



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:00 am BST

PDB ID : 5A0U
Title : Structure of CutC choline lyase choline bound form from *Klebsiella pneumoniae*.
Authors : Kalnins, G.; Tars, K.
Deposited on : 2015-04-23
Resolution : 2.40 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

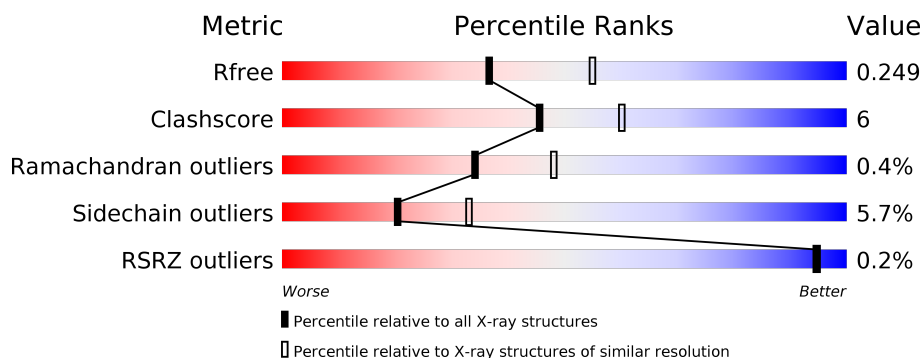
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	795	<div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	B	795	<div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	C	795	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	D	795	<div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	E	795	<div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	F	795	<div> <div>%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	795	<div><div></div><div>85%</div><div>13%</div><div></div></div>
1	H	795	<div><div></div><div>79%</div><div>19%</div><div></div></div>

2 Entry composition

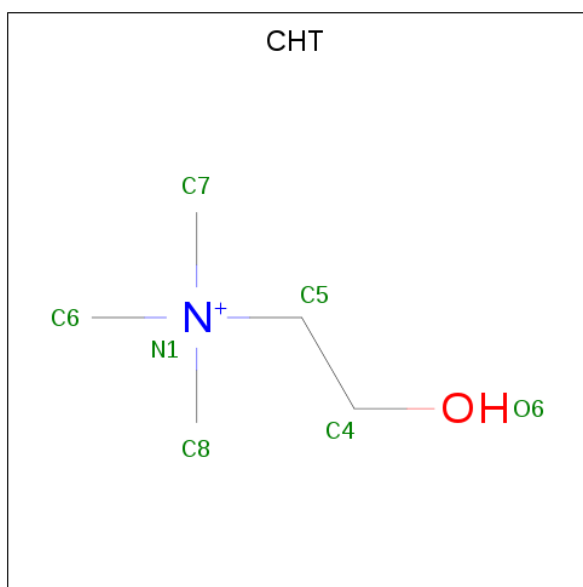
There are 3 unique types of molecules in this entry. The entry contains 52127 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	B	793	Total	C	N	O	S	0	0	0
			6261	3959	1078	1182	42			
1	C	793	Total	C	N	O	S	0	0	0
			6261	3959	1078	1182	42			
1	D	793	Total	C	N	O	S	0	0	0
			6261	3959	1078	1182	42			
1	E	793	Total	C	N	O	S	0	0	0
			6261	3959	1078	1182	42			
1	F	793	Total	C	N	O	S	0	0	0
			6261	3959	1078	1182	42			
1	G	793	Total	C	N	O	S	0	0	0
			6261	3959	1078	1182	42			
1	H	795	Total	C	N	O	S	0	0	0
			6275	3968	1080	1185	42			

- Molecule 2 is CHOLINE ION (three-letter code: CHT) (formula: C₅H₁₄NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	5	1	1		
2	B	1	Total	C	N	O	0	0
			7	5	1	1		
2	C	1	Total	C	N	O	0	0
			7	5	1	1		
2	D	1	Total	C	N	O	0	0
			7	5	1	1		
2	E	1	Total	C	N	O	0	0
			7	5	1	1		
2	F	1	Total	C	N	O	0	0
			7	5	1	1		
2	G	1	Total	C	N	O	0	0
			7	5	1	1		
2	H	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	344	Total	O	0	0
			344	344		
3	B	294	Total	O	0	0
			294	294		
3	C	297	Total	O	0	0
			297	297		
3	D	307	Total	O	0	0
			307	307		

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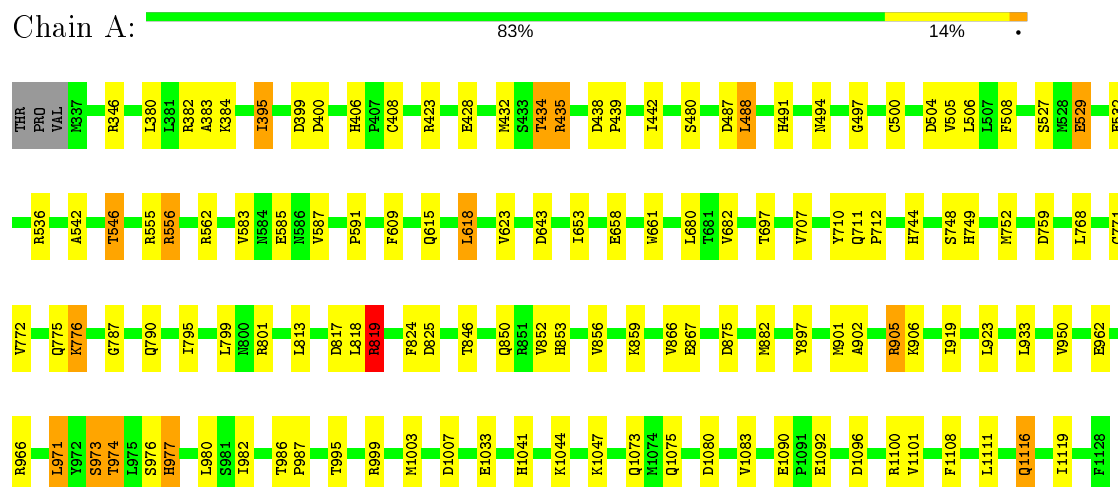
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	163	Total 163	O 163	0	0
3	F	152	Total 152	O 152	0	0
3	G	217	Total 217	O 217	0	0
3	H	202	Total 202	O 202	0	0

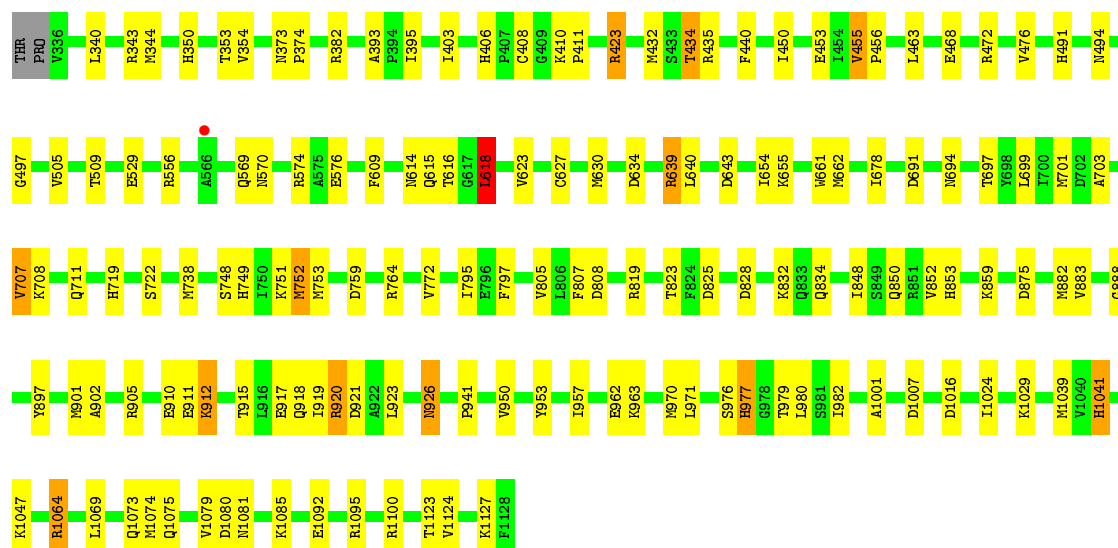
3 Residue-property plots

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

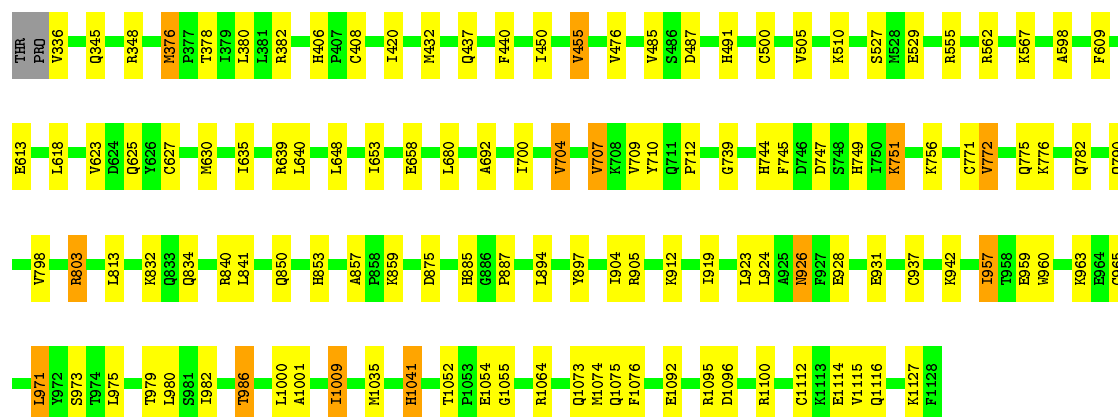


Chain C:  81% 17%



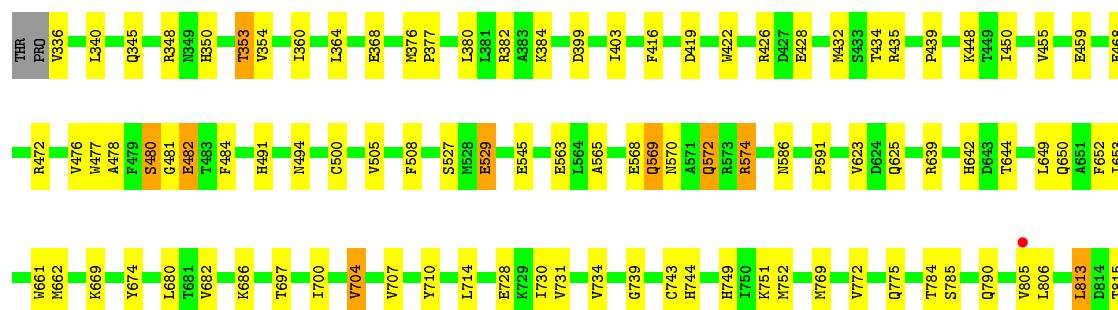
• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

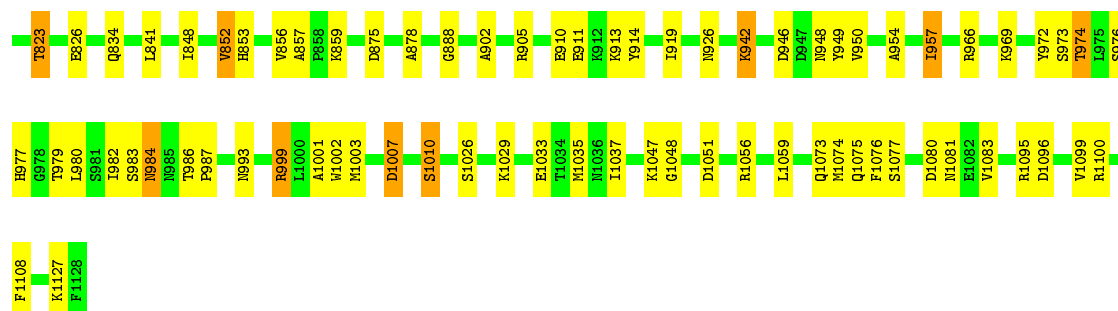
Chain D:  84% 14%



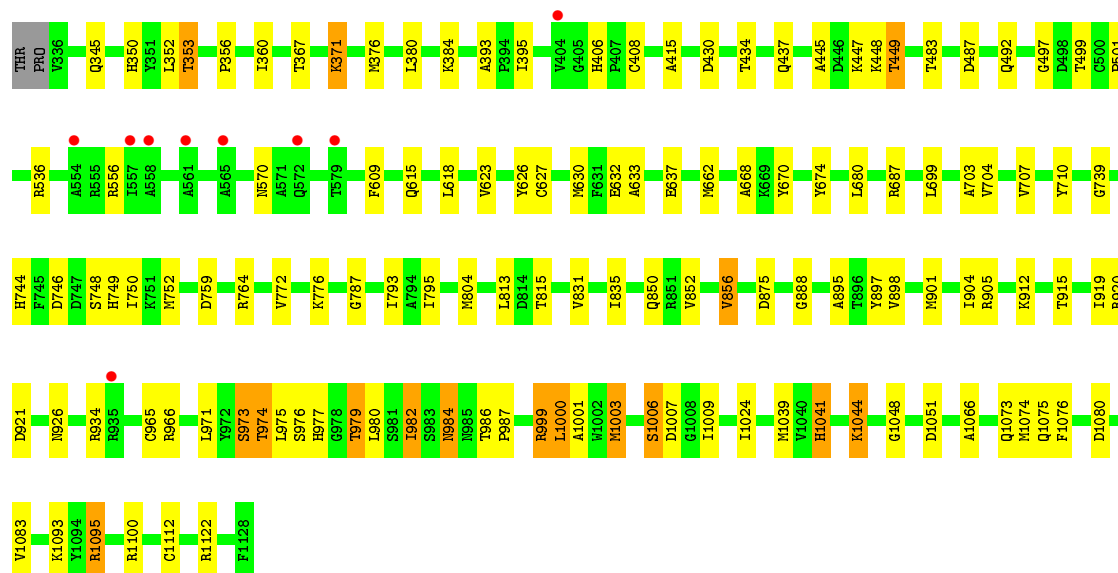
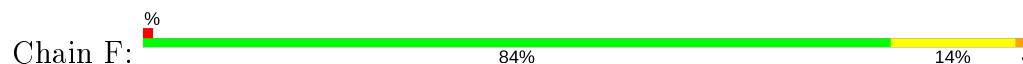
• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

Chain E:  78% 19%

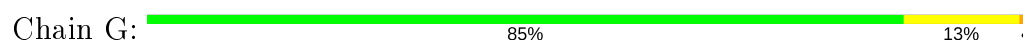





• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

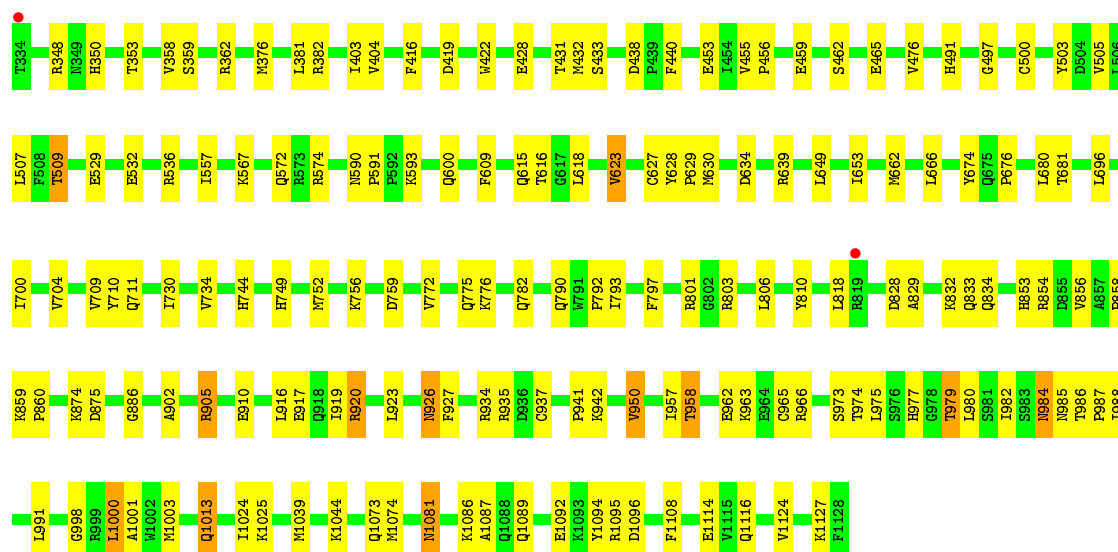


• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE



• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

Chain H:  79% 19%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.41Å 221.87Å 419.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	209.74 – 2.40 76.21 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.6 (209.74-2.40) 93.6 (76.21-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.188 , 0.247 0.194 , 0.249	Depositor DCC
R_{free} test set	15197 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	52127	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.65	0/6385	0.84	10/8640 (0.1%)
1	B	0.61	0/6392	0.80	7/8650 (0.1%)
1	C	0.62	0/6392	0.82	7/8650 (0.1%)
1	D	0.65	0/6392	0.82	6/8650 (0.1%)
1	E	0.57	0/6392	0.76	1/8650 (0.0%)
1	F	0.58	0/6392	0.75	1/8650 (0.0%)
1	G	0.59	0/6392	0.78	6/8650 (0.1%)
1	H	0.60	0/6407	0.77	3/8672 (0.0%)
All	All	0.61	0/51144	0.79	41/69212 (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	E	0	1
1	G	0	2
All	All	0	3

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	764	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	A	382	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	C	764	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	382	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	C	753	MET	CG-SD-CE	-7.57	88.08	100.20
1	H	362	ARG	NE-CZ-NH1	7.56	124.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	536	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	G	980	LEU	CA-CB-CG	7.29	132.07	115.30
1	G	854	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	536	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	A	556	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	D	803	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	D	487	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	779	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	536	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	F	536	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	G	348	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	779	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	G	1095	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	C	382	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	423	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	H	854	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	1080	ASP	CB-CG-OD1	5.54	123.29	118.30
1	E	382	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	556	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	618	LEU	CA-CB-CG	-5.38	102.94	115.30
1	H	536	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	643	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	825	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	618	LEU	CA-CB-CG	-5.27	103.17	115.30
1	D	382	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	D	382	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	819	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	376	MET	CG-SD-CE	-5.16	91.95	100.20
1	A	1096	ASP	CB-CG-OD1	5.14	122.92	118.30
1	B	762	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	B	764	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	G	854	ARG	CG-CD-NE	-5.08	101.13	111.80
1	G	999	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	643	ASP	CB-CG-OD1	5.05	122.85	118.30
1	D	803	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	480	SER	Peptide
1	G	377	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	G	789	THR	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	6254	0	6171	73	0
1	B	6261	0	6180	75	0
1	C	6261	0	6180	94	0
1	D	6261	0	6180	71	0
1	E	6261	0	6180	88	0
1	F	6261	0	6180	85	0
1	G	6261	0	6180	66	0
1	H	6275	0	6194	90	0
2	A	7	0	14	1	0
2	B	7	0	14	0	0
2	C	7	0	14	1	0
2	D	7	0	14	0	0
2	E	7	0	14	0	0
2	F	7	0	14	0	0
2	G	7	0	14	2	0
2	H	7	0	14	0	0
3	A	344	0	0	5	0
3	B	294	0	0	7	0
3	C	297	0	0	4	0
3	D	307	0	0	6	0
3	E	163	0	0	1	0
3	F	152	0	0	10	0
3	G	217	0	0	6	0
3	H	202	0	0	4	0
All	All	52127	0	49557	642	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 6.

All (642) 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:G:979:THR:HG21	1:G:1009:ILE:HD11	1.44	0.97
1:C:722:SER:O	1:C:1064:ARG:NH2	2.01	0.92
1:E:999:ARG:NH2	1:E:1003:MET:O	2.03	0.92
1:F:999:ARG:NH1	1:F:1003:MET:O	2.02	0.91
1:E:568:GLU:O	1:E:574:ARG:NH1	2.04	0.89
1:H:497:GLY:H	1:H:615:GLN:HE21	1.22	0.87
1:D:376:MET:HE1	1:D:380:LEU:HG	1.56	0.85
1:E:477:TRP:O	1:E:481:GLY:HA3	1.77	0.84
1:C:941:PRO:O	1:C:950:VAL:HG11	1.80	0.81
1:H:350:HIS:O	1:H:353:THR:HB	1.79	0.80
1:C:795:ILE:HD11	1:C:901:MET:HE2	1.62	0.80
1:G:784:THR:HG22	3:G:2148:HOH:O	1.81	0.80
1:B:637:GLU:OE1	1:B:639:ARG:NH2	2.17	0.77
1:G:979:THR:CG2	1:G:1009:ILE:HD11	2.14	0.76
1:A:966:ARG:HH11	1:A:974:THR:HG22	1.50	0.76
1:A:897:TYR:CZ	1:A:901:MET:HE3	2.21	0.75
1:C:902:ALA:CB	1:C:950:VAL:HG12	2.17	0.75
1:B:1075:GLN:HE22	1:B:1103:GLY:H	1.34	0.74
1:G:497:GLY:H	1:G:615:GLN:HE21	1.34	0.74
1:A:999:ARG:NH1	1:A:1003:MET:O	2.21	0.73
1:G:962:GLU:OE1	1:G:977:HIS:HD2	1.71	0.73
1:F:897:TYR:CZ	1:F:901:MET:HE3	2.23	0.72
1:G:432:MET:HE3	1:G:440:PHE:HB2	1.70	0.72
1:B:350:HIS:O	1:B:353:THR:HB	1.89	0.72
1:E:478:ALA:HA	1:E:482:GLU:HG3	1.72	0.72
1:C:1024:ILE:HD11	1:C:1074:MET:HE1	1.72	0.72
1:H:984:ASN:C	1:H:984:ASN:HD22	1.91	0.72
1:B:999:ARG:NH1	1:B:1003:MET:O	2.23	0.72
1:A:744:HIS:HD2	1:A:749:HIS:CE1	2.09	0.71
1:E:805:VAL:HG11	1:E:993:ASN:HB2	1.73	0.69
1:E:682:VAL:CG2	1:E:697:THR:HG23	2.22	0.69
1:D:527:SER:HB2	1:D:529:GLU:OE2	1.91	0.69
1:A:682:VAL:HG13	1:A:697:THR:HG23	1.75	0.69
1:A:711:GLN:NE2	3:A:2173:HOH:O	2.25	0.69
1:E:572:GLN:HE21	1:E:572:GLN:HA	1.58	0.69
1:A:795:ILE:HD11	1:A:901:MET:HE2	1.74	0.68
1:F:430:ASP:OD1	1:F:447:LYS:NZ	2.26	0.68
1:G:509:THR:HG21	3:G:2072:HOH:O	1.92	0.68
1:E:813:LEU:N	1:E:834:GLN:OE1	2.27	0.68
1:C:1024:ILE:HD11	1:C:1074:MET:CE	2.24	0.68
1:H:491:HIS:O	1:H:853:HIS:HE1	1.76	0.68
1:A:380:LEU:O	1:A:384:LYS:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:ASP:HB3	3:A:2212:HOH:O	1.95	0.66
1:F:979:THR:HG22	1:F:1039:MET:HA	1.78	0.66
1:G:773:GLU:OE2	1:G:784:THR:HG21	1.95	0.66
1:F:895:ALA:HB3	1:F:1006:SER:OG	1.95	0.66
1:G:1009:ILE:HG22	1:G:1009:ILE:O	1.95	0.66
1:H:627:CYS:HA	1:H:630:MET:HE2	1.78	0.66
1:D:1052:THR:CG2	1:D:1054:GLU:CD	2.64	0.66
1:E:743:CYS:HB2	1:E:1074:MET:O	1.95	0.66
1:E:731:VAL:HG22	1:E:1059:LEU:HD23	1.77	0.66
1:H:431:THR:HG23	3:H:2037:HOH:O	1.96	0.66
1:B:1080:ASP:HB3	1:B:1083:VAL:HG23	1.76	0.66
1:H:1108:PHE:CZ	1:H:1116:GLN:HB2	2.31	0.66
1:D:894:LEU:HD22	1:D:1009:ILE:CD1	2.26	0.65
1:F:395:ILE:HD11	1:F:556:ARG:HB3	1.78	0.65
1:F:746:ASP:O	1:F:750:ILE:HG12	1.97	0.65
1:B:920:ARG:NH1	1:B:921:ASP:OD1	2.30	0.65
1:C:748:SER:O	1:C:752:MET:HG2	1.96	0.65
1:F:966:ARG:HH11	1:F:974:THR:HG22	1.62	0.65
1:A:897:TYR:CE1	1:A:901:MET:CE	2.80	0.64
1:D:627:CYS:HA	1:D:630:MET:CE	2.27	0.64
1:F:497:GLY:H	1:F:615:GLN:HE21	1.43	0.64
1:E:1073:GLN:HE22	1:E:1075:GLN:HE21	1.43	0.64
1:E:857:ALA:O	1:E:859:LYS:NZ	2.28	0.64
1:H:404:VAL:H	1:H:600:GLN:HE22	1.44	0.64
1:A:497:GLY:H	1:A:615:GLN:HE21	1.45	0.64
1:E:682:VAL:HG22	1:E:697:THR:HG23	1.80	0.64
1:H:627:CYS:HA	1:H:630:MET:CE	2.28	0.64
1:E:902:ALA:HB2	1:E:950:VAL:HG23	1.79	0.64
1:B:419:ASP:OD1	1:B:419:ASP:N	2.30	0.63
1:C:423:ARG:NH2	1:C:468:GLU:OE1	2.31	0.63
1:A:962:GLU:OE2	1:A:976:SER:HB2	1.97	0.63
1:E:1048:GLY:HA2	1:E:1051:ASP:OD2	1.98	0.63
1:C:491:HIS:O	1:C:853:HIS:HE1	1.82	0.63
1:A:542:ALA:O	1:A:546:THR:HG23	1.99	0.63
1:A:795:ILE:HD11	1:A:901:MET:CE	2.29	0.63
1:B:346:ARG:NH1	1:B:400:ASP:OD1	2.31	0.63
1:D:1073:GLN:HE22	1:D:1075:GLN:HE21	1.45	0.63
1:E:700:ILE:O	1:E:704:VAL:HG12	1.99	0.62
1:B:691:ASP:OD1	1:B:719:HIS:HE1	1.82	0.62
1:H:979:THR:HG22	1:H:1039:MET:HA	1.81	0.62
1:C:627:CYS:HA	1:C:630:MET:CE	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:ILE:HD11	1:C:556:ARG:HB3	1.80	0.62
1:F:350:HIS:O	1:F:353:THR:HB	2.00	0.61
1:H:984:ASN:O	1:H:988:ILE:HG12	2.00	0.61
1:A:487:ASP:O	1:A:787:GLY:HA2	2.01	0.61
1:A:406:HIS:HD2	1:A:408:CYS:H	1.49	0.61
1:A:682:VAL:CG1	1:A:697:THR:HG23	2.29	0.60
1:B:966:ARG:HH11	1:B:974:THR:CG2	2.14	0.60
1:E:478:ALA:HA	1:E:482:GLU:CG	2.31	0.60
1:B:744:HIS:HD2	1:B:749:HIS:CE1	2.19	0.60
1:E:954:ALA:HA	1:E:957:ILE:HD11	1.83	0.60
1:F:966:ARG:HH11	1:F:974:THR:CG2	2.13	0.60
1:H:358:VAL:HG21	1:H:432:MET:HE3	1.84	0.60
1:B:942:LYS:HG2	1:B:1015:ALA:HB1	1.84	0.60
1:E:569:GLN:HA	1:E:569:GLN:OE1	2.01	0.60
1:E:984:ASN:C	1:E:984:ASN:HD22	2.05	0.60
1:G:350:HIS:O	1:G:353:THR:HB	2.01	0.60
1:C:627:CYS:HA	1:C:630:MET:HE1	1.84	0.60
1:F:483:THR:HB	1:F:804:MET:HE1	1.83	0.60
1:H:382:ARG:HD2	3:H:2017:HOH:O	2.02	0.60
1:E:979:THR:HG21	1:E:1035:MET:SD	2.41	0.59
1:F:926:ASN:HD21	1:F:1001:ALA:H	1.50	0.59
1:D:432:MET:HE3	1:D:440:PHE:HB2	1.83	0.59
1:F:1024:ILE:HD11	1:F:1074:MET:HE2	1.83	0.59
1:H:696:LEU:HD12	1:H:700:ILE:HG13	1.84	0.59
1:B:885:HIS:HE2	1:B:966:ARG:HH12	1.49	0.59
1:H:358:VAL:HG21	1:H:432:MET:CE	2.31	0.59
1:A:897:TYR:CE1	1:A:901:MET:HE1	2.38	0.59
1:D:406:HIS:HD2	1:D:408:CYS:H	1.48	0.59
1:D:623:VAL:HG22	1:D:680:LEU:HD21	1.85	0.59
1:D:897:TYR:CE1	1:D:957:ILE:HG12	2.38	0.59
1:A:383:ALA:HB1	1:A:546:THR:HG22	1.84	0.58
1:E:1099:VAL:HG11	1:E:1108:PHE:CD1	2.37	0.58
1:D:857:ALA:O	1:D:859:LYS:NZ	2.35	0.58
1:E:913:LYS:HD3	1:E:914:TYR:CZ	2.38	0.58
1:C:614:ASN:HD21	1:C:662:MET:H	1.51	0.58
1:H:934:ARG:NH1	1:H:1000:LEU:HD13	2.19	0.58
1:G:404:VAL:H	1:G:600:GLN:HE22	1.52	0.58
1:E:403:ILE:HD13	1:E:652:PHE:HB2	1.85	0.58
1:E:744:HIS:HD2	1:E:749:HIS:CE1	2.22	0.57
1:F:627:CYS:HA	1:F:630:MET:CE	2.34	0.57
1:F:973:SER:OG	1:F:974:THR:N	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:934:ARG:NH1	1:H:998:GLY:O	2.36	0.57
1:F:759:ASP:HB3	3:F:2080:HOH:O	2.03	0.57
1:H:966:ARG:HH11	1:H:974:THR:CG2	2.16	0.57
1:D:926:ASN:HD21	1:D:1000:LEU:HB2	1.69	0.57
1:H:680:LEU:HD23	1:H:681:THR:N	2.20	0.57
1:C:823:THR:HG22	1:C:825:ASP:N	2.19	0.57
1:C:406:HIS:HD2	1:C:408:CYS:H	1.52	0.57
1:B:785:SER:HB3	3:B:2202:HOH:O	2.03	0.56
1:C:902:ALA:HB2	1:C:950:VAL:HG12	1.87	0.56
1:D:813:LEU:H	1:D:834:GLN:HE22	1.52	0.56
1:D:500:CYS:H	1:D:775:GLN:HE22	1.53	0.56
1:H:730:ILE:O	1:H:734:VAL:HG23	2.05	0.56
1:H:1013:GLN:HE21	1:H:1013:GLN:H	1.51	0.56
1:H:965:CYS:O	1:H:975:LEU:HB3	2.06	0.56
1:E:491:HIS:O	1:E:853:HIS:HE1	1.87	0.56
1:G:785:SER:HA	1:G:888:GLY:O	2.05	0.56
1:F:356:PRO:HG2	1:F:674:TYR:CE2	2.40	0.56
1:F:850:GLN:HB3	1:F:971:LEU:HD22	1.88	0.56
1:D:894:LEU:HD22	1:D:1009:ILE:HD13	1.87	0.56
1:G:362:ARG:NH2	1:G:419:ASP:OD1	2.38	0.56
1:H:902:ALA:CB	1:H:950:VAL:HG12	2.35	0.56
1:E:348:ARG:NH1	1:E:707:VAL:O	2.40	0.55
1:H:1013:GLN:NE2	1:H:1013:GLN:H	2.04	0.55
1:E:650:GLN:HB3	1:E:707:VAL:HG21	1.89	0.55
1:H:416:PHE:HA	1:H:662:MET:HE1	1.89	0.55
1:C:905:ARG:HD2	1:C:953:TYR:OH	2.07	0.55
1:F:749:HIS:HA	1:F:752:MET:HG2	1.87	0.55
1:C:897:TYR:CZ	1:C:901:MET:HE3	2.39	0.55
1:C:639:ARG:O	1:C:640:LEU:HD23	2.06	0.55
1:H:497:GLY:H	1:H:615:GLN:NE2	2.00	0.55
1:E:376:MET:HE1	1:E:380:LEU:HG	1.87	0.55
1:F:934:ARG:HH12	1:F:1000:LEU:HG	1.70	0.55
2:G:2000:CHT:H82	2:G:2000:CHT:O6	2.07	0.55
1:D:627:CYS:HA	1:D:630:MET:HE1	1.87	0.54
1:E:1080:ASP:HB3	1:E:1083:VAL:HG23	1.88	0.54
1:C:1074:MET:CE	3:C:2280:HOH:O	2.55	0.54
1:G:399:ASP:O	1:G:400:ASP:HB2	2.07	0.54
1:D:1041:HIS:HD2	3:D:2294:HOH:O	1.89	0.54
1:E:749:HIS:HA	1:E:752:MET:HG2	1.89	0.54
1:B:462:SER:OG	1:B:465:GLU:OE1	2.24	0.54
1:B:974:THR:HG21	3:B:2186:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1073:GLN:HE22	1:C:1075:GLN:HE21	1.55	0.54
1:D:450:ILE:O	1:D:455:VAL:HG13	2.07	0.54
1:C:897:TYR:CE1	1:C:901:MET:CE	2.90	0.54
1:G:931:GLU:H	1:G:931:GLU:CD	2.11	0.54
1:B:700:ILE:O	1:B:704:VAL:HG13	2.06	0.54
1:B:749:HIS:HA	1:B:752:MET:HG2	1.89	0.54
1:D:609:PHE:CG	1:D:618:LEU:HD22	2.43	0.54
1:B:404:VAL:CG2	1:B:557:ILE:HD13	2.37	0.54
1:G:785:SER:HB3	1:G:890:ILE:HD12	1.90	0.54
1:H:1044:LYS:NZ	1:H:1081:ASN:HD21	2.06	0.54
1:F:437:GLN:HG3	1:F:668:ALA:HB1	1.89	0.53
1:G:739:GLY:HA3	1:G:1100:ARG:HB2	1.90	0.53
1:B:609:PHE:CD2	1:B:618:LEU:HD22	2.43	0.53
1:E:416:PHE:HA	1:E:662:MET:HE1	1.91	0.53
1:H:937:CYS:O	1:H:942:LYS:NZ	2.41	0.53
1:A:609:PHE:HB3	1:A:618:LEU:HD21	1.91	0.53
1:B:404:VAL:HG23	1:B:557:ILE:HD13	1.89	0.53
1:C:697:THR:HG22	1:C:701:MET:CE	2.39	0.53
1:E:1073:GLN:HE22	1:E:1075:GLN:NE2	2.06	0.53
1:H:962:GLU:OE1	1:H:977:HIS:HD2	1.91	0.53
1:C:1075:GLN:HE22	1:C:1100:ARG:HH21	1.57	0.53
1:A:749:HIS:HA	1:A:752:MET:HG2	1.90	0.53
1:F:850:GLN:OE1	1:F:971:LEU:HB2	2.09	0.53
1:B:399:ASP:O	1:B:400:ASP:HB2	2.08	0.53
1:D:437:GLN:HE22	1:D:1112:CYS:H	1.57	0.53
1:A:432:MET:HA	1:A:435:ARG:HD3	1.90	0.53
1:A:434:THR:HB	3:A:2062:HOH:O	2.09	0.53
1:B:979:THR:HG21	1:B:1009:ILE:CG2	2.39	0.53
1:A:395:ILE:CD1	1:A:556:ARG:CZ	2.87	0.53
1:H:428:GLU:HA	1:H:431:THR:HG22	1.91	0.53
1:H:790:GLN:HG2	1:H:792:PRO:HD2	1.90	0.53
1:F:445:ALA:O	1:F:449:THR:HG22	2.09	0.53
1:G:749:HIS:HA	1:G:752:MET:HG2	1.90	0.53
1:H:966:ARG:HH11	1:H:974:THR:HG23	1.74	0.53
1:B:823:THR:HG22	1:B:826:GLU:H	1.74	0.52
1:D:850:GLN:HB3	1:D:971:LEU:HD22	1.92	0.52
1:A:497:GLY:H	1:A:615:GLN:NE2	2.07	0.52
1:C:828:ASP:OD2	1:C:832:LYS:HE2	2.09	0.52
1:A:1075:GLN:NE2	1:A:1100:ARG:HH21	2.07	0.52
1:E:476:VAL:HG12	1:E:841:LEU:HD12	1.90	0.52
1:G:1044:LYS:NZ	1:G:1081:ASN:HD21	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ILE:HD11	1:B:584:ASN:CG	2.30	0.52
1:F:449:THR:HG21	3:F:2021:HOH:O	2.09	0.52
1:H:505:VAL:O	1:H:509:THR:HG21	2.10	0.52
1:B:426:ARG:HD2	1:B:426:ARG:C	2.30	0.52
1:B:979:THR:CG2	1:B:1009:ILE:HG23	2.40	0.52
1:F:750:ILE:CD1	1:F:764:ARG:HA	2.40	0.52
1:G:700:ILE:O	1:G:704:VAL:HG13	2.10	0.52
1:F:1048:GLY:HA2	1:F:1051:ASP:OD2	2.10	0.52
1:H:634:ASP:OD1	1:H:639:ARG:NH1	2.39	0.52
1:C:1074:MET:HE2	3:C:2280:HOH:O	2.10	0.52
1:C:902:ALA:HB1	1:C:950:VAL:HG12	1.89	0.52
1:F:915:THR:HG21	3:F:2117:HOH:O	2.09	0.52
1:A:933:LEU:HD23	1:A:933:LEU:C	2.31	0.51
1:F:395:ILE:CD1	1:F:556:ARG:HB3	2.41	0.51
1:B:491:HIS:O	1:B:853:HIS:HE1	1.94	0.51
1:E:966:ARG:HH11	1:E:974:THR:CG2	2.24	0.51
1:F:609:PHE:CG	1:F:618:LEU:HD22	2.46	0.51
1:H:615:GLN:HG3	1:H:618:LEU:HD11	1.93	0.51
1:F:483:THR:HB	1:F:804:MET:CE	2.41	0.51
1:G:498:ASP:OD1	2:G:2000:CHT:H61	2.11	0.51
1:C:823:THR:HG22	1:C:825:ASP:H	1.76	0.51
1:A:428:GLU:O	1:A:432:MET:HB2	2.11	0.51
1:C:403:ILE:HG22	1:C:655:LYS:HG3	1.92	0.51
1:E:1099:VAL:HG11	1:E:1108:PHE:HD1	1.76	0.51
1:G:1009:ILE:HD11	1:G:1035:MET:HE2	1.92	0.51
1:G:1009:ILE:CB	3:G:2130:HOH:O	2.59	0.51
1:G:632:GLU:OE2	1:G:636:ARG:NH1	2.44	0.51
1:G:854:ARG:HB2	1:G:877:ALA:O	2.11	0.51
1:F:920:ARG:NH1	1:F:921:ASP:OD1	2.43	0.50
1:A:897:TYR:CZ	1:A:901:MET:CE	2.94	0.50
1:C:797:PHE:HB2	1:C:834:GLN:HG2	1.93	0.50
1:F:965:CYS:O	1:F:975:LEU:HB3	2.11	0.50
1:D:609:PHE:CD2	1:D:618:LEU:HD22	2.46	0.50
1:H:759:ASP:HB3	3:H:2134:HOH:O	2.11	0.50
1:E:468:GLU:O	1:E:472:ARG:HG2	2.11	0.50
1:B:948:ASN:HD22	1:B:1029:LYS:HE2	1.76	0.50
1:F:1041:HIS:HD2	3:F:2150:HOH:O	1.93	0.50
1:H:497:GLY:N	1:H:615:GLN:HE21	2.01	0.50
1:C:915:THR:HG22	1:C:918:GLN:OE1	2.11	0.50
1:F:497:GLY:N	1:F:615:GLN:HE21	2.07	0.50
1:B:553:TYR:O	1:B:557:ILE:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:ASP:HB3	3:B:2191:HOH:O	2.12	0.50
1:H:348:ARG:NH2	1:H:1096:ASP:OD2	2.44	0.50
1:C:609:PHE:CG	1:C:618:LEU:HD22	2.46	0.49
1:E:848:ILE:O	1:E:852:VAL:HG13	2.11	0.49
1:B:632:GLU:OE1	1:B:636:ARG:NH2	2.44	0.49
1:D:832:LYS:HB3	1:D:960:TRP:CZ2	2.46	0.49
1:E:336:VAL:HA	1:E:345:GLN:HG3	1.94	0.49
1:A:434:THR:HG22	3:A:2066:HOH:O	2.13	0.49
1:C:432:MET:HE3	1:C:440:PHE:HB2	1.95	0.49
1:C:848:ILE:O	1:C:852:VAL:HG13	2.12	0.49
1:F:1024:ILE:HD11	1:F:1074:MET:CE	2.43	0.49
1:G:720:ASN:ND2	1:G:1067:SER:OG	2.45	0.49
1:H:984:ASN:C	1:H:984:ASN:ND2	2.64	0.49
1:E:730:ILE:O	1:E:734:VAL:HG23	2.12	0.49
1:G:1009:ILE:HG13	3:G:2130:HOH:O	2.12	0.49
1:C:920:ARG:HG3	1:C:921:ASP:N	2.28	0.49
1:D:491:HIS:O	1:D:853:HIS:HE1	1.96	0.49
1:C:1075:GLN:NE2	1:C:1100:ARG:HH21	2.11	0.49
1:F:1074:MET:CE	3:F:2148:HOH:O	2.60	0.49
1:F:449:THR:CG2	3:F:2021:HOH:O	2.61	0.49
1:F:497:GLY:H	1:F:615:GLN:NE2	2.08	0.49
1:G:1075:GLN:NE2	1:G:1100:ARG:HH21	2.10	0.49
1:A:986:THR:HB	1:A:987:PRO:CD	2.42	0.49
1:C:850:GLN:HB3	1:C:971:LEU:HD22	1.93	0.49
1:D:598:ALA:HB2	1:D:630:MET:HE3	1.95	0.49
1:F:748:SER:O	1:F:752:MET:HG2	2.12	0.49
1:G:497:GLY:N	1:G:615:GLN:HE21	2.07	0.49
1:H:649:LEU:O	1:H:653:ILE:HG12	2.12	0.49
1:A:771:CYS:SG	2:A:2000:CHT:HC42	2.53	0.49
1:B:1088:GLN:HG2	1:B:1116:GLN:OE1	2.13	0.49
1:D:919:ILE:O	1:D:923:LEU:HG	2.13	0.49
1:F:912:LYS:O	1:F:912:LYS:HD3	2.13	0.49
1:B:942:LYS:CG	1:B:1015:ALA:HB1	2.43	0.48
1:E:966:ARG:HH11	1:E:974:THR:HG22	1.78	0.48
1:G:745:PHE:HZ	1:G:1074:MET:HE3	1.77	0.48
1:A:1080:ASP:HB3	1:A:1083:VAL:HG23	1.93	0.48
1:D:1052:THR:HG23	1:D:1054:GLU:CD	2.33	0.48
1:B:744:HIS:CD2	1:B:749:HIS:CE1	3.00	0.48
1:C:897:TYR:CE1	1:C:901:MET:HE1	2.48	0.48
1:D:700:ILE:O	1:D:704:VAL:HG13	2.13	0.48
1:D:747:ASP:O	1:D:751:LYS:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:691:ASP:OD1	1:G:719:HIS:HE1	1.95	0.48
1:G:745:PHE:CZ	1:G:1074:MET:CE	2.96	0.48
1:B:993:ASN:O	1:B:999:ARG:NH2	2.47	0.48
1:E:739:GLY:HA3	1:E:1100:ARG:HB2	1.95	0.48
1:E:946:ASP:OD1	1:E:1029:LYS:NZ	2.45	0.48
1:B:857:ALA:O	1:B:859:LYS:NZ	2.46	0.48
1:C:1073:GLN:HE22	1:C:1075:GLN:NE2	2.10	0.48
1:C:853:HIS:HD2	1:C:859:LYS:NZ	2.12	0.48
1:C:915:THR:HG23	1:C:918:GLN:H	1.78	0.48
1:E:669:LYS:O	1:E:983:SER:OG	2.31	0.48
1:H:797:PHE:HB2	1:H:834:GLN:HG2	1.94	0.48
1:A:850:GLN:HB3	1:A:971:LEU:HD22	1.94	0.48
1:E:942:LYS:C	1:E:950:VAL:HG11	2.34	0.48
1:F:1075:GLN:HE22	1:F:1100:ARG:HH21	1.60	0.48
1:C:1016:ASP:OD2	1:C:1123:THR:HG21	2.14	0.48
1:E:500:CYS:H	1:E:775:GLN:HE22	1.62	0.48
1:B:962:GLU:OE1	1:B:977:HIS:HD2	1.96	0.48
1:C:395:ILE:CD1	1:C:556:ARG:HB3	2.44	0.48
1:C:962:GLU:OE1	1:C:977:HIS:HD2	1.97	0.47
1:H:680:LEU:C	1:H:680:LEU:HD23	2.34	0.47
1:E:419:ASP:N	1:E:419:ASP:OD1	2.46	0.47
1:A:966:ARG:HH11	1:A:974:THR:CG2	2.23	0.47
1:H:1087:ALA:HA	1:H:1094:TYR:CD2	2.49	0.47
1:B:406:HIS:HD2	1:B:408:CYS:H	1.62	0.47
1:C:570:ASN:O	1:C:574:ARG:HB2	2.14	0.47
1:B:785:SER:OG	1:B:787:GLY:O	2.33	0.47
1:G:1009:ILE:HG21	3:G:2130:HOH:O	2.14	0.47
1:G:739:GLY:HA3	1:G:1100:ARG:HD3	1.97	0.47
1:H:419:ASP:OD1	1:H:419:ASP:N	2.47	0.47
1:E:428:GLU:OE1	1:E:435:ARG:NH1	2.47	0.47
1:F:1066:ALA:HB2	1:F:1074:MET:HE1	1.96	0.47
1:G:628:TYR:N	1:G:629:PRO:CD	2.77	0.47
1:A:799:LEU:HA	1:A:818:LEU:HD21	1.97	0.47
1:B:358:VAL:CG2	1:B:432:MET:HE3	2.44	0.47
1:A:748:SER:O	1:A:752:MET:HG2	2.15	0.47
1:F:1080:ASP:HB3	1:F:1083:VAL:HG23	1.96	0.47
1:G:371:LYS:O	1:G:374:PRO:HD3	2.14	0.47
1:H:756:LYS:NZ	1:H:782:GLN:HE22	2.12	0.47
1:A:1044:LYS:NZ	1:A:1119:ILE:O	2.48	0.47
1:D:745:PHE:CZ	1:D:1074:MET:CE	2.98	0.47
1:D:979:THR:HG21	1:D:1035:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:653:ILE:HG23	1:D:712:PRO:HD2	1.97	0.47
1:G:438:ASP:HA	1:G:674:TYR:CZ	2.50	0.47
1:G:745:PHE:HZ	1:G:1074:MET:CE	2.28	0.47
1:F:352:LEU:O	1:F:1095:ARG:NH1	2.47	0.47
1:A:962:GLU:OE1	1:A:977:HIS:HD2	1.98	0.46
1:F:744:HIS:HD2	1:F:749:HIS:CE1	2.33	0.46
1:G:491:HIS:O	1:G:853:HIS:HE1	1.97	0.46
1:B:649:LEU:O	1:B:653:ILE:HG12	2.14	0.46
1:C:450:ILE:O	1:C:455:VAL:HG13	2.15	0.46
1:C:627:CYS:HA	1:C:630:MET:HE2	1.97	0.46
1:D:965:CYS:HB3	1:D:975:LEU:HB3	1.96	0.46
1:F:633:ALA:O	1:F:637:GLU:HG2	2.15	0.46
1:A:432:MET:HE1	1:A:442:ILE:HB	1.96	0.46
1:C:343:ARG:NH2	1:C:576:GLU:OE2	2.46	0.46
1:C:759:ASP:HB3	3:C:2177:HOH:O	2.14	0.46
1:D:627:CYS:HA	1:D:630:MET:HE2	1.96	0.46
1:G:900:SER:HB2	1:G:996:PRO:HD2	1.98	0.46
1:A:399:ASP:O	1:A:400:ASP:HB2	2.15	0.46
2:C:2000:CHT:H82	2:C:2000:CHT:O6	2.16	0.46
1:C:694:ASN:O	1:C:697:THR:HB	2.15	0.46
1:D:1112:CYS:O	1:D:1116:GLN:HG3	2.16	0.46
1:D:376:MET:CE	1:D:380:LEU:HG	2.39	0.46
1:E:384:LYS:NZ	1:E:545:GLU:OE2	2.37	0.46
1:G:348:ARG:NH2	1:G:1096:ASP:OD2	2.49	0.46
1:A:480:SER:HB3	1:A:488:LEU:HD22	1.97	0.46
1:D:926:ASN:HD21	1:D:1001:ALA:H	1.64	0.46
1:F:367:THR:O	1:F:371:LYS:HB2	2.15	0.46
1:F:406:HIS:HD2	1:F:408:CYS:H	1.64	0.46
1:A:902:ALA:HB2	1:A:950:VAL:HG23	1.97	0.46
1:D:639:ARG:O	1:D:640:LEU:HD23	2.15	0.46
1:F:749:HIS:HA	1:F:752:MET:CG	2.46	0.46
1:H:1086:LYS:HA	1:H:1086:LYS:HE2	1.97	0.46
1:A:867:GLU:HB2	1:A:882:MET:CE	2.46	0.46
1:B:966:ARG:HH11	1:B:974:THR:HG22	1.79	0.46
1:D:959:GLU:CG	3:D:2252:HOH:O	2.64	0.46
1:B:951:ASP:OD2	1:B:1026:SER:OG	2.25	0.46
1:C:697:THR:HG22	1:C:701:MET:HE2	1.98	0.46
1:E:948:ASN:O	1:E:949:TYR:C	2.54	0.46
1:H:905:ARG:NH1	1:H:910:GLU:OE2	2.48	0.46
1:A:346:ARG:NH1	1:A:400:ASP:OD1	2.50	0.46
1:C:609:PHE:CD2	1:C:618:LEU:HD22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:627:CYS:HA	1:F:630:MET:HE2	1.97	0.46
1:B:848:ILE:O	1:B:852:VAL:HG13	2.16	0.45
1:F:1074:MET:HE2	3:F:2148:HOH:O	2.16	0.45
1:A:406:HIS:HE1	1:A:658:GLU:O	1.98	0.45
1:B:527:SER:HB2	3:B:2089:HOH:O	2.16	0.45
1:D:406:HIS:HE1	1:D:658:GLU:O	2.00	0.45
1:E:527:SER:OG	1:E:529:GLU:HG2	2.17	0.45
1:E:805:VAL:HG13	1:E:806:LEU:N	2.32	0.45
1:H:984:ASN:HD22	1:H:985:ASN:N	2.14	0.45
1:B:790:GLN:HE21	1:B:792:PRO:HB2	1.81	0.45
1:D:336:VAL:HA	1:D:345:GLN:HG3	1.97	0.45
1:F:487:ASP:O	1:F:787:GLY:HA2	2.16	0.45
1:A:542:ALA:O	1:A:546:THR:CG2	2.64	0.45
1:C:393:ALA:O	1:C:556:ARG:NH2	2.50	0.45
1:D:1041:HIS:CD2	3:D:2294:HOH:O	2.68	0.45
1:F:623:VAL:HG22	1:F:680:LEU:HD21	1.98	0.45
1:D:745:PHE:CE2	1:D:1074:MET:HE2	2.52	0.45
1:H:958:THR:CG2	3:H:2174:HOH:O	2.64	0.45
1:D:1052:THR:HG22	1:D:1055:GLY:H	1.80	0.45
1:B:979:THR:HG23	1:B:1009:ILE:HG23	1.99	0.45
1:D:510:LYS:HE2	3:D:2096:HOH:O	2.16	0.45
1:D:623:VAL:CG2	1:D:680:LEU:HD21	2.46	0.45
1:E:823:THR:HG22	1:E:826:GLU:H	1.80	0.45
1:D:420:ILE:HD13	1:D:613:GLU:HB2	1.98	0.45
1:B:790:GLN:CG	1:B:792:PRO:HD2	2.47	0.45
1:B:853:HIS:HD2	1:B:859:LYS:NZ	2.15	0.45
1:H:853:HIS:HD2	1:H:859:LYS:HZ1	1.64	0.45
1:H:926:ASN:O	1:H:927:PHE:HB2	2.16	0.45
1:A:749:HIS:HA	1:A:752:MET:CG	2.47	0.45
1:B:756:LYS:NZ	1:B:782:GLN:HE22	2.14	0.45
1:B:790:GLN:NE2	1:B:793:ILE:N	2.65	0.45
1:C:494:ASN:ND2	1:C:661:TRP:HE1	2.15	0.45
1:E:508:PHE:O	1:E:591:PRO:HB3	2.17	0.45
1:G:1075:GLN:HE22	1:G:1103:GLY:HA2	1.82	0.45
1:C:497:GLY:H	1:C:615:GLN:NE2	2.15	0.44
1:G:999:ARG:CG	1:G:999:ARG:HH11	2.30	0.44
1:H:986:THR:HB	1:H:987:PRO:CD	2.46	0.44
1:A:504:ASP:OD2	1:A:776:LYS:NZ	2.49	0.44
1:B:790:GLN:NE2	1:B:793:ILE:H	2.14	0.44
1:E:680:LEU:C	1:E:680:LEU:HD23	2.37	0.44
1:F:1041:HIS:HE1	3:F:2141:HOH:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1075:GLN:NE2	1:F:1100:ARG:HH21	2.14	0.44
1:G:695:ASP:O	1:G:699:LEU:HD12	2.16	0.44
1:H:455:VAL:O	1:H:456:PRO:C	2.54	0.44
1:H:828:ASP:O	1:H:832:LYS:HG2	2.16	0.44
1:G:984:ASN:C	1:G:984:ASN:OD1	2.56	0.44
1:E:426:ARG:C	1:E:426:ARG:HD2	2.37	0.44
1:E:986:THR:HB	1:E:987:PRO:HD3	2.00	0.44
1:D:885:HIS:HA	1:D:973:SER:OG	2.17	0.44
1:E:422:TRP:CZ2	1:E:459:GLU:HB2	2.52	0.44
1:E:986:THR:HB	1:E:987:PRO:CD	2.48	0.44
1:H:744:HIS:HD2	1:H:749:HIS:CE1	2.35	0.44
1:C:616:THR:HB	1:C:661:TRP:CG	2.52	0.44
1:D:744:HIS:HD2	1:D:749:HIS:CE1	2.35	0.44
1:F:376:MET:HE1	1:F:380:LEU:HG	1.98	0.44
1:B:348:ARG:NH2	1:B:1096:ASP:OD2	2.51	0.44
1:B:470:GLN:NE2	3:B:2059:HOH:O	2.50	0.44
1:C:1041:HIS:HD2	3:C:2281:HOH:O	2.00	0.44
1:C:1081:ASN:O	1:C:1085:LYS:HG3	2.17	0.44
1:C:350:HIS:O	1:C:353:THR:HB	2.17	0.44
1:F:897:TYR:CE2	1:F:901:MET:CE	3.01	0.44
1:G:745:PHE:CZ	1:G:1074:MET:HE3	2.51	0.44
1:C:455:VAL:N	1:C:456:PRO:CD	2.81	0.44
1:D:562:ARG:NH2	3:D:2112:HOH:O	2.50	0.44
1:E:984:ASN:C	1:E:984:ASN:ND2	2.71	0.44
1:F:1044:LYS:NZ	1:F:1122:ARG:O	2.43	0.44
1:F:670:TYR:CD2	1:F:984:ASN:HB2	2.52	0.44
1:C:344:MET:CE	1:C:654:ILE:CD1	2.96	0.44
1:D:680:LEU:HD23	1:D:680:LEU:C	2.38	0.44
1:E:350:HIS:O	1:E:353:THR:HB	2.18	0.44
1:H:358:VAL:CG2	1:H:432:MET:HE3	2.48	0.44
1:D:756:LYS:NZ	1:D:782:GLN:HE22	2.15	0.43
1:F:852:VAL:O	1:F:856:VAL:HG13	2.17	0.43
1:H:806:LEU:HD22	1:H:991:LEU:HA	2.00	0.43
1:A:680:LEU:CD2	1:A:682:VAL:HG23	2.47	0.43
1:B:828:ASP:OD2	1:B:832:LYS:HE2	2.18	0.43
1:C:941:PRO:HB2	1:C:950:VAL:HG13	2.00	0.43
1:D:887:PRO:O	1:D:975:LEU:HD23	2.18	0.43
1:G:419:ASP:N	1:G:419:ASP:OD1	2.51	0.43
1:H:917:GLU:O	1:H:920:ARG:HG3	2.18	0.43
1:D:437:GLN:NE2	1:D:1112:CYS:H	2.16	0.43
1:E:586:ASN:N	1:E:586:ASN:HD22	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:623:VAL:O	1:F:627:CYS:HB2	2.19	0.43
1:G:1001:ALA:HB1	1:G:1002:TRP:CE2	2.52	0.43
1:A:817:ASP:OD1	1:A:819:ARG:HB2	2.18	0.43
1:C:463:LEU:HG	1:C:852:VAL:HG23	2.00	0.43
1:H:500:CYS:H	1:H:775:GLN:HE22	1.65	0.43
1:H:941:PRO:HB2	1:H:950:VAL:HG13	1.99	0.43
1:A:824:PHE:CD1	1:A:905:ARG:HG2	2.54	0.43
1:C:529:GLU:OE2	1:D:840:ARG:NE	2.44	0.43
1:A:1075:GLN:HE22	1:A:1100:ARG:HH21	1.66	0.43
1:A:853:HIS:HD2	1:A:859:LYS:NZ	2.16	0.43
1:B:539:TYR:CD1	1:B:539:TYR:C	2.92	0.43
1:B:536:ARG:HD3	1:B:872:SER:O	2.19	0.43
1:C:343:ARG:HH22	1:C:576:GLU:CD	2.22	0.43
1:C:795:ILE:HD11	1:C:901:MET:CE	2.41	0.43
1:D:348:ARG:NH2	1:D:1096:ASP:OD2	2.44	0.43
1:D:1075:GLN:NE2	1:D:1100:ARG:HH21	2.17	0.43
1:E:376:MET:O	1:E:377:PRO:C	2.55	0.43
1:E:494:ASN:ND2	1:E:661:TRP:HE1	2.17	0.43
1:H:902:ALA:HB2	1:H:950:VAL:HG12	2.01	0.43
1:B:403:ILE:HG22	1:B:655:LYS:HG3	2.00	0.43
1:E:751:LYS:HG3	1:E:1033:GLU:HG2	2.00	0.43
1:H:966:ARG:HD3	1:H:975:LEU:O	2.18	0.43
1:A:973:SER:OG	1:A:974:THR:N	2.50	0.43
1:F:434:THR:HG22	1:F:434:THR:O	2.19	0.43
1:H:858:PRO:O	1:H:860:PRO:HD3	2.18	0.43
1:B:444:GLU:HG2	1:E:563:GLU:OE2	2.19	0.43
1:B:937:CYS:O	1:B:942:LYS:NZ	2.51	0.43
1:C:691:ASP:OD1	1:C:719:HIS:HE1	2.01	0.43
1:G:677:PHE:O	1:G:770:GLY:HA2	2.19	0.43
1:H:628:TYR:N	1:H:629:PRO:CD	2.81	0.43
1:C:1024:ILE:HG23	1:C:1069:LEU:HD12	2.01	0.42
1:C:888:GLY:HA2	1:C:976:SER:O	2.18	0.42
1:E:432:MET:HE2	1:E:432:MET:HB3	1.86	0.42
1:E:439:PRO:HD2	1:E:674:TYR:OH	2.19	0.42
1:F:1000:LEU:O	1:F:1003:MET:HB2	2.18	0.42
1:F:746:ASP:O	1:F:750:ILE:CG1	2.66	0.42
1:G:487:ASP:O	1:G:787:GLY:HA2	2.19	0.42
1:G:957:ILE:HD12	1:G:958:THR:H	1.84	0.42
1:A:1108:PHE:CZ	1:A:1116:GLN:HB3	2.54	0.42
1:B:528:MET:HE3	1:B:537:ILE:HG21	2.00	0.42
1:C:373:ASN:N	1:C:374:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2065:HOH:O	1:C:434:THR:HB	2.19	0.42
1:C:807:PHE:O	1:C:808:ASP:C	2.56	0.42
1:F:1041:HIS:CE1	3:F:2141:HOH:O	2.72	0.42
1:F:986:THR:HB	1:F:987:PRO:CD	2.50	0.42
1:H:749:HIS:HA	1:H:752:MET:HG2	2.00	0.42
1:H:941:PRO:O	1:H:950:VAL:HG11	2.19	0.42
1:F:415:ALA:C	1:F:662:MET:CE	2.88	0.42
1:A:491:HIS:O	1:A:853:HIS:HE1	2.02	0.42
1:B:562:ARG:NH1	3:B:2112:HOH:O	2.53	0.42
1:C:432:MET:HB3	1:C:432:MET:HE3	1.92	0.42
1:C:468:GLU:OE2	1:C:472:ARG:NH1	2.49	0.42
1:E:1007:ASP:O	1:E:1010:SER:HB3	2.20	0.42
1:F:984:ASN:C	1:F:984:ASN:OD1	2.56	0.42
1:H:623:VAL:HG13	1:H:680:LEU:HD21	2.01	0.42
1:H:829:ALA:O	1:H:833:GLN:HG3	2.18	0.42
1:H:886:GLY:O	1:H:973:SER:HB3	2.20	0.42
1:A:583:VAL:O	1:A:587:VAL:HG22	2.19	0.42
1:A:850:GLN:CB	1:A:971:LEU:HD22	2.49	0.42
1:C:703:ALA:O	1:C:707:VAL:HG23	2.20	0.42
1:D:500:CYS:N	1:D:775:GLN:HE22	2.15	0.42
1:E:360:ILE:HD12	1:E:364:LEU:HD21	2.01	0.42
1:E:565:ALA:O	1:E:574:ARG:HD3	2.19	0.42
1:E:728:GLU:OE1	1:E:1056:ARG:NE	2.53	0.42
1:G:1009:ILE:CG1	3:G:2130:HOH:O	2.67	0.42
1:H:590:ASN:HB3	1:H:591:PRO:HD2	2.01	0.42
1:A:529:GLU:HG2	1:A:529:GLU:H	1.66	0.42
1:C:707:VAL:O	1:C:708:LYS:C	2.57	0.42
1:E:878:ALA:HA	1:E:972:TYR:OH	2.20	0.42
1:E:888:GLY:HA3	1:E:1037:ILE:HG13	2.01	0.42
1:H:919:ILE:O	1:H:923:LEU:HG	2.19	0.42
1:H:986:THR:HB	1:H:987:PRO:HD3	2.02	0.42
1:E:769:MET:SD	1:E:769:MET:C	2.98	0.42
1:F:888:GLY:HA2	1:F:976:SER:O	2.19	0.42
1:H:376:MET:HB3	1:H:381:LEU:HD13	2.01	0.42
1:H:803:ARG:HG3	1:H:810:TYR:CE2	2.54	0.42
1:A:919:ILE:O	1:A:923:LEU:HG	2.20	0.42
1:C:797:PHE:HB2	1:C:834:GLN:CG	2.49	0.42
1:F:986:THR:HB	1:F:987:PRO:HD3	2.02	0.42
1:H:422:TRP:CZ2	1:H:459:GLU:HA	2.55	0.42
1:B:500:CYS:H	1:B:775:GLN:HE22	1.66	0.42
1:D:798:VAL:HG23	1:D:834:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:897:TYR:CD1	1:D:957:ILE:HG12	2.55	0.42
1:E:348:ARG:NH2	1:E:1096:ASP:OD2	2.53	0.42
1:E:888:GLY:HA2	1:E:976:SER:O	2.20	0.42
1:G:749:HIS:HA	1:G:752:MET:CG	2.50	0.42
1:H:433:SER:HA	1:H:440:PHE:O	2.20	0.42
1:A:562:ARG:NH2	1:A:585:GLU:OE2	2.53	0.42
1:A:986:THR:HB	1:A:987:PRO:HD3	2.01	0.42
1:B:1047:LYS:HD3	1:B:1047:LYS:HA	1.98	0.42
1:B:790:GLN:HG3	1:B:792:PRO:HD2	2.02	0.42
1:C:678:ILE:H	1:C:711:GLN:NE2	2.18	0.42
1:E:1001:ALA:HB1	1:E:1002:TRP:CE2	2.55	0.42
1:F:615:GLN:HG3	1:F:618:LEU:HD11	2.02	0.42
1:C:850:GLN:HE22	1:C:970:MET:HB3	1.85	0.41
1:D:739:GLY:HA3	1:D:1100:ARG:HB2	2.01	0.41
1:D:771:CYS:C	1:D:772:VAL:HG13	2.40	0.41
1:D:986:THR:HG21	1:D:1115:VAL:HA	2.02	0.41
1:E:784:THR:O	1:E:785:SER:HB3	2.20	0.41
1:F:570:ASN:C	1:F:570:ASN:OD1	2.56	0.41
1:G:348:ARG:NH2	1:G:1096:ASP:OD1	2.53	0.41
1:G:919:ILE:O	1:G:923:LEU:HG	2.20	0.41
1:H:438:ASP:HA	1:H:674:TYR:CZ	2.55	0.41
1:C:410:LYS:HG2	1:C:411:PRO:N	2.33	0.41
1:D:336:VAL:HG13	1:D:345:GLN:HG3	2.02	0.41
1:E:1047:LYS:HG3	1:E:1080:ASP:HB2	2.02	0.41
1:E:416:PHE:HA	1:E:662:MET:CE	2.49	0.41
1:E:805:VAL:HG13	1:E:1002:TRP:HH2	1.85	0.41
1:F:831:VAL:O	1:F:835:ILE:HG13	2.19	0.41
1:H:503:TYR:HA	1:H:507:LEU:HB3	2.03	0.41
1:B:979:THR:HG22	1:B:1039:MET:HA	2.02	0.41
1:B:966:ARG:HD3	1:B:974:THR:HG23	2.01	0.41
1:E:739:GLY:HA2	1:E:1076:PHE:O	2.20	0.41
1:F:360:ILE:HA	3:F:2007:HOH:O	2.20	0.41
1:F:979:THR:HG23	1:F:979:THR:O	2.21	0.41
1:G:748:SER:O	1:G:752:MET:HG2	2.20	0.41
1:H:609:PHE:CG	1:H:618:LEU:HD22	2.55	0.41
1:A:768:LEU:N	1:A:768:LEU:HD22	2.36	0.41
1:D:937:CYS:O	1:D:942:LYS:NZ	2.54	0.41
1:H:462:SER:OG	1:H:465:GLU:HG3	2.20	0.41
1:H:627:CYS:HA	1:H:630:MET:HE1	2.01	0.41
1:C:634:ASP:OD1	1:C:639:ARG:NH2	2.52	0.41
1:C:853:HIS:HD2	1:C:859:LYS:HZ1	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:497:GLY:H	1:G:615:GLN:NE2	2.09	0.41
1:H:567:LYS:O	1:H:567:LYS:HG3	2.19	0.41
1:H:793:ILE:HG12	1:H:797:PHE:CZ	2.55	0.41
1:A:653:ILE:HG23	1:A:712:PRO:HD2	2.02	0.41
1:C:926:ASN:ND2	1:C:1001:ALA:H	2.19	0.41
1:G:351:TYR:O	1:G:354:VAL:HG12	2.20	0.41
1:G:500:CYS:H	1:G:775:GLN:HE22	1.67	0.41
1:H:1044:LYS:HZ2	1:H:1081:ASN:HD21	1.69	0.41
1:H:818:LEU:HD23	1:H:916:LEU:HB3	2.01	0.41
1:A:438:ASP:N	1:A:439:PRO:CD	2.84	0.41
1:A:500:CYS:H	1:A:775:GLN:HE22	1.69	0.41
1:B:438:ASP:HA	1:B:674:TYR:CZ	2.55	0.41
1:A:506:LEU:HD11	1:A:867:GLU:HG2	2.03	0.41
1:B:815:THR:HG22	1:B:833:GLN:HE21	1.85	0.41
1:C:882:MET:HG2	1:C:883:VAL:HG23	2.02	0.41
1:E:450:ILE:O	1:E:455:VAL:HG13	2.20	0.41
1:E:682:VAL:HG11	1:E:714:LEU:HD11	2.02	0.41
1:G:362:ARG:HD2	1:G:611:ILE:O	2.21	0.41
1:H:1024:ILE:HD12	1:H:1074:MET:HE1	2.03	0.41
1:A:508:PHE:O	1:A:591:PRO:HB3	2.21	0.41
1:D:476:VAL:HG23	1:D:841:LEU:HB3	2.02	0.41
1:F:376:MET:HE1	1:F:384:LYS:CE	2.50	0.41
1:G:731:VAL:HG22	1:G:1059:LEU:HD23	2.03	0.41
1:G:853:HIS:HD2	1:G:859:LYS:NZ	2.19	0.41
1:H:926:ASN:HD21	1:H:1001:ALA:H	1.69	0.41
1:A:846:THR:O	1:A:850:GLN:HG3	2.21	0.41
1:B:1079:VAL:O	1:B:1079:VAL:HG23	2.20	0.41
1:B:1092:GLU:H	1:B:1092:GLU:CD	2.24	0.41
1:F:393:ALA:O	1:F:556:ARG:NH2	2.54	0.41
1:G:598:ALA:HB2	1:G:630:MET:HE3	2.03	0.41
1:A:623:VAL:HG13	1:A:680:LEU:HG	2.03	0.41
1:A:494:ASN:ND2	1:A:661:TRP:HE1	2.19	0.41
1:C:979:THR:CG2	1:C:1039:MET:HA	2.51	0.41
1:F:739:GLY:HA2	1:F:1076:PHE:O	2.22	0.41
1:F:499:THR:O	1:F:501:PRO:HD3	2.21	0.41
1:B:358:VAL:HG21	1:B:432:MET:CE	2.51	0.40
1:C:699:LEU:HA	1:C:699:LEU:HD12	1.92	0.40
1:C:915:THR:HG22	1:C:918:GLN:HG3	2.03	0.40
1:D:1052:THR:HG23	1:D:1054:GLU:OE1	2.21	0.40
1:G:969:LYS:O	1:G:970:MET:HE2	2.21	0.40
1:H:358:VAL:HG21	1:H:432:MET:HE1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:616:THR:OG1	1:H:676:PRO:HA	2.21	0.40
1:A:776:LYS:HD3	1:A:776:LYS:C	2.41	0.40
1:C:432:MET:HA	1:C:435:ARG:HD3	2.02	0.40
1:C:708:LYS:HA	1:C:738:MET:SD	2.61	0.40
1:C:749:HIS:HA	1:C:752:MET:CG	2.51	0.40
3:B:2180:HOH:O	1:C:751:LYS:HE3	2.21	0.40
1:D:1041:HIS:HE1	3:D:2277:HOH:O	2.02	0.40
1:D:739:GLY:HA2	1:D:1076:PHE:O	2.20	0.40
1:E:434:THR:HG22	3:E:2026:HOH:O	2.22	0.40
1:E:480:SER:O	1:E:484:PHE:HA	2.21	0.40
1:G:659:LEU:HD23	1:G:678:ILE:HD11	2.02	0.40
1:H:700:ILE:O	1:H:704:VAL:HG23	2.21	0.40
1:C:917:GLU:OE1	1:C:917:GLU:N	2.51	0.40
1:C:919:ILE:O	1:C:923:LEU:HG	2.21	0.40
1:D:625:GLN:NE2	1:D:692:ALA:HB1	2.36	0.40
1:F:623:VAL:HA	1:F:626:TYR:CE1	2.56	0.40
1:C:911:GLU:O	1:C:912:LYS:HB2	2.22	0.40
1:D:348:ARG:HD2	1:D:707:VAL:O	2.21	0.40
1:F:376:MET:CE	1:F:380:LEU:HG	2.51	0.40
1:F:434:THR:O	1:F:434:THR:CG2	2.69	0.40
1:F:795:ILE:HD11	1:F:901:MET:HE2	2.03	0.40
1:G:786:THR:HG21	1:G:849:SER:OG	2.22	0.40
1:B:943:TYR:O	1:B:1011:PRO:HB3	2.22	0.40
1:B:616:THR:HB	1:B:661:TRP:CG	2.57	0.40
1:E:805:VAL:CG1	1:E:806:LEU:N	2.85	0.40
1:F:703:ALA:O	1:F:707:VAL:HG23	2.21	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	790/795 (99%)	761 (96%)	24 (3%)	5 (1%)	25	36
1	B	791/795 (100%)	756 (96%)	32 (4%)	3 (0%)	34	48
1	C	791/795 (100%)	756 (96%)	33 (4%)	2 (0%)	41	55
1	D	791/795 (100%)	761 (96%)	28 (4%)	2 (0%)	41	55
1	E	791/795 (100%)	755 (95%)	33 (4%)	3 (0%)	34	48
1	F	791/795 (100%)	750 (95%)	36 (5%)	5 (1%)	25	36
1	G	791/795 (100%)	760 (96%)	28 (4%)	3 (0%)	34	48
1	H	793/795 (100%)	765 (96%)	26 (3%)	2 (0%)	41	55
All	All	6329/6360 (100%)	6064 (96%)	240 (4%)	25 (0%)	34	48

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	772	VAL
1	F	1112	CYS
1	G	982	ILE
1	H	772	VAL
1	A	435	ARG
1	A	982	ILE
1	B	973	SER
1	B	982	ILE
1	C	982	ILE
1	D	982	ILE
1	E	973	SER
1	E	982	ILE
1	F	982	ILE
1	F	1006	SER
1	H	982	ILE
1	A	772	VAL
1	A	973	SER
1	G	973	SER
1	G	1112	CYS
1	F	973	SER
1	B	772	VAL
1	E	772	VAL
1	A	1101	VAL
1	F	772	VAL
1	C	772	VAL

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	668/671 (100%)	631 (94%)	37 (6%)	21	35
1	B	669/671 (100%)	632 (94%)	37 (6%)	21	35
1	C	669/671 (100%)	633 (95%)	36 (5%)	22	36
1	D	669/671 (100%)	633 (95%)	36 (5%)	22	36
1	E	669/671 (100%)	619 (92%)	50 (8%)	13	21
1	F	669/671 (100%)	632 (94%)	37 (6%)	21	35
1	G	669/671 (100%)	641 (96%)	28 (4%)	30	47
1	H	671/671 (100%)	627 (93%)	44 (7%)	16	26
All	All	5353/5368 (100%)	5048 (94%)	305 (6%)	20	33

All (305) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	ILE
1	A	434	THR
1	A	488	LEU
1	A	505	VAL
1	A	527	SER
1	A	529	GLU
1	A	532	GLU
1	A	546	THR
1	A	555	ARG
1	A	618	LEU
1	A	707	VAL
1	A	710	TYR
1	A	776	LYS
1	A	790	GLN
1	A	801	ARG
1	A	813	LEU
1	A	819	ARG
1	A	852	VAL
1	A	856	VAL

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Mol	Chain	Res	Type
1	A	866	VAL
1	A	875	ASP
1	A	905	ARG
1	A	906	LYS
1	A	971	LEU
1	A	974	THR
1	A	977	HIS
1	A	980	LEU
1	A	995	THR
1	A	1007	ASP
1	A	1033	GLU
1	A	1041	HIS
1	A	1047	LYS
1	A	1073	GLN
1	A	1090	GLU
1	A	1092	GLU
1	A	1111	LEU
1	A	1116	GLN
1	B	348	ARG
1	B	434	THR
1	B	505	VAL
1	B	529	GLU
1	B	557	ILE
1	B	567	LYS
1	B	572	GLN
1	B	593	LYS
1	B	618	LEU
1	B	625	GLN
1	B	630	MET
1	B	699	LEU
1	B	704	VAL
1	B	710	TYR
1	B	815	THR
1	B	823	THR
1	B	856	VAL
1	B	875	ASP
1	B	901	MET
1	B	904	ILE
1	B	926	ASN
1	B	928	GLU
1	B	971	LEU
1	B	974	THR

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Mol	Chain	Res	Type
1	B	977	HIS
1	B	979	THR
1	B	980	LEU
1	B	1000	LEU
1	B	1003	MET
1	B	1017	LYS
1	B	1026	SER
1	B	1029	LYS
1	B	1041	HIS
1	B	1092	GLU
1	B	1095	ARG
1	B	1126	GLU
1	B	1127	LYS
1	C	340	LEU
1	C	354	VAL
1	C	423	ARG
1	C	434	THR
1	C	453	GLU
1	C	455	VAL
1	C	476	VAL
1	C	505	VAL
1	C	509	THR
1	C	569	GLN
1	C	618	LEU
1	C	623	VAL
1	C	639	ARG
1	C	707	VAL
1	C	752	MET
1	C	805	VAL
1	C	819	ARG
1	C	875	ASP
1	C	910	GLU
1	C	912	LYS
1	C	920	ARG
1	C	926	ASN
1	C	957	ILE
1	C	963	LYS
1	C	977	HIS
1	C	980	LEU
1	C	1007	ASP
1	C	1029	LYS
1	C	1041	HIS

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Mol	Chain	Res	Type
1	C	1047	LYS
1	C	1064	ARG
1	C	1079	VAL
1	C	1092	GLU
1	C	1095	ARG
1	C	1124	VAL
1	C	1127	LYS
1	D	378	THR
1	D	455	VAL
1	D	485	VAL
1	D	505	VAL
1	D	555	ARG
1	D	567	LYS
1	D	635	ILE
1	D	648	LEU
1	D	704	VAL
1	D	707	VAL
1	D	709	VAL
1	D	710	TYR
1	D	751	LYS
1	D	776	LYS
1	D	790	GLN
1	D	803	ARG
1	D	875	ASP
1	D	904	ILE
1	D	905	ARG
1	D	912	LYS
1	D	924	LEU
1	D	926	ASN
1	D	928	GLU
1	D	931	GLU
1	D	957	ILE
1	D	963	LYS
1	D	971	LEU
1	D	980	LEU
1	D	986	THR
1	D	1009	ILE
1	D	1041	HIS
1	D	1064	ARG
1	D	1092	GLU
1	D	1095	ARG
1	D	1114	GLU

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Mol	Chain	Res	Type
1	D	1127	LYS
1	E	340	LEU
1	E	353	THR
1	E	354	VAL
1	E	368	GLU
1	E	399	ASP
1	E	448	LYS
1	E	482	GLU
1	E	505	VAL
1	E	529	GLU
1	E	569	GLN
1	E	570	ASN
1	E	572	GLN
1	E	574	ARG
1	E	623	VAL
1	E	625	GLN
1	E	639	ARG
1	E	642	HIS
1	E	644	THR
1	E	649	LEU
1	E	653	ILE
1	E	686	LYS
1	E	704	VAL
1	E	710	TYR
1	E	790	GLN
1	E	813	LEU
1	E	815	THR
1	E	823	THR
1	E	852	VAL
1	E	856	VAL
1	E	875	ASP
1	E	905	ARG
1	E	910	GLU
1	E	911	GLU
1	E	919	ILE
1	E	926	ASN
1	E	942	LYS
1	E	957	ILE
1	E	969	LYS
1	E	974	THR
1	E	977	HIS
1	E	980	LEU

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Mol	Chain	Res	Type
1	E	984	ASN
1	E	999	ARG
1	E	1007	ASP
1	E	1010	SER
1	E	1026	SER
1	E	1077	SER
1	E	1081	ASN
1	E	1095	ARG
1	E	1127	LYS
1	F	345	GLN
1	F	353	THR
1	F	371	LYS
1	F	448	LYS
1	F	449	THR
1	F	492	GLN
1	F	632	GLU
1	F	687	ARG
1	F	699	LEU
1	F	704	VAL
1	F	710	TYR
1	F	776	LYS
1	F	793	ILE
1	F	813	LEU
1	F	815	THR
1	F	856	VAL
1	F	875	ASP
1	F	898	VAL
1	F	904	ILE
1	F	905	ARG
1	F	919	ILE
1	F	974	THR
1	F	977	HIS
1	F	979	THR
1	F	980	LEU
1	F	982	ILE
1	F	984	ASN
1	F	999	ARG
1	F	1000	LEU
1	F	1003	MET
1	F	1007	ASP
1	F	1009	ILE
1	F	1041	HIS

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Mol	Chain	Res	Type
1	F	1044	LYS
1	F	1073	GLN
1	F	1093	LYS
1	F	1095	ARG
1	G	378	THR
1	G	516	LYS
1	G	555	ARG
1	G	569	GLN
1	G	593	LYS
1	G	687	ARG
1	G	699	LEU
1	G	704	VAL
1	G	710	TYR
1	G	751	LYS
1	G	801	ARG
1	G	815	THR
1	G	852	VAL
1	G	854	ARG
1	G	866	VAL
1	G	875	ASP
1	G	905	ARG
1	G	920	ARG
1	G	957	ILE
1	G	958	THR
1	G	980	LEU
1	G	999	ARG
1	G	1029	LYS
1	G	1033	GLU
1	G	1047	LYS
1	G	1073	GLN
1	G	1093	LYS
1	G	1095	ARG
1	H	359	SER
1	H	403	ILE
1	H	453	GLU
1	H	476	VAL
1	H	509	THR
1	H	529	GLU
1	H	532	GLU
1	H	557	ILE
1	H	572	GLN
1	H	574	ARG

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Mol	Chain	Res	Type
1	H	593	LYS
1	H	623	VAL
1	H	666	LEU
1	H	709	VAL
1	H	710	TYR
1	H	711	GLN
1	H	776	LYS
1	H	801	ARG
1	H	856	VAL
1	H	874	LYS
1	H	875	ASP
1	H	905	ARG
1	H	920	ARG
1	H	926	ASN
1	H	935	ARG
1	H	950	VAL
1	H	957	ILE
1	H	958	THR
1	H	963	LYS
1	H	979	THR
1	H	980	LEU
1	H	984	ASN
1	H	1000	LEU
1	H	1003	MET
1	H	1013	GLN
1	H	1025	LYS
1	H	1073	GLN
1	H	1081	ASN
1	H	1089	GLN
1	H	1092	GLU
1	H	1095	ARG
1	H	1114	GLU
1	H	1124	VAL
1	H	1127	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	HIS
1	A	470	GLN
1	A	492	GLN
1	A	494	ASN

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Mol	Chain	Res	Type
1	A	615	GLN
1	A	642	HIS
1	A	719	HIS
1	A	724	GLN
1	A	744	HIS
1	A	749	HIS
1	A	775	GLN
1	A	790	GLN
1	A	853	HIS
1	A	952	GLN
1	A	977	HIS
1	A	993	ASN
1	A	1041	HIS
1	A	1073	GLN
1	A	1075	GLN
1	A	1081	ASN
1	B	350	HIS
1	B	406	HIS
1	B	470	GLN
1	B	522	HIS
1	B	552	ASN
1	B	586	ASN
1	B	615	GLN
1	B	719	HIS
1	B	744	HIS
1	B	749	HIS
1	B	775	GLN
1	B	782	GLN
1	B	790	GLN
1	B	833	GLN
1	B	853	HIS
1	B	918	GLN
1	B	926	ASN
1	B	948	ASN
1	B	952	GLN
1	B	977	HIS
1	C	406	HIS
1	C	494	ASN
1	C	513	ASN
1	C	522	HIS
1	C	552	ASN
1	C	570	ASN

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Mol	Chain	Res	Type
1	C	586	ASN
1	C	596	GLN
1	C	614	ASN
1	C	615	GLN
1	C	711	GLN
1	C	719	HIS
1	C	744	HIS
1	C	749	HIS
1	C	775	GLN
1	C	850	GLN
1	C	853	HIS
1	C	926	ASN
1	C	977	HIS
1	C	1018	GLN
1	C	1041	HIS
1	C	1075	GLN
1	C	1089	GLN
1	D	345	GLN
1	D	406	HIS
1	D	437	GLN
1	D	470	GLN
1	D	492	GLN
1	D	494	ASN
1	D	552	ASN
1	D	625	GLN
1	D	642	HIS
1	D	711	GLN
1	D	719	HIS
1	D	724	GLN
1	D	744	HIS
1	D	749	HIS
1	D	775	GLN
1	D	782	GLN
1	D	790	GLN
1	D	834	GLN
1	D	853	HIS
1	D	926	ASN
1	D	952	GLN
1	D	977	HIS
1	D	1041	HIS
1	D	1075	GLN
1	E	349	ASN

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Mol	Chain	Res	Type
1	E	406	HIS
1	E	470	GLN
1	E	494	ASN
1	E	522	HIS
1	E	552	ASN
1	E	570	ASN
1	E	572	GLN
1	E	586	ASN
1	E	600	GLN
1	E	625	GLN
1	E	642	HIS
1	E	719	HIS
1	E	744	HIS
1	E	749	HIS
1	E	775	GLN
1	E	790	GLN
1	E	837	HIS
1	E	853	HIS
1	E	926	ASN
1	E	952	GLN
1	E	977	HIS
1	E	984	ASN
1	E	1075	GLN
1	E	1081	ASN
1	F	406	HIS
1	F	552	ASN
1	F	560	HIS
1	F	586	ASN
1	F	600	GLN
1	F	615	GLN
1	F	642	HIS
1	F	719	HIS
1	F	720	ASN
1	F	744	HIS
1	F	749	HIS
1	F	790	GLN
1	F	853	HIS
1	F	926	ASN
1	F	977	HIS
1	F	993	ASN
1	F	1041	HIS
1	F	1073	GLN

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Mol	Chain	Res	Type
1	F	1075	GLN
1	F	1089	GLN
1	G	406	HIS
1	G	437	GLN
1	G	492	GLN
1	G	494	ASN
1	G	552	ASN
1	G	600	GLN
1	G	615	GLN
1	G	625	GLN
1	G	720	ASN
1	G	724	GLN
1	G	744	HIS
1	G	749	HIS
1	G	775	GLN
1	G	782	GLN
1	G	790	GLN
1	G	853	HIS
1	G	939	ASN
1	G	952	GLN
1	G	977	HIS
1	G	1031	ASN
1	G	1081	ASN
1	H	350	HIS
1	H	398	GLN
1	H	406	HIS
1	H	600	GLN
1	H	615	GLN
1	H	711	GLN
1	H	724	GLN
1	H	744	HIS
1	H	749	HIS
1	H	775	GLN
1	H	782	GLN
1	H	853	HIS
1	H	926	ASN
1	H	948	ASN
1	H	977	HIS
1	H	984	ASN
1	H	1013	GLN
1	H	1071	ASN
1	H	1073	GLN

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Mol	Chain	Res	Type
1	H	1075	GLN
1	H	1081	ASN
1	H	1116	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CHT	G	2000	-	6,6,6	0.68	0	8,8,8	0.78	0
2	CHT	A	2000	-	6,6,6	0.57	0	8,8,8	0.55	0
2	CHT	C	2000	-	6,6,6	0.75	0	8,8,8	0.57	0
2	CHT	B	2000	-	6,6,6	0.74	0	8,8,8	0.47	0
2	CHT	D	2000	-	6,6,6	1.20	0	8,8,8	1.04	0
2	CHT	F	2000	-	6,6,6	0.65	0	8,8,8	0.81	0
2	CHT	H	2000	-	6,6,6	0.62	0	8,8,8	0.68	0
2	CHT	E	2000	-	6,6,6	0.74	0	8,8,8	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CHT	G	2000	-	-	4/4/4/4	-
2	CHT	A	2000	-	-	0/4/4/4	-
2	CHT	C	2000	-	-	0/4/4/4	-
2	CHT	B	2000	-	-	3/4/4/4	-
2	CHT	D	2000	-	-	1/4/4/4	-
2	CHT	F	2000	-	-	4/4/4/4	-
2	CHT	H	2000	-	-	3/4/4/4	-
2	CHT	E	2000	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2000	CHT	O6-C4-C5-N1
2	F	2000	CHT	O6-C4-C5-N1
2	H	2000	CHT	C4-C5-N1-C6
2	H	2000	CHT	C4-C5-N1-C7
2	H	2000	CHT	C4-C5-N1-C8
2	G	2000	CHT	C4-C5-N1-C6
2	G	2000	CHT	C4-C5-N1-C8
2	F	2000	CHT	C4-C5-N1-C8
2	F	2000	CHT	C4-C5-N1-C6
2	F	2000	CHT	C4-C5-N1-C7
2	G	2000	CHT	C4-C5-N1-C7
2	G	2000	CHT	O6-C4-C5-N1
2	B	2000	CHT	C4-C5-N1-C6
2	B	2000	CHT	C4-C5-N1-C8
2	B	2000	CHT	C4-C5-N1-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2000	CHT	2	0
2	A	2000	CHT	1	0
2	C	2000	CHT	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	792/795 (99%)	-0.69	0 100 100	12, 20, 34, 67	0
1	B	793/795 (99%)	-0.67	0 100 100	15, 24, 39, 59	0
1	C	793/795 (99%)	-0.59	1 (0%) 95 95	13, 24, 42, 73	0
1	D	793/795 (99%)	-0.67	0 100 100	12, 21, 34, 50	0
1	E	793/795 (99%)	-0.43	1 (0%) 95 95	18, 32, 52, 71	0
1	F	793/795 (99%)	-0.35	9 (1%) 80 79	18, 34, 55, 84	0
1	G	793/795 (99%)	-0.58	0 100 100	15, 27, 45, 65	0
1	H	795/795 (100%)	-0.56	2 (0%) 94 93	16, 28, 46, 77	0
All	All	6345/6360 (99%)	-0.57	13 (0%) 95 94	12, 26, 46, 84	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	819	ARG	3.1
1	F	561	ALA	3.0
1	F	572	GLN	2.5
1	H	334	THR	2.5
1	F	557	ILE	2.4
1	F	404	VAL	2.2
1	F	554	ALA	2.2
1	F	565	ALA	2.2
1	F	579	THR	2.2
1	F	558	ALA	2.1
1	C	566	ALA	2.1
1	F	935	ARG	2.1
1	E	805	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CHT	F	2000	7/7	0.92	0.20	42,45,47,48	0
2	CHT	D	2000	7/7	0.94	0.18	25,29,30,33	0
2	CHT	H	2000	7/7	0.95	0.14	27,30,30,33	0
2	CHT	E	2000	7/7	0.96	0.13	30,31,32,32	0
2	CHT	G	2000	7/7	0.97	0.11	24,24,25,27	0
2	CHT	C	2000	7/7	0.97	0.11	17,18,18,18	0
2	CHT	A	2000	7/7	0.98	0.12	14,14,15,16	0
2	CHT	B	2000	7/7	0.98	0.11	19,19,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.