



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:37 am BST

PDB ID : 5A0Z
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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

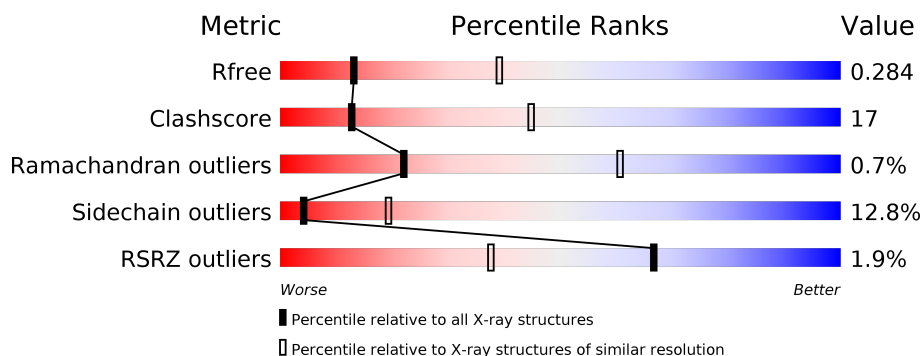
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on 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	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>25%</div> <div>5%</div> <div>5%</div> </div> </div>
1	B	792	<div> <div>65%</div> <div>25%</div> <div>6%</div> </div>
1	C	792	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>24%</div> <div>6%</div> </div> </div>
1	D	792	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>22%</div> <div>5%</div> <div>10%</div> </div> </div>

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.

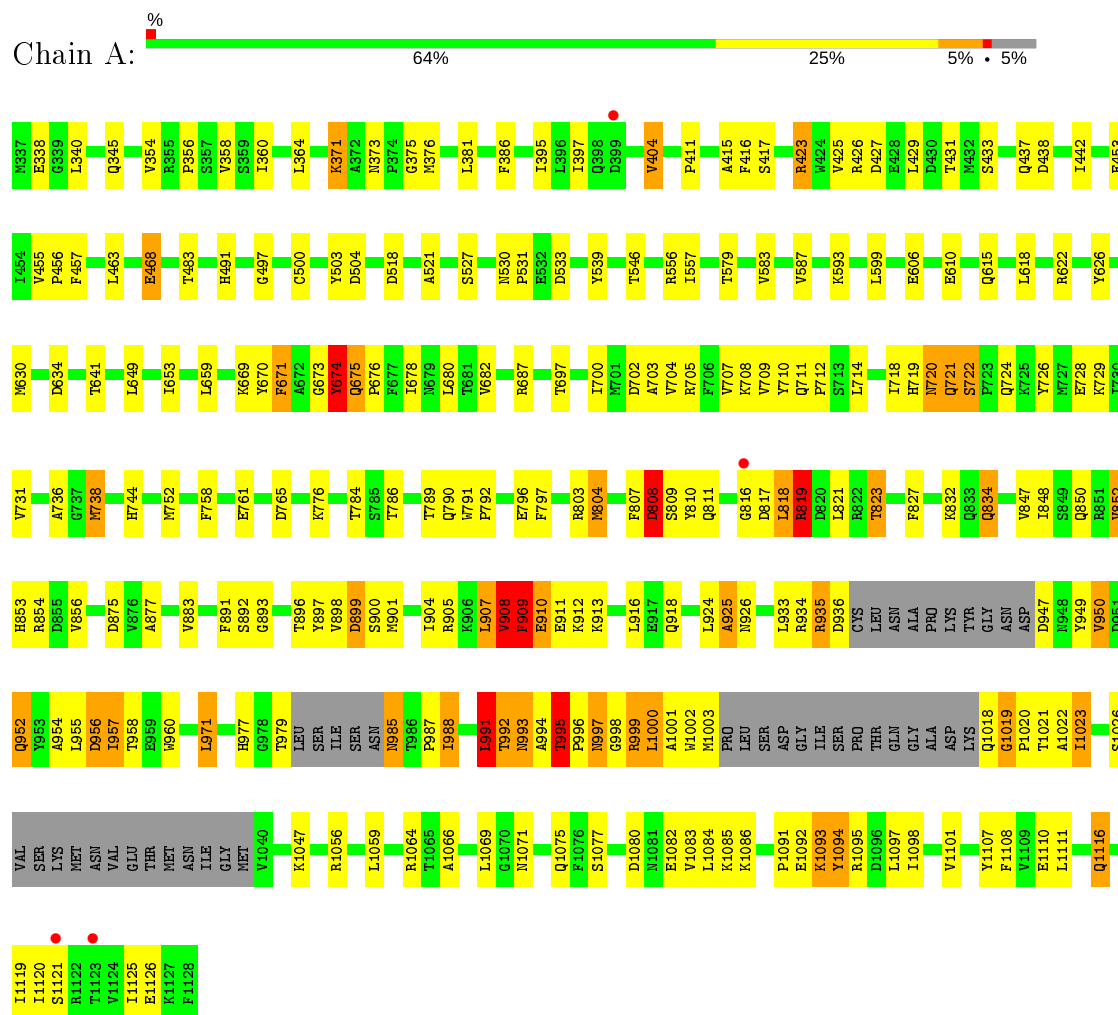
- Molecule 1 is a protein called CHOLINE TRIMETHYLAMINE LYASE.

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

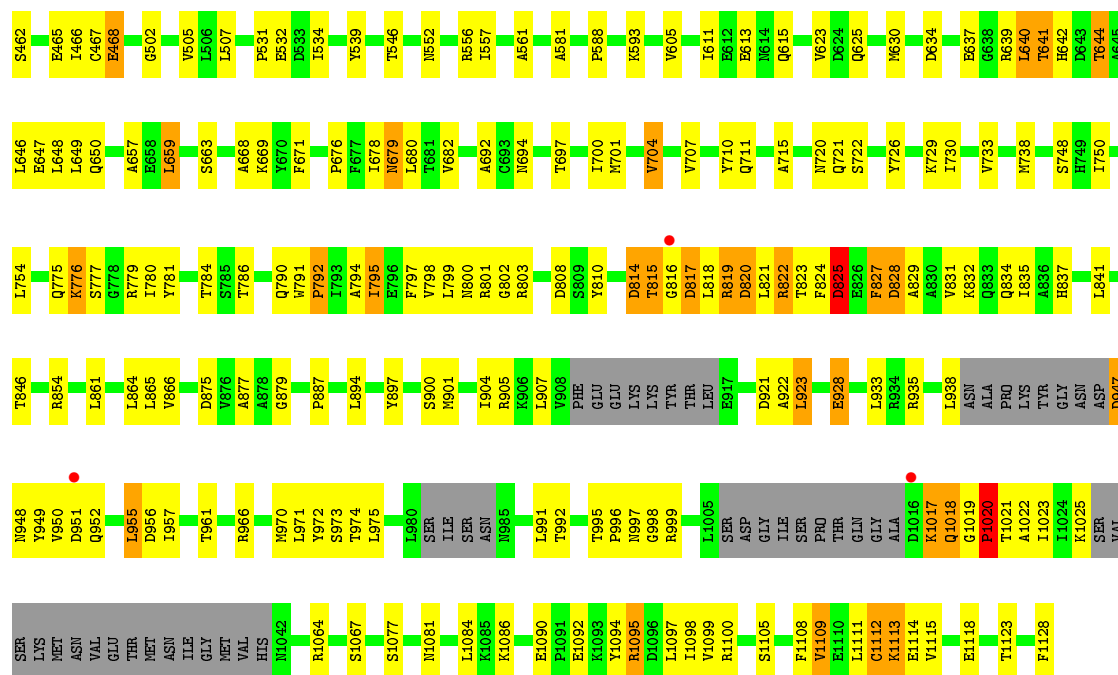
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

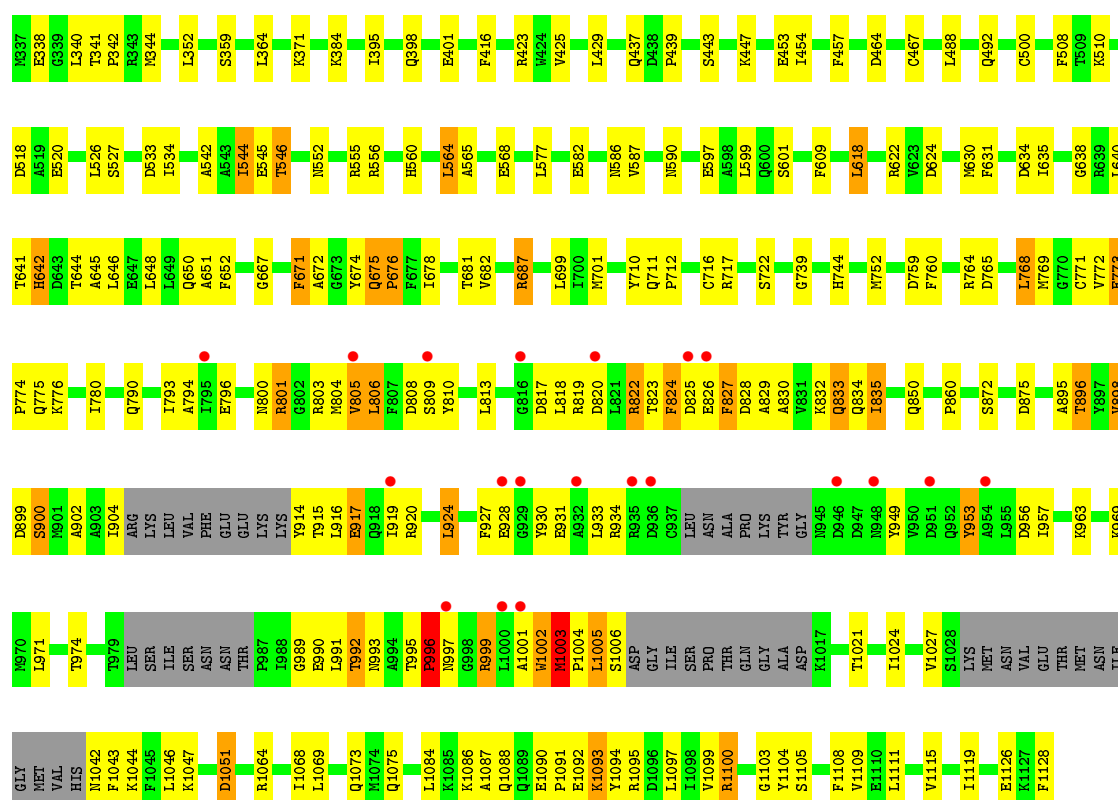


• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE



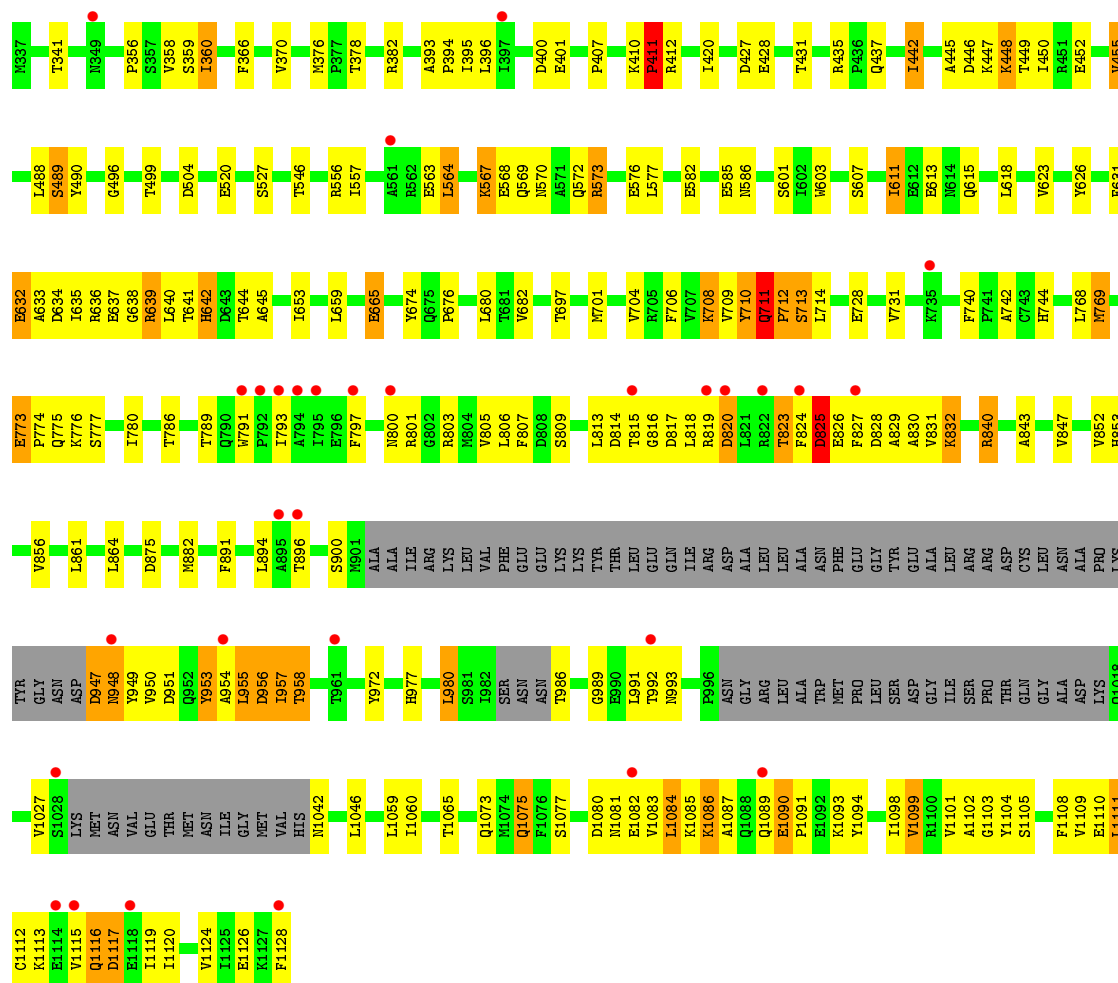


• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE



• 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 56.60 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.5 (119.92-3.00) 88.5 (56.60-3.00)	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)	0.33 , 51.2	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	0.84	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	0.80	2/6041 (0.0%)	0.87	13/8170 (0.2%)
1	B	0.73	1/5987 (0.0%)	0.85	5/8099 (0.1%)
1	C	0.73	2/5977 (0.0%)	0.84	10/8089 (0.1%)
1	D	0.63	3/5649 (0.1%)	0.81	6/7652 (0.1%)
All	All	0.72	8/23654 (0.0%)	0.84	34/32010 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	4
1	D	0	2
All	All	0	15

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	726	TYR	CE1-CZ	-5.62	1.31	1.38
1	B	468	GLU	CD-OE2	-5.40	1.19	1.25
1	D	774	PRO	N-CD	5.26	1.55	1.47
1	C	342	PRO	N-CD	5.22	1.55	1.47
1	A	674	TYR	CE1-CZ	-5.09	1.31	1.38
1	D	411	PRO	N-CD	5.09	1.54	1.47
1	D	712	PRO	N-CD	5.06	1.54	1.47
1	C	774	PRO	N-CD	5.06	1.54	1.47

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	996	PRO	CA-N-CD	-7.46	101.05	111.50
1	C	675	GLN	C-N-CD	6.72	142.51	128.40
1	B	1019	GLY	C-N-CD	6.40	141.85	128.40
1	A	675	GLN	C-N-CD	6.35	141.74	128.40
1	A	1019	GLY	C-N-CD	6.31	141.65	128.40
1	C	1003	MET	C-N-CD	6.23	141.48	128.40
1	A	423	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	D	455	VAL	C-N-CD	6.20	141.42	128.40
1	C	1109	VAL	CG1-CB-CG2	6.12	120.69	110.90
1	D	711	GLN	N-CA-C	-6.03	94.73	111.00
1	B	827	PHE	N-CA-C	5.93	127.01	111.00
1	A	995	THR	C-N-CD	5.92	140.83	128.40
1	B	640	LEU	CB-CG-CD1	-5.84	101.07	111.00
1	C	676	PRO	CA-N-CD	-5.84	103.33	111.50
1	A	722	SER	C-N-CD	5.79	140.56	128.40
1	B	952	GLN	N-CA-C	5.67	126.32	111.00
1	A	819	ARG	N-CA-C	-5.67	95.69	111.00
1	D	382	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	808	ASP	CB-CG-OD1	5.61	123.34	118.30
1	D	410	LYS	C-N-CD	5.58	140.13	128.40
1	B	435	ARG	C-N-CD	5.50	139.96	128.40
1	D	773	GLU	C-N-CD	5.49	139.92	128.40
1	A	531	PRO	CA-N-CD	-5.47	103.84	111.50
1	A	676	PRO	CA-N-CD	-5.46	103.86	111.50
1	C	773	GLU	C-N-CD	5.45	139.84	128.40
1	A	530	ASN	C-N-CD	5.42	139.78	128.40
1	C	341	THR	C-N-CD	5.37	139.68	128.40
1	C	1109	VAL	CA-CB-CG1	5.28	118.82	110.90
1	A	991	LEU	CA-CB-CG	5.21	127.28	115.30
1	C	996	PRO	N-CA-C	5.20	125.62	112.10
1	A	533	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	908	VAL	CB-CA-C	5.10	121.08	111.40
1	D	712	PRO	CA-N-CD	-5.08	104.38	111.50
1	C	898	VAL	CB-CA-C	-5.07	101.77	111.40

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

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Mol	Chain	Res	Type	Group
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	173	0
1	B	5868	0	5753	166	0
1	C	5856	0	5720	214	0
1	D	5534	0	5388	211	0
All	All	23177	0	22664	762	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 17.

All (762) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:947:ASP:OD1	1:D:949:TYR:N	1.87	1.07
1:B:641:THR:N	1:B:644:THR:OG1	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: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:D:1116:GLN:C	1:D:1120:ILE:HG13	1.81	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:A:905:ARG:HG3	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:NH1	1:C:822:ARG:HA	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
1:D:632:GLU:O	1:D:636:ARG:HB2	1.78	0.82
1:A:1093:LYS:HD2	1:A:1093:LYS:N	1.95	0.82
1:A:995:THR:OG1	1:A:998:GLY:HA3	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:632:GLU:OE1	1:D:636:ARG:NH2	2.12	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: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:989:GLY:CA	1:C:1005:LEU:HD21	1.87	0.77
1:D:1116:GLN:C	1:D:1120:ILE:CG1	2.47	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:D:706:PHE:O	1:D:708:LYS:HD2	1.85	0.76
1:B:462:SER:OG	1:B:465:GLU:HG3	1.84	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:C:830:ALA:HA	1:C:833:GLN:OE1	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:955:LEU:HD23	1:B:956:ASP:N	2.01	0.75
1:D:826:GLU:C	1:D:829:ALA:H	1.90	0.75
1:D:957:ILE:H	1:D:957:ILE:HD12	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: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:822:ARG:C	1:C:822:ARG:HH11	1.90	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:H	1:D:1084:LEU:HD12	1.53	0.73
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:B:795:ILE:HA	1:B:798:VAL:CG1	2.19	0.72
1:C:819:ARG:HD3	1:C:917:GLU:CD	2.04	0.71
1:C:796:GLU:CD	1:C:805:VAL:CG2	2.58	0.71
1:C:800:ASN:O	1:C:801:ARG:NE	2.23	0.71
1:A:900:SER:C	1:A:904:ILE:HG23	2.12	0.71
1:D:817:ASP:OD2	1:D:819:ARG:CB	2.39	0.70
1:C:1027:VAL:HG23	1:C:1069:LEU:HD22	1.72	0.70
1:C:769:MET:CB	1:C:775:GLN:HG3	2.20	0.70
1:A:905:ARG:NH1	1:A:905:ARG:HG3	2.01	0.70
1:A:904:ILE:O	1:A:904:ILE:HD12	1.91	0.70
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:C:822:ARG:C	1:C:822:ARG:HD3	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:800:ASN:C	1:C:801:ARG:HG3	2.12	0.69
1:D:445:ALA:O	1:D:449:THR:OG1	2.09	0.69
1:B:794:ALA:O	1:B:798:VAL:CG1	2.35	0.68
1:C:822:ARG:HH11	1:C:823:THR:N	1.92	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:1075:GLN:HE22	1:C:1103:GLY:HA2	1.58	0.68
1:C:823:THR:HB	1:C:826:GLU:HB2	1.75	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:D:400:ASP:C	1:D:573:ARG:NH2	2.47	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:C:835:ILE:C	1:C:835:ILE:HD12	2.15	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:B:422:TRP:NE1	1:B:465:GLU:OE2	2.27	0.67
1:C:676:PRO:HD2	1:C:711:GLN:CD	2.15	0.67
1:C:822:ARG:HA	1:C:822:ARG:HH11	1.58	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
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:N	1:A:721:GLN:HE21	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:D:843:ALA:O	1:D:847:VAL:HG23	1.97	0.65
1:D:1084:LEU:HA	1:D:1087:ALA:CB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:817:ASP:CG	1:D:819:ARG:HG2	2.13	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:D:828:ASP:HB3	1:D:832:LYS:HZ3	1.62	0.64
1:C:646:LEU:HD12	1:C:699:LEU:HD22	1.79	0.64
1:D:828:ASP:C	1:D:832:LYS:HD3	2.17	0.64
1:C:1003:MET:HG2	1:C:1004:PRO:CD	2.28	0.63
1:C:818:LEU:CD1	1:C:819:ARG:H	2.10	0.63
1:A:673:GLY:C	1:A:674:TYR:HD1	2.02	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:1022:ALA:O	1:B:1025:LYS:N	2.23	0.62
1:B:854:ARG:HA	1:B:877:ALA:HB1	1.79	0.62
1:A:934:ARG:HD2	1:A:999:ARG:HA	1.82	0.62
1:D:697:THR:HG22	1:D:701:MET:HE2	1.82	0.62
1:B:822:ARG:CB	1:B:823:THR:HA	2.29	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: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:N	1:A:899:ASP:OD1	2.32	0.61
1:B:738:MET:O	1:B:1098:ILE:HG22	2.00	0.61
1:D:1083:VAL:HG12	1:D:1083:VAL:O	2.00	0.61
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:999:ARG:HH11	1:C:1005:LEU:HA	1.60	0.60
1:C:995:THR:HA	1:C:996:PRO:C	2.21	0.60
1:C:829:ALA:O	1:C:833:GLN:N	2.31	0.60
1:D:826:GLU:C	1:D:830:ALA:H	2.04	0.60
1:B:821:LEU:HD23	1:B:821:LEU:O	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:A:682:VAL:CG1	1:A:697:THR:HG23	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:GLN:CG	1:C:1104:TYR:CD2	2.84	0.60
1:B:827:PHE:HA	1:B:828:ASP:C	2.22	0.59
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:C:796:GLU:CD	1:C:805:VAL:HG21	2.23	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:CD1	1:D:953:TYR:N	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:C:1002:TRP:CD1	1:C:1002:TRP:N	2.72	0.58
1:A:1023:ILE:HD13	1:A:1023:ILE:O	2.04	0.58
1:A:491:HIS:O	1:A:853:HIS:CE1	2.56	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:1084:LEU:N	1:D:1084:LEU:HD12	2.20	0.57
1:D:708:LYS:O	1:D:1098:ILE:CD1	2.51	0.57
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:HA	1:A:819:ARG:NH1	2.20	0.57
1:A:1094:TYR:CD1	1:A:1094:TYR:N	2.72	0.57
1:A:674:TYR:CD1	1:A:674:TYR:N	2.73	0.57
1:D:1099:VAL:HG21	1:D:1108:PHE:CD1	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:676:PRO:CD	1:C:711:GLN:CD	2.74	0.56
1:D:828:ASP:O	1:D:832:LYS:HD3	2.06	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:1117:ASP:N	1:D:1120:ILE:HG13	2.20	0.56
1:D:815:THR:CB	1:D:816:GLY:CA	2.84	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:708:LYS:O	1:D:1098:ILE:HD12	2.07	0.55
1:D:411:PRO:O	1:D:412:ARG:HB2	2.05	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:C:1002:TRP:O	1:C:1003:MET:C	2.45	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: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
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:D:950:VAL:HG13	1:D:951:ASP:N	2.22	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:A:1101:VAL:HG22	1:A:1111:LEU:HD21	1.90	0.55
1:A:687:ARG:NH2	1:A:761:GLU:OE1	2.39	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:B:1113:LYS:HG3	1:B:1114:GLU:H	1.71	0.54
1:B:561:ALA:HB3	1:B:581:ALA:HB2	1.89	0.54
1:C:1094:TYR:N	1:C:1094:TYR:CD1	2.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:631:PHE:CE1	1:D:635:ILE:HG13	2.42	0.54
1:C:1095:ARG:HD2	1:C:1095:ARG:C	2.24	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: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:HD1	1:D:953:TYR:H	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:C:641:THR:O	1:C:644:THR:OG1	2.24	0.53
1:A:1091:PRO:HD2	1:A:1092:GLU:H	1.73	0.53
1:B:900:SER:CB	1:B:997:ASN:CG	2.77	0.53
1:C:822:ARG:CA	1:C:822:ARG:HH11	2.20	0.53
1:D:828:ASP:HB3	1:D:832:LYS:NZ	2.22	0.53
1:C:1046:LEU:HD22	1:C:1126:GLU:CG	2.39	0.53
1:C:631:PHE:CZ	1:C:635:ILE:HG13	2.44	0.53
1:D:828:ASP:HA	1:D:832:LYS:HD3	1.89	0.53
1:A:483:THR:HB	1:A:804:MET:HE1	1.90	0.53
1:D:896:THR:O	1:D:900:SER:OG	2.21	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:HD1	1:A:1094:TYR:N	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:D:731:VAL:HG13	1:D:1059:LEU:HD23	1.92	0.52
1:D:1116:GLN:C	1:D:1120:ILE:CD1	2.77	0.52
1:D:826:GLU:N	1:D:829:ALA:HB3	2.23	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:1075:GLN:NE2	1:C:1103:GLY:HA2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1021:THR:HG23	1:C:1024:ILE:HD11	1.92	0.52
1:C:920:ARG:O	1:C:924:LEU:N	2.38	0.52
1:D:744:HIS:CD2	1:D:768:LEU:CD2	2.92	0.52
1:A:1091:PRO:CG	1:A:1092:GLU:N	2.73	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:C:822:ARG:HD3	1:C:822:ARG:O	2.10	0.51
1:B:605:VAL:HG11	1:B:865:LEU:HD11	1.93	0.51
1:C:818:LEU:CG	1:C:819:ARG:N	2.73	0.51
1:C:930:TYR:CE2	1:C:933:LEU:HB2	2.45	0.51
1:C:1090:GLU:HG2	1:C:1094:TYR:CE1	2.45	0.51
1:C:675:GLN:HG2	1:C:1104:TYR:CE2	2.45	0.51
1:A:789:THR:O	1:A:892:SER:CB	2.58	0.51
1:A:999:ARG:HG2	1:A:999:ARG:O	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: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:835:ILE:O	1:C:835:ILE:HD12	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:1066:ALA:HB1	1:A:1071:ASN:ND2	2.23	0.51
1:A:504:ASP:HB3	1:A:626:TYR:CG	2.46	0.51
1:A:904:ILE:C	1:A:904:ILE:HD12	2.30	0.51
1:A:911:GLU:OE2	1:A:913:LYS:HE3	2.11	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:C:642:HIS:C	1:C:642:HIS:CD2	2.85	0.50
1:D:1046:LEU:HD13	1:D:1124:VAL:HG11	1.93	0.50
1:D:711:GLN:HG3	1:D:712:PRO:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:819:ARG:HD2	1:B:819:ARG:C	2.32	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
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:D:642:HIS:CD2	1:D:642:HIS:C	2.85	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:824:PHE:C	1:C:824:PHE:CD1	2.86	0.49
1:B:820:ASP:CA	1:B:821:LEU:CB	2.85	0.49
1:C:1001:ALA:HB3	1:C:1003:MET:HB3	1.94	0.49
1:C:609:PHE:HB3	1:C:618:LEU:HD21	1.94	0.49
1:A:1093:LYS:H	1:A:1093:LYS:HD2	1.73	0.49
1:A:935:ARG:CG	1:A:999:ARG:HD3	2.42	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:1111:LEU:HB3	1:C:1115:VAL:CG2	2.43	0.49
1:C:917:GLU:HA	1:C:917:GLU:OE1	2.13	0.49
1:C:850:GLN:OE1	1:C:971:LEU:HB2	2.13	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:D:400:ASP:C	1:D:573:ARG:HH22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:991:LEU:HD22	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:1093:LYS:C	1:C:1094:TYR:CD1	2.85	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:D:1116:GLN:C	1:D:1120:ILE:HD11	2.34	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:A:673:GLY:C	1:A:674:TYR:CD1	2.85	0.48
1:B:726:TYR:CE2	1:B:730:ILE:HD11	2.48	0.48
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:C:902:ALA:C	1:C:904:ILE:H	2.17	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:1017:LYS:N	1:B:1018:GLN:OE1	2.47	0.47
1:B:827:PHE:N	1:B:827:PHE:CD1	2.81	0.47
1:B:827:PHE:HA	1:B:829:ALA:H	1.78	0.47
1:A:993:ASN:HB2	1:A:1001:ALA:HA	1.96	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:671:PHE:CD1	1:A:671:PHE:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:822:ARG:CZ	1:C:822:ARG:HA	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:A:907:LEU:HD12	1:A:907:LEU:C	2.34	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: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: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:955:LEU:HA	1:D:958:THR:OG1	2.15	0.47
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:B:539:TYR:CD1	1:B:539:TYR:C	2.88	0.47
1:C:1002:TRP:O	1:C:1005:LEU:HD22	2.14	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: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:B:362:ARG:O	1:B:363:ALA:C	2.53	0.46
1:B:646:LEU:HG	1:B:650:GLN:HE21	1.80	0.46
1:C:1002:TRP:O	1:C:1003:MET:O	2.32	0.46
1:D:489:SER:O	1:D:490:TYR:C	2.53	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:A:893:GLY:C	1:A:898:VAL:H	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:822:ARG:NH1	1:C:823:THR:N	2.61	0.46
1:A:1020:PRO:O	1:A:1023:ILE:HG22	2.16	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:801:ARG:O	1:C:810:TYR:CZ	2.69	0.45
1:C:546:THR:HG21	1:C:860:PRO:HB2	1.98	0.45
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:848:ILE:O	1:A:852:VAL:HG13	2.17	0.45
1:A:791:TRP:HB3	1:A:901:MET:HG3	1.99	0.45
1:A:997:ASN:ND2	1:A:997:ASN:O	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: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:C:995:THR:CA	1:C:996:PRO:C	2.86	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:1090:GLU:O	1:D:1093:LYS:N	2.50	0.45
1:D:713:SER:CB	1:D:1103:GLY:O	2.65	0.45
1:D:825:ASP:C	1:D:829:ALA:CB	2.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:TYR:CD1	1:A:949:TYR:O	2.70	0.44
1:B:1114:GLU:HG2	1:B:1115:VAL:N	2.32	0.44
1:B:396:LEU:HG	1:B:396:LEU:O	2.16	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:1081:ASN:O	1:D:1084:LEU:HD11	2.17	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
1:D:697:THR:HG22	1:D:701:MET:CE	2.46	0.44
1:D:807:PHE:HB2	1:D:809:SER:HB2	1.98	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:D:573:ARG:HD2	1:D:577:LEU:CG	2.45	0.44
1:D:504:ASP:HB3	1:D:626:TYR:CD1	2.53	0.44
1:D:633:ALA:HB1	1:D:639:ARG:HH21	1.82	0.44
1:B:824:PHE:CD1	1:B:824:PHE:O	2.70	0.44
1:C:423:ARG:NH1	1:C:464:ASP:OD2	2.51	0.44
1:D:1087:ALA:CB	1:D:1108:PHE:CE2	2.95	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:A:910:GLU:HG3	1:A:910:GLU:O	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: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:1044:LYS:NZ	1:C:1119:ILE:O	2.51	0.43
1:C:520:GLU:CG	1:C:544:ILE:HD11	2.47	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:A:423:ARG:HG3	1:A:423:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:947:ASP:OD1	1:D:948:ASN:N	2.51	0.43
1:B:721:GLN:NE2	1:C:1069:LEU:HA	2.34	0.43
1:D:636:ARG:HB3	1:D:636:ARG:NH1	2.34	0.43
1:D:640:LEU:HD13	1:D:645:ALA:CA	2.49	0.43
1:D:824:PHE:C	1:D:826:GLU:H	2.17	0.43
1:D:1111:LEU:HD13	1:D:1111:LEU:N	2.34	0.43
1:A:397:ILE:HG23	1:A:404:VAL:HG21	2.01	0.43
1:A:395:ILE:HG13	1:A:557:ILE:HD13	1.99	0.43
1:B:434:THR:O	1:B:434:THR:HG22	2.18	0.43
1:B:502:GLY:HA3	1:B:505:VAL:HG12	2.01	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:C:687:ARG:HD2	1:C:765:ASP:OD2	2.19	0.43
1:D:573:ARG:HD2	1:D:577:LEU:CD2	2.48	0.43
1:D:636:ARG:C	1:D:638:GLY:H	2.20	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: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: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:1075:GLN:HE22	1:D:1103:GLY:H	1.66	0.42
1:C:819:ARG:HG3	1:C:819:ARG:O	2.19	0.42
1:D:1112:CYS:SG	1:D:1112:CYS:O	2.77	0.42
1:D:773:GLU:OE2	1:D:980:LEU:HD13	2.19	0.42
1:D:817:ASP:CG	1:D:818:LEU:N	2.73	0.42
1:A:935:ARG:HG2	1:A:999:ARG:HD3	2.00	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: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
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:708:LYS:HD2	1:A:736:ALA:HB1	2.02	0.42
1:A:622:ARG:HD3	1:A:765:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:947:ASP:CG	1:D:948:ASN:N	2.73	0.42
1:A:358:VAL:CG1	1:A:442:ILE:HD12	2.49	0.42
1:A:819:ARG:CZ	1:A:819:ARG:HA	2.50	0.42
1:C:526:LEU:HD22	1:C:533:ASP:CG	2.40	0.42
1:C:542:ALA:O	1:C:546:THR:HG23	2.19	0.42
1:C:827:PHE:C	1:C:829:ALA:N	2.73	0.42
1:D:634:ASP:O	1:D:639:ARG:N	2.51	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: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:C:996:PRO:HA	1:C:997:ASN:C	2.40	0.42
1:A:1082:GLU:OE1	1:A:1086:LYS:NZ	2.53	0.41
1:A:803:ARG:HD2	1:A:808:ASP:HB2	2.02	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: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:C:1051:ASP:N	1:C:1051:ASP:OD1	2.53	0.41
1:D:640:LEU:HD21	1:D:644:THR:HG22	2.02	0.41
1:A:995:THR:HG1	1:A:998:GLY:HA3	1.82	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: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:HG12	1:D:455:VAL:O	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
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:1084:LEU:HD22	1:A:1097:LEU:CD2	2.50	0.41
1:A:416:PHE:CE1	1:A:425:VAL:HG11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:504:ASP:HB3	1:D:626:TYR:CG	2.55	0.41
1:A:1095:ARG:HG3	1:A:1095:ARG:NH1	2.36	0.41
1:A:710:TYR:HD1	1:A:1107:TYR:CE2	2.36	0.41
1:A:395:ILE:HD13	1:A:556:ARG:NH1	2.35	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:437:GLN:CD	1:C:672:ALA:HB1	2.41	0.41
1:C:800:ASN:C	1:C:801:ARG:CG	2.85	0.41
1:C:1090:GLU:N	1:C:1091:PRO:CD	2.84	0.41
1:C:344:MET:HE1	1:C:651:ALA:HB2	2.02	0.41
1:D:490:TYR:C	1:D:490:TYR:CD1	2.93	0.41
1:D:708:LYS:O	1:D:1098:ILE:HD11	2.20	0.41
1:A:680:LEU:C	1:A:680:LEU:HD23	2.42	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:O	1:B:819:ARG:HD2	2.20	0.41
1:C:352:LEU:HD23	1:C:1095:ARG:HH21	1.85	0.41
1:C:644:THR:HG1	1:C:645:ALA:H	1.68	0.41
1:A:653:ILE:HG23	1:A:712:PRO:HD2	2.03	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:769:MET:HE3	1:D:773:GLU:OE1	2.21	0.41
1:D:827:PHE:O	1:D:831:VAL:HG12	2.20	0.41
1:A:1093:LYS:CD	1:A:1093:LYS:N	2.73	0.40
1:A:1108:PHE:CE1	1:A:1116:GLN:HB2	2.56	0.40
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:832:LYS:NZ	1:A:956:ASP:OD1	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:539:TYR:C	1:A:539:TYR:CD2	2.94	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:680:LEU:C	1:B:680:LEU:HD23	2.41	0.40
1:B:837:HIS:CE1	1:B:841:LEU:HD13	2.56	0.40
1:C:895:ALA:O	1:C:896:THR:C	2.58	0.40
1:D:582:GLU:O	1:D:586:ASN:ND2	2.55	0.40
1:C:1090:GLU:CG	1:C:1094:TYR:CE1	3.04	0.40
1:C:429:LEU:HB3	1:C:447:LYS:HD2	2.04	0.40
1:C:675:GLN:HG3	1:C:1104:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

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	740/792 (93%)	656 (89%)	76 (10%)	8 (1%)	14	50
1	B	734/792 (93%)	664 (90%)	66 (9%)	4 (0%)	29	68
1	C	734/792 (93%)	661 (90%)	69 (9%)	4 (0%)	29	68
1	D	700/792 (88%)	635 (91%)	60 (9%)	5 (1%)	22	60
All	All	2908/3168 (92%)	2616 (90%)	271 (9%)	21 (1%)	22	60

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%)	544 (87%)	80 (13%)	4	19
1	B	618/668 (92%)	544 (88%)	74 (12%)	5	22
1	C	617/668 (92%)	542 (88%)	75 (12%)	5	21
1	D	580/668 (87%)	496 (86%)	84 (14%)	3	15
All	All	2439/2672 (91%)	2126 (87%)	313 (13%)	4	19

All (313) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	GLU

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Mol	Chain	Res	Type
1	A	371	LYS
1	A	404	VAL
1	A	417	SER
1	A	429	LEU
1	A	431	THR
1	A	433	SER
1	A	453	GLU
1	A	468	GLU
1	A	527	SER
1	A	593	LYS
1	A	618	LEU
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	776	LYS
1	A	784	THR
1	A	786	THR
1	A	807	PHE
1	A	808	ASP
1	A	809	SER
1	A	818	LEU
1	A	819	ARG
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	908	VAL
1	A	909	PHE
1	A	910	GLU

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Mol	Chain	Res	Type
1	A	916	LEU
1	A	918	GLN
1	A	933	LEU
1	A	935	ARG
1	A	936	ASP
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	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
1	A	1085	LYS
1	A	1093	LYS
1	A	1094	TYR
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	426	ARG
1	B	431	THR

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Mol	Chain	Res	Type
1	B	441	GLU
1	B	443	SER
1	B	453	GLU
1	B	467	CYS
1	B	532	GLU
1	B	557	ILE
1	B	593	LYS
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	669	LYS
1	B	671	PHE
1	B	679	ASN
1	B	704	VAL
1	B	710	TYR
1	B	748	SER
1	B	775	GLN
1	B	776	LYS
1	B	777	SER
1	B	784	THR
1	B	791	TRP
1	B	795	ILE
1	B	814	ASP
1	B	815	THR
1	B	819	ARG
1	B	820	ASP
1	B	825	ASP
1	B	828	ASP
1	B	834	GLN
1	B	866	VAL
1	B	875	ASP
1	B	894	LEU
1	B	901	MET
1	B	905	ARG
1	B	907	LEU
1	B	921	ASP
1	B	923	LEU
1	B	928	GLU
1	B	935	ARG

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Mol	Chain	Res	Type
1	B	947	ASP
1	B	948	ASN
1	B	949	TYR
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	1017	LYS
1	B	1018	GLN
1	B	1020	PRO
1	B	1077	SER
1	B	1081	ASN
1	B	1084	LEU
1	B	1086	LYS
1	B	1090	GLU
1	B	1092	GLU
1	B	1094	TYR
1	B	1095	ARG
1	B	1097	LEU
1	B	1109	VAL
1	B	1111	LEU
1	B	1112	CYS
1	B	1113	LYS
1	B	1123	THR
1	B	1128	PHE
1	C	359	SER
1	C	384	LYS
1	C	401	GLU
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	544	ILE
1	C	546	THR
1	C	555	ARG
1	C	564	LEU
1	C	590	ASN
1	C	618	LEU

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Mol	Chain	Res	Type
1	C	624	ASP
1	C	630	MET
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	710	TYR
1	C	716	CYS
1	C	752	MET
1	C	759	ASP
1	C	760	PHE
1	C	768	LEU
1	C	771	CYS
1	C	772	VAL
1	C	776	LYS
1	C	780	ILE
1	C	790	GLN
1	C	801	ARG
1	C	805	VAL
1	C	806	LEU
1	C	813	LEU
1	C	817	ASP
1	C	822	ARG
1	C	824	PHE
1	C	825	ASP
1	C	833	GLN
1	C	835	ILE
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	953	TYR
1	C	956	ASP
1	C	957	ILE
1	C	963	LYS

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Mol	Chain	Res	Type
1	C	969	LYS
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	1073	GLN
1	C	1086	LYS
1	C	1088	GLN
1	C	1093	LYS
1	C	1100	ARG
1	C	1128	PHE
1	D	341	THR
1	D	366	PHE
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	448	LYS
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

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Mol	Chain	Res	Type
1	D	611	ILE
1	D	618	LEU
1	D	632	GLU
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
1	D	769	MET
1	D	776	LYS
1	D	777	SER
1	D	786	THR
1	D	791	TRP
1	D	800	ASN
1	D	803	ARG
1	D	805	VAL
1	D	806	LEU
1	D	814	ASP
1	D	820	ASP
1	D	823	THR
1	D	832	LYS
1	D	840	ARG
1	D	852	VAL
1	D	853	HIS
1	D	856	VAL
1	D	875	ASP
1	D	882	MET
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

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Mol	Chain	Res	Type
1	D	993	ASN
1	D	1027	VAL
1	D	1042	ASN
1	D	1065	THR
1	D	1073	GLN
1	D	1075	GLN
1	D	1077	SER
1	D	1084	LEU
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	1117	ASP
1	D	1126	GLU
1	D	1128	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	GLN
1	A	470	GLN
1	A	491	HIS
1	A	560	HIS
1	A	615	GLN
1	A	675	GLN
1	A	721	GLN
1	A	744	HIS
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	1073	GLN
1	B	406	HIS
1	B	470	GLN
1	B	494	ASN

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Mol	Chain	Res	Type
1	B	615	GLN
1	B	625	GLN
1	B	642	HIS
1	B	721	GLN
1	B	790	GLN
1	B	800	ASN
1	B	837	HIS
1	B	985	ASN
1	C	345	GLN
1	C	437	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	724	GLN
1	C	749	HIS
1	C	800	ASN
1	C	977	HIS
1	C	1073	GLN
1	D	437	GLN
1	D	470	GLN
1	D	494	ASN
1	D	560	HIS
1	D	569	GLN
1	D	586	ASN
1	D	615	GLN
1	D	642	HIS
1	D	775	GLN
1	D	790	GLN
1	D	833	GLN
1	D	993	ASN
1	D	1042	ASN
1	D	1071	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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%)	-0.35	4 (0%)	91 75	6, 27, 56, 87	0
1	B	746/792 (94%)	-0.34	3 (0%)	92 79	3, 26, 65, 91	0
1	C	746/792 (94%)	-0.17	20 (2%)	54 26	14, 34, 82, 146	0
1	D	710/792 (89%)	0.11	30 (4%)	36 14	17, 51, 91, 115	0
All	All	2952/3168 (93%)	-0.19	57 (1%)	66 37	3, 33, 78, 146	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	827	PHE	5.0
1	C	1001	ALA	4.5
1	C	816	GLY	4.4
1	D	992	THR	4.3
1	D	822	ARG	4.3
1	C	935	ARG	4.1
1	C	932	ALA	4.1
1	D	800	ASN	3.8
1	D	1089	GLN	3.6
1	C	1000	LEU	3.6
1	D	819	ARG	3.5
1	A	1121	SER	3.4
1	D	795	ILE	3.3
1	D	1114	GLU	3.3
1	D	349	ASN	3.2
1	C	928	GLU	3.0
1	D	561	ALA	3.0
1	D	1028	SER	3.0
1	C	951	ASP	3.0
1	B	816	GLY	3.0
1	D	797	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	895	ALA	2.6
1	D	954	ALA	2.5
1	C	936	ASP	2.5
1	C	795	ILE	2.5
1	D	815	THR	2.5
1	C	820	ASP	2.5
1	D	792	PRO	2.5
1	D	1128	PHE	2.4
1	D	1082	GLU	2.4
1	D	791	TRP	2.4
1	B	951	ASP	2.4
1	C	929	GLY	2.4
1	D	1118	GLU	2.3
1	C	805	VAL	2.3
1	D	820	ASP	2.3
1	C	809	SER	2.3
1	C	954	ALA	2.3
1	D	948	ASN	2.2
1	C	948	ASN	2.2
1	C	825	ASP	2.2
1	D	397	ILE	2.2
1	D	735	LYS	2.2
1	D	794	ALA	2.2
1	A	1123	THR	2.1
1	C	946	ASP	2.1
1	D	1115	VAL	2.1
1	D	961	THR	2.1
1	D	793	ILE	2.1
1	A	816	GLY	2.1
1	C	997	ASN	2.1
1	A	399	ASP	2.1
1	D	896	THR	2.1
1	C	919	ILE	2.0
1	B	1016	ASP	2.0
1	D	824	PHE	2.0
1	C	826	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.