	0.53
1:B:657:ALA:HB2	1:B:711:GLN:O	2.09	0.52
1:C:1004:PRO:O	1:C:1005:LEU:HD13	2.09	0.52
1:A:1094:TYR:N	1:A:1094:TYR:HD1	2.08	0.52
1:B:750:ILE:O	1:B:754:LEU:HG	2.09	0.52
1:B:682:VAL:HG13	1:B:697:THR:HG23	1.91	0.52
1:C:552:ASN:O	1:C:556:ARG:HG3	2.10	0.52
1:C:804:MET:HE2	1:C:807:PHE:HB2	1.92	0.52
1:D:731:VAL:HG13	1:D:1059:LEU:HD23	1.92	0.52
1:D:826:GLU:N	1:D:829:ALA:HB3	2.23	0.52
1:A:907:LEU:HD12	1:A:907:LEU:C	2.34	0.52
1:A:1019:GLY:HA3	1:A:1022:ALA:HB3	1.92	0.52
1:D:1084:LEU:O	1:D:1087:ALA:HB3	2.10	0.52
1:C:969:LYS:O	1:C:970:MET:HE2	2.10	0.52
1:C:1075:GLN:NE2	1:C:1103:GLY:HA2	2.25	0.52
1:D:775:GLN:NE2	1:D:780:ILE:HG21	2.24	0.52
1:B:393:ALA:O	1:B:556:ARG:NH2	2.41	0.52
1:C:920:ARG:O	1:C:924:LEU:N	2.38	0.52
1:C:1021:THR:HG23	1:C:1024:ILE:HD11	1.92	0.52
1:D:744:HIS:CD2	1:D:768:LEU:CD2	2.92	0.52
1:D:1109:VAL:HG23	1:D:1110:GLU:HG3	1.92	0.52
1:C:599:LEU:HD22	1:C:652:PHE:CD2	2.45	0.51
1:B:539:TYR:CD1	1:B:539:TYR:C	2.88	0.51
1:B:605:VAL:HG11	1:B:865:LEU:HD11	1.93	0.51
1:C:930:TYR:CE2	1:C:933:LEU:HB2	2.45	0.51
1:B:362:ARG:O	1:B:363:ALA:C	2.53	0.51
1:C:675:GLN:HG2	1:C:1104:TYR:CE2	2.45	0.51
1:C:1090:GLU:HG2	1:C:1094:TYR:CE1	2.45	0.51
1:A:789:THR:O	1:A:892:SER:CB	2.58	0.51
1:A:999:ARG:O	1:A:999:ARG:HG2	2.11	0.51
1:B:1020:PRO:CG	1:B:1021:THR:N	2.73	0.51
1:D:401:GLU:O	1:D:573:ARG:NH2	2.44	0.51
1:D:489:SER:O	1:D:490:TYR:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:623:VAL:CG2	1:D:680:LEU:HD21	2.41	0.51
1:A:1020:PRO:HA	1:A:1023:ILE:HG22	1.92	0.51
1:A:1094:TYR:HD1	1:A:1094:TYR:H	1.58	0.51
1:B:799:LEU:HD12	1:B:923:LEU:HD23	1.93	0.51
1:D:613:GLU:O	1:D:615:GLN:HG2	2.10	0.51
1:C:818:LEU:CG	1:C:819:ARG:N	2.73	0.51
1:C:835:ILE:HD12	1:C:835:ILE:O	2.11	0.51
1:C:898:VAL:CG1	1:C:953:TYR:CG	2.93	0.51
1:B:613:GLU:O	1:B:615:GLN:OE1	2.28	0.51
1:D:640:LEU:CD2	1:D:644:THR:CG2	2.89	0.51
1:A:504:ASP:HB3	1:A:626:TYR:CG	2.46	0.51
1:A:911:GLU:OE2	1:A:913:LYS:HE3	2.11	0.51
1:A:1066:ALA:HB1	1:A:1071:ASN:ND2	2.23	0.51
1:C:822:ARG:HD3	1:C:822:ARG:O	2.10	0.51
1:C:1100:ARG:HA	1:C:1105:SER:HA	1.93	0.51
1:D:894:LEU:HD12	1:D:954:ALA:O	2.11	0.51
1:B:1114:GLU:HG2	1:B:1115:VAL:CG2	2.41	0.50
1:C:995:THR:HA	1:C:996:PRO:O	2.12	0.50
1:C:364:LEU:HD21	1:C:454:ILE:HD11	1.93	0.50
1:D:793:ILE:HG13	1:D:797:PHE:CE2	2.46	0.50
1:A:708:LYS:O	1:A:709:VAL:HG13	2.11	0.50
1:D:711:GLN:HG3	1:D:712:PRO:HA	1.92	0.50
1:D:1046:LEU:HD13	1:D:1124:VAL:HG11	1.93	0.50
1:C:829:ALA:HA	1:C:832:LYS:HB3	1.93	0.50
1:D:775:GLN:NE2	1:D:780:ILE:CG2	2.75	0.50
1:B:342:PRO:HA	1:B:345:GLN:HB2	1.94	0.50
1:B:729:LYS:O	1:B:733:VAL:HG23	2.11	0.50
1:C:500:CYS:SG	1:C:769:MET:HA	2.51	0.50
1:C:794:ALA:HB1	1:C:834:GLN:HB3	1.92	0.50
1:C:809:SER:OG	1:C:810:TYR:N	2.44	0.50
1:C:818:LEU:CD1	1:C:916:LEU:HD12	2.42	0.50
1:A:925:ALA:N	1:A:926:ASN:OD1	2.45	0.50
1:A:386:PHE:CE2	1:A:546:THR:HG23	2.46	0.50
1:A:718:ILE:N	1:A:744:HIS:O	2.44	0.50
1:B:827:PHE:N	1:B:828:ASP:HB2	2.27	0.50
1:D:789:THR:HG23	1:D:891:PHE:CE1	2.46	0.50
1:D:828:ASP:CA	1:D:832:LYS:HD3	2.41	0.50
1:A:893:GLY:CA	1:A:897:TYR:H	2.25	0.50
1:A:1091:PRO:CG	1:A:1092:GLU:N	2.73	0.50
1:C:806:LEU:HB2	1:C:991:LEU:HA	1.94	0.50
1:D:1075:GLN:NE2	1:D:1103:GLY:H	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ARG:HH22	1:A:468:GLU:HG3	1.77	0.50
1:C:675:GLN:CG	1:C:1104:TYR:CE2	2.95	0.50
1:C:1111:LEU:HD23	1:C:1115:VAL:HG23	1.94	0.50
1:C:819:ARG:CB	1:C:917:GLU:OE2	2.60	0.49
1:A:358:VAL:HG11	1:A:442:ILE:HD12	1.94	0.49
1:A:908:VAL:HG23	1:A:909:PHE:CE1	2.46	0.49
1:C:995:THR:CA	1:C:996:PRO:C	2.86	0.49
1:C:609:PHE:HB3	1:C:618:LEU:HD21	1.94	0.49
1:C:1001:ALA:HB3	1:C:1003:MET:HB3	1.94	0.49
1:D:825:ASP:C	1:D:829:ALA:CB	2.85	0.49
1:A:935:ARG:CG	1:A:999:ARG:HD3	2.42	0.49
1:A:1093:LYS:HD2	1:A:1093:LYS:H	1.73	0.49
1:C:376:MET:HE1	1:D:473:GLU:HG2	1.95	0.49
1:C:997:ASN:ND2	1:C:999:ARG:N	2.60	0.49
1:D:401:GLU:N	1:D:573:ARG:NH2	2.60	0.49
1:A:710:TYR:CD1	1:A:1107:TYR:CE2	3.01	0.49
1:C:850:GLN:OE1	1:C:971:LEU:HB2	2.13	0.49
1:C:917:GLU:OE1	1:C:917:GLU:HA	2.13	0.49
1:C:1111:LEU:HB3	1:C:1115:VAL:CG2	2.43	0.49
1:D:358:VAL:HG21	1:D:432:MET:HE1	1.94	0.49
1:D:825:ASP:O	1:D:828:ASP:N	2.45	0.49
1:A:909:PHE:HB3	1:A:912:LYS:HA	1.95	0.49
1:D:1075:GLN:NE2	1:D:1103:GLY:HA2	2.27	0.49
1:A:947:ASP:O	1:A:950:VAL:N	2.46	0.49
1:B:1114:GLU:HG3	1:B:1118:GLU:OE1	2.13	0.49
1:C:667:GLY:O	1:C:671:PHE:CD1	2.66	0.49
1:A:659:LEU:HD23	1:A:678:ILE:HD11	1.95	0.49
1:A:991:LEU:HD22	1:A:991:LEU:H	1.78	0.49
1:B:824:PHE:O	1:B:824:PHE:HD1	1.96	0.49
1:D:1083:VAL:O	1:D:1087:ALA:HB2	2.13	0.49
1:A:993:ASN:CB	1:A:994:ALA:HA	2.16	0.49
1:C:744:HIS:CD2	1:C:768:LEU:HD11	2.47	0.49
1:A:463:LEU:HD11	1:A:853:HIS:ND1	2.28	0.48
1:C:818:LEU:CD1	1:C:819:ARG:N	2.72	0.48
1:C:995:THR:HB	1:C:997:ASN:N	2.28	0.48
1:C:1046:LEU:HD22	1:C:1126:GLU:HG3	1.95	0.48
1:A:955:LEU:HA	1:A:958:THR:OG1	2.13	0.48
1:C:701:MET:HE1	1:C:726:TYR:CE2	2.48	0.48
1:C:800:ASN:C	1:C:801:ARG:CG	2.85	0.48
1:B:726:TYR:CE2	1:B:730:ILE:HD11	2.48	0.48
1:C:609:PHE:CE1	1:C:862:MET:HE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:PRO:HA	1:D:412:ARG:O	2.13	0.48
1:A:659:LEU:CD2	1:A:678:ILE:HD11	2.43	0.48
1:B:814:ASP:CB	1:B:815:THR:HA	2.44	0.48
1:C:587:VAL:HG21	1:C:597:GLU:O	2.14	0.48
1:A:340:LEU:HD12	1:A:345:GLN:HE21	1.78	0.48
1:A:985:ASN:HA	1:A:988:ILE:HG13	1.96	0.48
1:C:828:ASP:OD1	1:C:832:LYS:HB2	2.14	0.48
1:D:957:ILE:HD12	1:D:957:ILE:N	2.22	0.48
1:C:1003:MET:HB3	1:C:1004:PRO:HD2	1.95	0.48
1:D:817:ASP:OD2	1:D:819:ARG:CA	2.62	0.48
1:B:1114:GLU:HG2	1:B:1115:VAL:HG23	1.95	0.48
1:C:899:ASP:HB2	1:C:997:ASN:HB3	1.95	0.48
1:C:340:LEU:HD23	1:C:650:GLN:HE22	1.78	0.47
1:D:446:ASP:O	1:D:450:ILE:HD12	2.14	0.47
1:A:901:MET:SD	1:A:957:ILE:HD13	2.54	0.47
1:B:820:ASP:CA	1:B:821:LEU:CB	2.85	0.47
1:B:827:PHE:HA	1:B:829:ALA:H	1.78	0.47
1:B:827:PHE:N	1:B:827:PHE:CD1	2.81	0.47
1:B:1017:LYS:N	1:B:1018:GLN:OE1	2.47	0.47
1:A:426:ARG:NH2	1:A:427:ASP:OD1	2.42	0.47
1:A:682:VAL:HG12	1:A:697:THR:HG23	1.96	0.47
1:A:993:ASN:HB2	1:A:1001:ALA:HA	1.96	0.47
1:B:412:ARG:HB3	1:B:660:MET:HE3	1.95	0.47
1:A:671:PHE:CD1	1:A:671:PHE:N	2.82	0.47
1:C:822:ARG:HA	1:C:822:ARG:CZ	2.42	0.47
1:D:640:LEU:HD13	1:D:645:ALA:HB2	1.95	0.47
1:A:897:TYR:HA	1:A:900:SER:HB2	1.96	0.47
1:B:780:ILE:HG12	1:B:781:TYR:N	2.28	0.47
1:B:897:TYR:CE1	1:B:957:ILE:HG21	2.49	0.47
1:D:824:PHE:C	1:D:826:GLU:N	2.73	0.47
1:A:854:ARG:HA	1:A:877:ALA:HB1	1.96	0.47
1:B:820:ASP:HA	1:B:821:LEU:HB2	1.93	0.47
1:C:634:ASP:O	1:C:638:GLY:N	2.47	0.47
1:C:818:LEU:HG	1:C:819:ARG:N	2.30	0.47
1:D:636:ARG:C	1:D:638:GLY:H	2.20	0.47
1:D:817:ASP:CG	1:D:818:LEU:N	2.73	0.47
1:D:1080:ASP:OD1	1:D:1082:GLU:N	2.30	0.47
1:B:722:SER:O	1:B:1064:ARG:NH1	2.44	0.47
1:C:768:LEU:N	1:C:768:LEU:CD2	2.77	0.47
1:D:947:ASP:CG	1:D:948:ASN:N	2.73	0.47
1:D:955:LEU:HA	1:D:958:THR:OG1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLY:HA2	1:A:615:GLN:HE21	1.79	0.47
1:B:406:HIS:CE1	1:B:411:PRO:HA	2.49	0.47
1:C:722:SER:O	1:C:1064:ARG:NH1	2.47	0.47
1:C:806:LEU:CD1	1:C:991:LEU:HA	2.45	0.47
1:C:1002:TRP:O	1:C:1005:LEU:HD22	2.14	0.47
1:A:789:THR:O	1:A:892:SER:HB2	2.14	0.47
1:B:396:LEU:HD22	1:B:409:GLY:O	2.14	0.47
1:C:526:LEU:HD22	1:C:533:ASP:CG	2.40	0.47
1:C:827:PHE:C	1:C:829:ALA:N	2.73	0.47
1:B:646:LEU:HG	1:B:650:GLN:HE21	1.80	0.46
1:C:996:PRO:HA	1:C:997:ASN:C	2.40	0.46
1:C:1002:TRP:O	1:C:1003:MET:O	2.32	0.46
1:D:653:ILE:HG22	1:D:709:VAL:HG21	1.97	0.46
1:A:816:GLY:O	1:A:821:LEU:HG	2.14	0.46
1:B:694:ASN:O	1:B:697:THR:HB	2.14	0.46
1:B:955:LEU:HD23	1:B:956:ASP:H	1.76	0.46
1:D:395:ILE:HG23	1:D:557:ILE:HD13	1.96	0.46
1:B:697:THR:O	1:B:701:MET:HG3	2.14	0.46
1:B:800:ASN:N	1:B:800:ASN:HD22	2.13	0.46
1:B:900:SER:CB	1:B:997:ASN:HA	2.45	0.46
1:D:356:PRO:HG2	1:D:674:TYR:CZ	2.51	0.46
1:D:713:SER:HB2	1:D:1104:TYR:HA	1.96	0.46
1:C:416:PHE:CE1	1:C:425:VAL:HG11	2.50	0.46
1:A:438:ASP:OD1	1:A:673:GLY:N	2.47	0.46
1:B:790:GLN:OE1	1:B:992:THR:OG1	2.34	0.46
1:D:420:ILE:HD11	1:D:613:GLU:OE1	2.15	0.46
1:B:370:VAL:HG13	1:B:381:LEU:HD21	1.97	0.46
1:A:437:GLN:NE2	1:A:1110:GLU:O	2.47	0.46
1:C:395:ILE:HG22	1:C:560:HIS:CD2	2.51	0.46
1:C:437:GLN:CD	1:C:672:ALA:HB1	2.41	0.46
1:A:997:ASN:HD22	1:A:997:ASN:C	2.24	0.46
1:C:822:ARG:NH1	1:C:823:THR:N	2.61	0.46
1:D:490:TYR:C	1:D:490:TYR:CD1	2.93	0.46
1:A:1020:PRO:O	1:A:1023:ILE:HG22	2.16	0.45
1:A:680:LEU:HD23	1:A:680:LEU:C	2.42	0.45
1:A:904:ILE:HB	1:A:996:PRO:HD2	1.99	0.45
1:B:386:PHE:CZ	1:B:861:LEU:HD22	2.51	0.45
1:C:501:PRO:HG3	1:C:862:MET:HE1	1.98	0.45
1:C:801:ARG:O	1:C:810:TYR:CZ	2.69	0.45
1:B:680:LEU:C	1:B:680:LEU:HD23	2.41	0.45
1:C:546:THR:HG21	1:C:860:PRO:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:PRO:CG	1:A:1092:GLU:H	2.29	0.45
1:B:1099:VAL:HG21	1:B:1108:PHE:CD1	2.51	0.45
1:C:510:LYS:NZ	1:C:518:ASP:OD2	2.48	0.45
1:D:546:THR:HG23	1:D:864:LEU:HD11	1.97	0.45
1:A:850:GLN:HB3	1:A:971:LEU:HD22	1.97	0.45
1:B:818:LEU:H	1:B:821:LEU:CD2	2.09	0.45
1:B:832:LYS:HA	1:B:835:ILE:HG22	1.97	0.45
1:A:728:GLU:OE2	1:A:1056:ARG:NH2	2.50	0.45
1:A:791:TRP:HB3	1:A:901:MET:HG3	1.99	0.45
1:A:848:ILE:O	1:A:852:VAL:HG13	2.17	0.45
1:A:997:ASN:O	1:A:997:ASN:ND2	2.46	0.45
1:B:824:PHE:O	1:B:825:ASP:CB	2.50	0.45
1:B:827:PHE:N	1:B:828:ASP:CB	2.80	0.45
1:C:646:LEU:CD1	1:C:699:LEU:CD2	2.90	0.45
1:D:450:ILE:C	1:D:455:VAL:HG23	2.42	0.45
1:A:539:TYR:CD2	1:A:539:TYR:C	2.94	0.45
1:B:803:ARG:HG3	1:B:810:TYR:CZ	2.52	0.45
1:C:997:ASN:OD1	1:C:999:ARG:HB2	2.16	0.45
1:C:992:THR:O	1:C:1002:TRP:CE3	2.70	0.45
1:D:697:THR:HG22	1:D:701:MET:CE	2.46	0.45
1:A:1091:PRO:HG2	1:A:1092:GLU:N	2.32	0.45
1:B:720:ASN:OD1	1:B:1067:SER:OG	2.33	0.45
1:C:544:ILE:HG22	1:C:545:GLU:N	2.32	0.45
1:D:713:SER:CB	1:D:1103:GLY:O	2.65	0.45
1:D:1090:GLU:O	1:D:1093:LYS:N	2.50	0.45
1:A:376:MET:HB3	1:A:381:LEU:HB2	1.99	0.45
1:B:887:PRO:HD2	1:B:970:MET:HG3	1.99	0.45
1:C:895:ALA:O	1:C:896:THR:C	2.58	0.45
1:C:915:THR:O	1:C:919:ILE:HG13	2.17	0.45
1:A:719:HIS:CD2	1:A:721:GLN:HB2	2.52	0.44
1:B:649:LEU:HD22	1:B:700:ILE:HG12	1.99	0.44
1:C:565:ALA:HB2	1:C:577:LEU:HB3	1.99	0.44
1:C:599:LEU:HD22	1:C:652:PHE:CG	2.52	0.44
1:A:797:PHE:HB2	1:A:834:GLN:HG2	1.99	0.44
1:A:949:TYR:CD1	1:A:949:TYR:O	2.70	0.44
1:B:396:LEU:HG	1:B:396:LEU:O	2.16	0.44
1:B:1114:GLU:HG2	1:B:1115:VAL:N	2.32	0.44
1:D:861:LEU:HD12	1:D:864:LEU:HD12	1.99	0.44
1:A:518:ASP:O	1:A:521:ALA:HB3	2.18	0.44
1:D:442:ILE:HG12	1:D:447:LYS:HG3	2.00	0.44
1:D:674:TYR:O	1:D:676:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:807:PHE:HB2	1:D:809:SER:HB2	1.98	0.44
1:D:950:VAL:HG13	1:D:951:ASP:CG	2.42	0.44
1:D:1081:ASN:O	1:D:1084:LEU:HD11	2.17	0.44
1:C:582:GLU:O	1:C:586:ASN:ND2	2.51	0.44
1:D:428:GLU:OE2	1:D:665:GLU:N	2.50	0.44
1:B:803:ARG:HG3	1:B:810:TYR:CE2	2.52	0.44
1:C:833:GLN:CD	1:C:833:GLN:C	2.85	0.44
1:D:504:ASP:HB3	1:D:626:TYR:CD1	2.53	0.44
1:D:573:ARG:HD2	1:D:577:LEU:CG	2.45	0.44
1:D:633:ALA:HB1	1:D:639:ARG:HH21	1.82	0.44
1:B:824:PHE:O	1:B:824:PHE:CD1	2.70	0.44
1:C:423:ARG:NH1	1:C:464:ASP:OD2	2.51	0.44
1:C:827:PHE:C	1:C:829:ALA:H	2.26	0.44
1:D:396:LEU:CD2	1:D:411:PRO:HD3	2.48	0.44
1:D:801:ARG:HA	1:D:815:THR:OG1	2.16	0.44
1:D:1087:ALA:CB	1:D:1108:PHE:CE2	2.95	0.44
1:A:910:GLU:O	1:A:910:GLU:HG3	2.18	0.44
1:C:565:ALA:O	1:C:568:GLU:HB3	2.18	0.44
1:D:728:GLU:HA	1:D:1060:ILE:HD11	1.99	0.44
1:D:825:ASP:C	1:D:829:ALA:HB3	2.42	0.44
1:A:1091:PRO:CD	1:A:1092:GLU:N	2.79	0.43
1:B:814:ASP:HB3	1:B:816:GLY:N	2.33	0.43
1:B:819:ARG:N	1:B:820:ASP:CA	2.79	0.43
1:C:800:ASN:HD21	1:C:924:LEU:CD1	2.31	0.43
1:A:952:GLN:HE21	1:A:952:GLN:HB3	1.63	0.43
1:C:520:GLU:CG	1:C:544:ILE:HD11	2.47	0.43
1:C:1044:LYS:NZ	1:C:1119:ILE:O	2.51	0.43
1:C:1062:LEU:HG	1:C:1074:MET:HE1	2.01	0.43
1:D:950:VAL:CG1	1:D:951:ASP:N	2.81	0.43
1:A:503:TYR:OH	1:A:606:GLU:OE1	2.26	0.43
1:A:704:VAL:HG11	1:A:714:LEU:HD22	1.99	0.43
1:B:792:PRO:HB2	1:B:795:ILE:HG12	2.00	0.43
1:A:1084:LEU:CD2	1:A:1097:LEU:CD2	2.92	0.43
1:B:904:ILE:HD11	1:B:996:PRO:CG	2.48	0.43
1:D:448:LYS:HZ3	1:D:452:GLU:CD	2.05	0.43
1:A:423:ARG:HH11	1:A:423:ARG:HG3	1.83	0.43
1:A:455:VAL:N	1:A:456:PRO:CD	2.81	0.43
1:A:599:LEU:HD11	1:A:649:LEU:HD23	2.01	0.43
1:A:900:SER:O	1:A:904:ILE:N	2.50	0.43
1:B:904:ILE:HD11	1:B:996:PRO:HG3	2.01	0.43
1:C:744:HIS:CD2	1:C:768:LEU:CD1	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:817:ASP:HB3	1:D:820:ASP:CG	2.37	0.43
1:D:947:ASP:OD1	1:D:948:ASN:N	2.51	0.43
1:A:805:VAL:O	1:A:806:LEU:C	2.61	0.43
1:B:721:GLN:NE2	1:C:1069:LEU:HA	2.34	0.43
1:C:344:MET:HE1	1:C:651:ALA:HB2	2.00	0.43
1:D:636:ARG:NH1	1:D:636:ARG:HB3	2.34	0.43
1:D:640:LEU:HD13	1:D:645:ALA:CA	2.49	0.43
1:B:819:ARG:C	1:B:819:ARG:CD	2.91	0.43
1:D:1111:LEU:HD13	1:D:1111:LEU:N	2.34	0.43
1:A:395:ILE:HG13	1:A:557:ILE:HD13	1.99	0.43
1:A:397:ILE:HG23	1:A:404:VAL:HG21	2.01	0.43
1:B:502:GLY:HA3	1:B:505:VAL:HG12	2.01	0.43
1:C:687:ARG:HD2	1:C:765:ASP:OD2	2.19	0.43
1:C:1064:ARG:O	1:C:1068:ILE:HD13	2.19	0.43
1:C:1099:VAL:HG11	1:C:1108:PHE:HD1	1.82	0.43
1:D:573:ARG:HD2	1:D:577:LEU:CD2	2.48	0.43
1:D:828:ASP:N	1:D:828:ASP:OD1	2.49	0.43
1:A:583:VAL:O	1:A:587:VAL:HG22	2.18	0.43
1:B:879:GLY:HA3	1:B:972:TYR:CD1	2.54	0.43
1:B:966:ARG:NH1	1:B:974:THR:O	2.52	0.43
1:C:848:ILE:O	1:C:849:SER:C	2.61	0.43
1:D:634:ASP:HB3	1:D:640:LEU:HB2	2.01	0.43
1:A:738:MET:CB	1:A:1098:ILE:HB	2.49	0.43
1:B:434:THR:O	1:B:434:THR:HG22	2.18	0.43
1:B:552:ASN:O	1:B:556:ARG:HG3	2.18	0.43
1:B:971:LEU:HD12	1:B:971:LEU:HA	1.87	0.43
1:D:358:VAL:CG2	1:D:432:MET:HE1	2.49	0.43
1:B:526:LEU:HD22	1:B:533:ASP:CG	2.43	0.42
1:D:1075:GLN:HE22	1:D:1103:GLY:H	1.66	0.42
1:C:819:ARG:O	1:C:819:ARG:HG3	2.19	0.42
1:D:773:GLU:OE2	1:D:980:LEU:HD13	2.19	0.42
1:D:1112:CYS:SG	1:D:1112:CYS:O	2.77	0.42
1:A:935:ARG:HG2	1:A:999:ARG:HD3	2.00	0.42
1:B:861:LEU:O	1:B:862:MET:C	2.60	0.42
1:C:340:LEU:HD23	1:C:650:GLN:NE2	2.33	0.42
1:C:622:ARG:NH1	1:C:765:ASP:OD1	2.41	0.42
1:D:986:THR:O	1:D:989:GLY:N	2.52	0.42
1:B:949:TYR:CD1	1:B:949:TYR:C	2.97	0.42
1:D:775:GLN:HE21	1:D:780:ILE:HG21	1.84	0.42
1:D:861:LEU:HA	1:D:864:LEU:HD12	2.01	0.42
1:B:663:SER:HB2	1:B:668:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1115:VAL:HG12	1:D:1119:ILE:HD11	2.01	0.42
1:C:678:ILE:CG2	1:C:712:PRO:HB3	2.49	0.42
1:A:483:THR:CB	1:A:804:MET:HE1	2.48	0.42
1:A:622:ARG:HD3	1:A:765:ASP:OD1	2.19	0.42
1:A:708:LYS:HD2	1:A:736:ALA:HB1	2.02	0.42
1:B:1020:PRO:CG	1:B:1021:THR:H	2.33	0.42
1:B:1099:VAL:HG12	1:B:1100:ARG:O	2.20	0.42
1:A:358:VAL:HG21	1:A:432:MET:HE1	2.01	0.42
1:A:358:VAL:CG1	1:A:442:ILE:HD12	2.49	0.42
1:A:819:ARG:HA	1:A:819:ARG:CZ	2.50	0.42
1:A:899:ASP:O	1:A:900:SER:C	2.63	0.42
1:C:542:ALA:O	1:C:546:THR:HG23	2.19	0.42
1:D:634:ASP:O	1:D:639:ARG:N	2.51	0.42
1:D:817:ASP:CG	1:D:818:LEU:H	2.27	0.42
1:A:758:PHE:CZ	1:A:883:VAL:HG21	2.55	0.42
1:B:442:ILE:HD11	1:B:450:ILE:HD12	2.01	0.42
1:C:915:THR:O	1:C:919:ILE:CG1	2.68	0.42
1:D:563:GLU:O	1:D:567:LYS:HD3	2.20	0.42
1:A:696:LEU:O	1:A:697:THR:C	2.62	0.42
1:B:820:ASP:CA	1:B:821:LEU:HB3	2.42	0.42
1:B:922:ALA:HB2	1:B:933:LEU:HD23	2.02	0.42
1:C:769:MET:N	1:C:773:GLU:O	2.46	0.42
1:A:803:ARG:HD2	1:A:808:ASP:HB2	2.02	0.41
1:A:1082:GLU:OE1	1:A:1086:LYS:NZ	2.53	0.41
1:B:625:GLN:NE2	1:B:692:ALA:HB1	2.35	0.41
1:B:799:LEU:HD12	1:B:923:LEU:CD2	2.50	0.41
1:B:879:GLY:HA3	1:B:972:TYR:CE1	2.55	0.41
1:B:1099:VAL:O	1:B:1105:SER:HA	2.20	0.41
1:B:1114:GLU:CG	1:B:1115:VAL:N	2.83	0.41
1:D:640:LEU:HD21	1:D:644:THR:HG22	2.02	0.41
1:C:640:LEU:HD11	1:C:648:LEU:HD12	2.01	0.41
1:C:800:ASN:HD21	1:C:924:LEU:HD12	1.85	0.41
1:D:358:VAL:HG12	1:D:359:SER:N	2.35	0.41
1:D:676:PRO:HD2	1:D:710:TYR:OH	2.20	0.41
1:D:680:LEU:HD23	1:D:680:LEU:C	2.45	0.41
1:D:840:ARG:O	1:D:843:ALA:HB3	2.21	0.41
1:A:371:LYS:HD3	1:A:457:PHE:CD1	2.56	0.41
1:B:704:VAL:HA	1:B:707:VAL:HG22	2.01	0.41
1:D:455:VAL:O	1:D:455:VAL:HG12	2.19	0.41
1:A:792:PRO:CD	1:A:897:TYR:CB	2.98	0.41
1:B:938:LEU:CD2	1:B:998:GLY:HA3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:PRO:O	1:C:674:TYR:OH	2.34	0.41
1:D:394:PRO:HG2	1:D:407:PRO:O	2.21	0.41
1:A:416:PHE:CE1	1:A:425:VAL:HG11	2.55	0.41
1:A:1084:LEU:HD22	1:A:1097:LEU:CD2	2.50	0.41
1:B:356:PRO:HA	1:B:412:ARG:O	2.21	0.41
1:B:679:ASN:OD1	1:B:715:ALA:HB2	2.21	0.41
1:C:676:PRO:HD3	1:C:711:GLN:CD	2.46	0.41
1:C:1051:ASP:OD1	1:C:1051:ASP:N	2.53	0.41
1:D:504:ASP:HB3	1:D:626:TYR:CG	2.55	0.41
1:A:395:ILE:HD13	1:A:556:ARG:NH1	2.35	0.41
1:A:710:TYR:HD1	1:A:1107:TYR:CE2	2.36	0.41
1:A:923:LEU:C	1:A:926:ASN:OD1	2.63	0.41
1:A:1095:ARG:NH1	1:A:1095:ARG:HG3	2.36	0.41
1:B:799:LEU:CD1	1:B:923:LEU:CD2	2.99	0.41
1:B:995:THR:HB	1:B:996:PRO:HD2	2.03	0.41
1:C:508:PHE:HE1	1:C:601:SER:HG	1.64	0.41
1:C:1090:GLU:N	1:C:1091:PRO:CD	2.84	0.41
1:A:823:THR:O	1:A:827:PHE:N	2.51	0.41
1:A:893:GLY:O	1:A:898:VAL:CB	2.69	0.41
1:B:814:ASP:HB3	1:B:815:THR:HA	2.03	0.41
1:B:819:ARG:HD2	1:B:819:ARG:O	2.20	0.41
1:C:352:LEU:HD23	1:C:1095:ARG:HH21	1.85	0.41
1:D:708:LYS:O	1:D:1098:ILE:HD11	2.20	0.41
1:D:769:MET:HE3	1:D:769:MET:HB3	1.85	0.41
1:A:653:ILE:HG23	1:A:712:PRO:HD2	2.03	0.41
1:B:350:HIS:O	1:B:351:TYR:C	2.64	0.41
1:C:830:ALA:O	1:C:834:GLN:HB2	2.20	0.41
1:D:359:SER:O	1:D:360:ILE:HG23	2.21	0.41
1:D:564:LEU:HB3	1:D:577:LEU:HD13	2.03	0.41
1:D:827:PHE:O	1:D:831:VAL:HG12	2.20	0.41
1:A:360:ILE:O	1:A:364:LEU:HG	2.21	0.40
1:A:504:ASP:HB3	1:A:626:TYR:CB	2.50	0.40
1:A:523:LEU:O	1:A:524:ALA:C	2.64	0.40
1:A:832:LYS:NZ	1:A:956:ASP:OD1	2.50	0.40
1:A:1093:LYS:N	1:A:1093:LYS:CD	2.73	0.40
1:A:1108:PHE:CE1	1:A:1116:GLN:HB2	2.56	0.40
1:B:1020:PRO:O	1:B:1023:ILE:CB	2.70	0.40
1:B:1099:VAL:HG21	1:B:1108:PHE:HD1	1.85	0.40
1:C:338:GLU:O	1:C:340:LEU:HG	2.22	0.40
1:D:1090:GLU:N	1:D:1091:PRO:HD3	2.36	0.40
1:B:407:PRO:HB2	1:B:611:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:ASP:O	1:B:831:VAL:HB	2.21	0.40
1:C:508:PHE:HE1	1:C:601:SER:OG	2.03	0.40
1:C:823:THR:HG22	1:C:826:GLU:N	2.36	0.40
1:D:428:GLU:OE1	1:D:435:ARG:NH1	2.54	0.40
1:D:742:ALA:HA	1:D:1075:GLN:HB3	2.03	0.40
1:A:894:LEU:HD11	1:A:979:THR:C	2.46	0.40
1:A:934:ARG:CD	1:A:999:ARG:HA	2.50	0.40
1:B:814:ASP:HB3	1:B:815:THR:CA	2.52	0.40
1:B:824:PHE:CD1	1:B:824:PHE:C	2.99	0.40
1:C:566:ALA:C	1:C:568:GLU:H	2.28	0.40
1:D:817:ASP:CB	1:D:820:ASP:OD1	2.47	0.40
1:D:947:ASP:HB3	1:D:950:VAL:HG12	2.02	0.40
1:A:415:ALA:HB3	1:A:610:GLU:O	2.22	0.40
1:B:341:THR:OG1	1:B:647:GLU:OE2	2.14	0.40
1:B:478:ALA:O	1:B:483:THR:OG1	2.35	0.40
1:B:837:HIS:CE1	1:B:841:LEU:HD13	2.56	0.40
1:D:582:GLU:O	1:D:586:ASN:ND2	2.55	0.40
1:C:429:LEU:HB3	1:C:447:LYS:HD2	2.04	0.40
1:C:588:PRO:O	1:C:589:ALA:C	2.64	0.40
1:C:675:GLN:HG3	1:C:1104:TYR:CE2	2.57	0.40
1:C:1090:GLU:CG	1:C:1094:TYR:CE1	3.04	0.40

There are no symmetry-related clashes.

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	740/792 (93%)	656 (89%)	76 (10%)	8 (1%)	11	43
1	B	734/792 (93%)	664 (90%)	66 (9%)	4 (0%)	24	60
1	C	734/792 (93%)	661 (90%)	69 (9%)	4 (0%)	24	60
1	D	700/792 (88%)	635 (91%)	60 (9%)	5 (1%)	18	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2908/3168 (92%)	2616 (90%)	271 (9%)	21 (1%)	18	53

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	825	ASP
1	C	996	PRO
1	C	1003	MET
1	D	825	ASP
1	A	810	TYR
1	A	993	ASN
1	D	496	GLY
1	A	907	LEU
1	A	1000	LEU
1	B	1020	PRO
1	C	934	ARG
1	A	804	MET
1	A	908	VAL
1	B	792	PRO
1	D	442	ILE
1	D	1113	LYS
1	B	442	ILE
1	C	534	ILE
1	D	360	ILE
1	A	373	ASN
1	A	500	CYS

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	624/668 (93%)	536 (86%)	88 (14%)	3	16
1	B	618/668 (92%)	540 (87%)	78 (13%)	4	20
1	C	617/668 (92%)	534 (86%)	83 (14%)	4	18
1	D	580/668 (87%)	488 (84%)	92 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2439/2672 (91%)	2098 (86%)	341 (14%)	3 16

All (341) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	GLU
1	A	404	VAL
1	A	417	SER
1	A	423	ARG
1	A	429	LEU
1	A	431	THR
1	A	433	SER
1	A	453	GLU
1	A	468	GLU
1	A	499	THR
1	A	527	SER
1	A	529	GLU
1	A	593	LYS
1	A	618	LEU
1	A	623	VAL
1	A	630	MET
1	A	634	ASP
1	A	641	THR
1	A	669	LYS
1	A	671	PHE
1	A	674	TYR
1	A	705	ARG
1	A	720	ASN
1	A	721	GLN
1	A	722	SER
1	A	724	GLN
1	A	738	MET
1	A	752	MET
1	A	768	LEU
1	A	776	LYS
1	A	784	THR
1	A	786	THR
1	A	798	VAL
1	A	803	ARG
1	A	807	PHE
1	A	808	ASP
1	A	809	SER

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Mol	Chain	Res	Type
1	A	818	LEU
1	A	823	THR
1	A	834	GLN
1	A	852	VAL
1	A	856	VAL
1	A	875	ASP
1	A	896	THR
1	A	899	ASP
1	A	904	ILE
1	A	905	ARG
1	A	908	VAL
1	A	909	PHE
1	A	910	GLU
1	A	912	LYS
1	A	916	LEU
1	A	918	GLN
1	A	933	LEU
1	A	935	ARG
1	A	952	GLN
1	A	956	ASP
1	A	957	ILE
1	A	971	LEU
1	A	977	HIS
1	A	979	THR
1	A	985	ASN
1	A	988	ILE
1	A	990	GLU
1	A	991	LEU
1	A	995	THR
1	A	997	ASN
1	A	999	ARG
1	A	1002	TRP
1	A	1003	MET
1	A	1018	GLN
1	A	1021	THR
1	A	1023	ILE
1	A	1026	SER
1	A	1047	LYS
1	A	1064	ARG
1	A	1069	LEU
1	A	1075	GLN
1	A	1077	SER

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Mol	Chain	Res	Type
1	A	1093	LYS
1	A	1094	TYR
1	A	1111	LEU
1	A	1116	GLN
1	A	1119	ILE
1	A	1120	ILE
1	A	1121	SER
1	A	1125	ILE
1	A	1126	GLU
1	B	355	ARG
1	B	359	SER
1	B	376	MET
1	B	377	PRO
1	B	431	THR
1	B	441	GLU
1	B	443	SER
1	B	453	GLU
1	B	467	CYS
1	B	505	VAL
1	B	515	ILE
1	B	529	GLU
1	B	532	GLU
1	B	557	ILE
1	B	593	LYS
1	B	623	VAL
1	B	630	MET
1	B	641	THR
1	B	642	HIS
1	B	644	THR
1	B	648	LEU
1	B	659	LEU
1	B	671	PHE
1	B	679	ASN
1	B	682	VAL
1	B	704	VAL
1	B	735	LYS
1	B	738	MET
1	B	748	SER
1	B	775	GLN
1	B	776	LYS
1	B	777	SER
1	B	780	ILE

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Mol	Chain	Res	Type
1	B	784	THR
1	B	786	THR
1	B	791	TRP
1	B	795	ILE
1	B	803	ARG
1	B	814	ASP
1	B	815	THR
1	B	819	ARG
1	B	825	ASP
1	B	828	ASP
1	B	834	GLN
1	B	856	VAL
1	B	866	VAL
1	B	875	ASP
1	B	894	LEU
1	B	901	MET
1	B	923	LEU
1	B	928	GLU
1	B	947	ASP
1	B	948	ASN
1	B	955	LEU
1	B	961	THR
1	B	973	SER
1	B	975	LEU
1	B	991	LEU
1	B	999	ARG
1	B	1018	GLN
1	B	1020	PRO
1	B	1077	SER
1	B	1081	ASN
1	B	1084	LEU
1	B	1090	GLU
1	B	1092	GLU
1	B	1094	TYR
1	B	1095	ARG
1	B	1097	LEU
1	B	1098	ILE
1	B	1109	VAL
1	B	1111	LEU
1	B	1112	CYS
1	B	1113	LYS
1	B	1115	VAL

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Mol	Chain	Res	Type
1	B	1121	SER
1	B	1123	THR
1	B	1128	PHE
1	C	340	LEU
1	C	353	THR
1	C	359	SER
1	C	384	LYS
1	C	395	ILE
1	C	401	GLU
1	C	435	ARG
1	C	443	SER
1	C	453	GLU
1	C	467	CYS
1	C	488	LEU
1	C	492	GLN
1	C	527	SER
1	C	537	ILE
1	C	544	ILE
1	C	546	THR
1	C	555	ARG
1	C	564	LEU
1	C	590	ASN
1	C	618	LEU
1	C	624	ASP
1	C	640	LEU
1	C	642	HIS
1	C	671	PHE
1	C	681	THR
1	C	682	VAL
1	C	687	ARG
1	C	701	MET
1	C	716	CYS
1	C	727	MET
1	C	752	MET
1	C	759	ASP
1	C	768	LEU
1	C	772	VAL
1	C	776	LYS
1	C	780	ILE
1	C	784	THR
1	C	790	GLN
1	C	801	ARG

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Mol	Chain	Res	Type
1	C	805	VAL
1	C	806	LEU
1	C	813	LEU
1	C	822	ARG
1	C	824	PHE
1	C	825	ASP
1	C	833	GLN
1	C	835	ILE
1	C	852	VAL
1	C	856	VAL
1	C	872	SER
1	C	875	ASP
1	C	896	THR
1	C	900	SER
1	C	914	TYR
1	C	917	GLU
1	C	924	LEU
1	C	927	PHE
1	C	931	GLU
1	C	957	ILE
1	C	963	LYS
1	C	969	LYS
1	C	971	LEU
1	C	974	THR
1	C	992	THR
1	C	993	ASN
1	C	999	ARG
1	C	1002	TRP
1	C	1005	LEU
1	C	1006	SER
1	C	1042	ASN
1	C	1043	PHE
1	C	1047	LYS
1	C	1051	ASP
1	C	1068	ILE
1	C	1073	GLN
1	C	1086	LYS
1	C	1088	GLN
1	C	1093	LYS
1	C	1100	ARG
1	C	1101	VAL
1	C	1109	VAL

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Mol	Chain	Res	Type
1	C	1114	GLU
1	C	1128	PHE
1	D	338	GLU
1	D	341	THR
1	D	370	VAL
1	D	376	MET
1	D	378	THR
1	D	411	PRO
1	D	427	ASP
1	D	431	THR
1	D	437	GLN
1	D	441	GLU
1	D	447	LYS
1	D	448	LYS
1	D	450	ILE
1	D	488	LEU
1	D	489	SER
1	D	499	THR
1	D	520	GLU
1	D	527	SER
1	D	564	LEU
1	D	567	LYS
1	D	568	GLU
1	D	569	GLN
1	D	570	ASN
1	D	572	GLN
1	D	573	ARG
1	D	585	GLU
1	D	601	SER
1	D	606	GLU
1	D	611	ILE
1	D	618	LEU
1	D	632	GLU
1	D	636	ARG
1	D	639	ARG
1	D	642	HIS
1	D	665	GLU
1	D	682	VAL
1	D	708	LYS
1	D	710	TYR
1	D	711	GLN
1	D	713	SER

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Mol	Chain	Res	Type
1	D	728	GLU
1	D	769	MET
1	D	772	VAL
1	D	773	GLU
1	D	776	LYS
1	D	777	SER
1	D	786	THR
1	D	791	TRP
1	D	800	ASN
1	D	805	VAL
1	D	806	LEU
1	D	814	ASP
1	D	820	ASP
1	D	823	THR
1	D	831	VAL
1	D	832	LYS
1	D	852	VAL
1	D	853	HIS
1	D	856	VAL
1	D	875	ASP
1	D	882	MET
1	D	883	VAL
1	D	898	VAL
1	D	947	ASP
1	D	948	ASN
1	D	953	TYR
1	D	955	LEU
1	D	956	ASP
1	D	957	ILE
1	D	958	THR
1	D	972	TYR
1	D	977	HIS
1	D	980	LEU
1	D	991	LEU
1	D	992	THR
1	D	993	ASN
1	D	1027	VAL
1	D	1042	ASN
1	D	1065	THR
1	D	1073	GLN
1	D	1077	SER
1	D	1084	LEU

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Mol	Chain	Res	Type
1	D	1085	LYS
1	D	1086	LYS
1	D	1090	GLU
1	D	1094	TYR
1	D	1099	VAL
1	D	1111	LEU
1	D	1116	GLN
1	D	1120	ILE
1	D	1126	GLU
1	D	1128	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	GLN
1	A	470	GLN
1	A	491	HIS
1	A	492	GLN
1	A	560	HIS
1	A	615	GLN
1	A	675	GLN
1	A	679	ASN
1	A	721	GLN
1	A	744	HIS
1	A	775	GLN
1	A	790	GLN
1	A	811	GLN
1	A	850	GLN
1	A	853	HIS
1	A	952	GLN
1	A	993	ASN
1	A	1018	GLN
1	A	1071	ASN
1	A	1075	GLN
1	B	470	GLN
1	B	494	ASN
1	B	560	HIS
1	B	615	GLN
1	B	625	GLN
1	B	675	GLN
1	B	721	GLN
1	B	749	HIS

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Mol	Chain	Res	Type
1	B	790	GLN
1	B	800	ASN
1	B	811	GLN
1	B	837	HIS
1	B	985	ASN
1	B	993	ASN
1	C	345	GLN
1	C	373	ASN
1	C	437	GLN
1	C	470	GLN
1	C	494	ASN
1	C	560	HIS
1	C	586	ASN
1	C	615	GLN
1	C	625	GLN
1	C	642	HIS
1	C	650	GLN
1	C	675	GLN
1	C	685	GLN
1	C	711	GLN
1	C	719	HIS
1	C	724	GLN
1	C	744	HIS
1	C	749	HIS
1	C	800	ASN
1	C	837	HIS
1	C	945	ASN
1	C	977	HIS
1	C	1018	GLN
1	C	1075	GLN
1	D	560	HIS
1	D	569	GLN
1	D	586	ASN
1	D	615	GLN
1	D	625	GLN
1	D	642	HIS
1	D	721	GLN
1	D	744	HIS
1	D	775	GLN
1	D	833	GLN
1	D	850	GLN
1	D	884	ASN

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Mol	Chain	Res	Type
1	D	1042	ASN
1	D	1071	ASN
1	D	1075	GLN

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	750/792 (94%)	0.06	21 (2%) 55 32	6, 27, 56, 87	0
1	B	746/792 (94%)	0.04	15 (2%) 65 41	3, 26, 65, 91	0
1	C	746/792 (94%)	0.36	37 (4%) 34 18	14, 34, 82, 146	0
1	D	710/792 (89%)	0.75	66 (9%) 14 7	17, 51, 91, 115	0
All	All	2952/3168 (93%)	0.30	139 (4%) 36 19	3, 33, 78, 146	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1001	ALA	6.3
1	D	895	ALA	5.6
1	C	1000	LEU	4.8
1	D	1087	ALA	4.8
1	A	908	VAL	4.6
1	D	955	LEU	4.6
1	A	816	GLY	4.2
1	D	561	ALA	4.1
1	D	818	LEU	3.9
1	D	795	ILE	3.9
1	D	954	ALA	3.8
1	A	1121	SER	3.8
1	D	1109	VAL	3.7
1	D	1089	GLN	3.5
1	A	820	ASP	3.4
1	D	982	ILE	3.3
1	D	822	ARG	3.3
1	D	1045	PHE	3.3
1	D	992	THR	3.3
1	C	953	TYR	3.3
1	B	951	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	1049	LEU	3.2
1	D	1083	VAL	3.2
1	B	816	GLY	3.2
1	B	953	TYR	3.2
1	C	951	ASP	3.1
1	C	1020	PRO	3.1
1	C	1023	ILE	3.1
1	D	675	GLN	3.1
1	D	349	ASN	3.1
1	C	1017	LYS	3.1
1	D	1077	SER	3.1
1	D	1112	CYS	3.0
1	D	1050	LEU	3.0
1	D	1114	GLU	3.0
1	A	998	GLY	2.9
1	C	997	ASN	2.9
1	C	896	THR	2.9
1	D	1046	LEU	2.9
1	D	1028	SER	2.9
1	A	935	ARG	2.9
1	C	954	ALA	2.9
1	C	994	ALA	2.9
1	C	894	LEU	2.9
1	A	936	ASP	2.9
1	D	663	SER	2.9
1	C	936	ASP	2.9
1	C	830	ALA	2.8
1	C	950	VAL	2.8
1	C	929	GLY	2.8
1	D	1126	GLU	2.8
1	C	988	ILE	2.8
1	D	827	PHE	2.8
1	C	816	GLY	2.8
1	A	1081	ASN	2.7
1	C	932	ALA	2.7
1	D	1082	GLU	2.7
1	C	934	ARG	2.7
1	C	935	ARG	2.7
1	D	800	ASN	2.7
1	D	671	PHE	2.6
1	C	809	SER	2.6
1	D	892	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	1118	GLU	2.6
1	D	1027	VAL	2.6
1	A	903	ALA	2.6
1	B	1124	VAL	2.6
1	C	1085	LYS	2.6
1	C	927	PHE	2.6
1	C	1018	GLN	2.5
1	C	796	GLU	2.5
1	C	1019	GLY	2.5
1	D	437	GLN	2.5
1	D	395	ILE	2.5
1	D	1128	PHE	2.5
1	D	1088	GLN	2.5
1	A	950	VAL	2.4
1	A	934	ARG	2.4
1	C	1096	ASP	2.4
1	B	958	THR	2.4
1	C	1027	VAL	2.4
1	C	933	LEU	2.4
1	B	690	GLY	2.3
1	D	628	TYR	2.3
1	C	805	VAL	2.3
1	A	1120	ILE	2.3
1	C	806	LEU	2.3
1	D	397	ILE	2.3
1	D	1024	ILE	2.3
1	D	791	TRP	2.3
1	D	1079	VAL	2.3
1	B	1020	PRO	2.3
1	A	825	ASP	2.2
1	D	1023	ILE	2.2
1	D	566	ALA	2.2
1	D	893	GLY	2.2
1	D	1123	THR	2.2
1	B	1121	SER	2.2
1	D	1020	PRO	2.2
1	D	1022	ALA	2.2
1	D	810	TYR	2.2
1	C	918	GLN	2.2
1	A	926	ASN	2.2
1	D	948	ASN	2.2
1	A	666	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1085	LYS	2.2
1	A	819	ARG	2.2
1	B	815	THR	2.1
1	D	797	PHE	2.1
1	C	1003	MET	2.1
1	D	1110	GLU	2.1
1	C	1128	PHE	2.1
1	C	1059	LEU	2.1
1	D	1044	LYS	2.1
1	D	1097	LEU	2.1
1	D	414	GLY	2.1
1	D	1108	PHE	2.1
1	B	908	VAL	2.1
1	A	1119	ILE	2.1
1	A	823	THR	2.1
1	A	909	PHE	2.1
1	D	1043	PHE	2.1
1	A	894	LEU	2.1
1	D	960	TRP	2.1
1	B	986	THR	2.1
1	B	1021	THR	2.1
1	D	995	THR	2.1
1	B	929	GLY	2.1
1	A	563	GLU	2.1
1	D	563	GLU	2.1
1	B	1083	VAL	2.0
1	D	646	LEU	2.0
1	D	1062	LEU	2.0
1	D	961	THR	2.0
1	D	667	GLY	2.0
1	B	985	ASN	2.0
1	D	365	ALA	2.0
1	D	1047	LYS	2.0
1	C	931	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.