



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:06 PM EDT

PDB ID : 3UGT / pdb_00003ugt
Title : Crystal structure of the yeast mitochondrial threonyl-tRNA synthetase - orthorhombic crystal form
Authors : Peterson, K.M.; Ling, J.; Simonovic, I.; Cho, C.; Soll, D.; Simonovic, M.
Deposited on : 2011-11-02
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

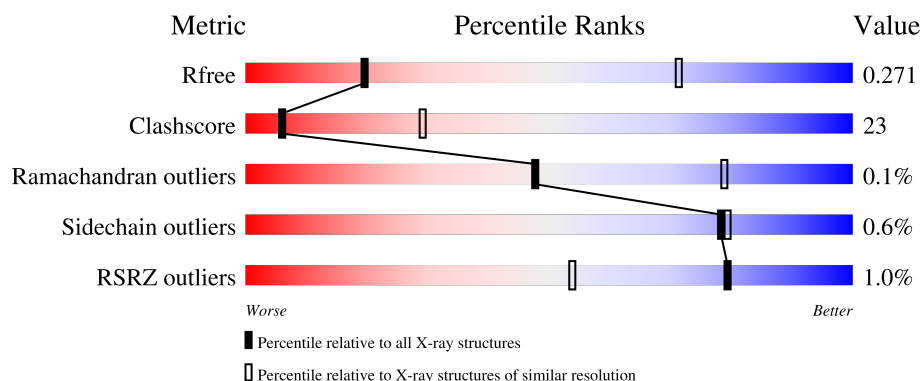
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	460	
1	B	460	
1	C	460	
1	D	460	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13459 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 Threonyl-tRNA synthetase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	3	0
			3397	2195	571	613	18			
1	B	419	Total	C	N	O	S	3	4	0
			3285	2115	553	601	16			
1	C	427	Total	C	N	O	S	1	2	0
			3432	2206	574	634	18			
1	D	418	Total	C	N	O	S	0	1	0
			3295	2121	552	605	17			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	expression tag	UNP P07236
A	4	GLY	-	expression tag	UNP P07236
A	5	SER	-	expression tag	UNP P07236
A	6	SER	-	expression tag	UNP P07236
A	7	HIS	-	expression tag	UNP P07236
A	8	HIS	-	expression tag	UNP P07236
A	9	HIS	-	expression tag	UNP P07236
A	10	HIS	-	expression tag	UNP P07236
A	11	HIS	-	expression tag	UNP P07236
A	12	HIS	-	expression tag	UNP P07236
A	13	SER	-	expression tag	UNP P07236
A	14	SER	-	expression tag	UNP P07236
A	15	GLY	-	expression tag	UNP P07236
A	16	LEU	-	expression tag	UNP P07236
A	17	VAL	-	expression tag	UNP P07236
A	18	PRO	-	expression tag	UNP P07236
A	19	ARG	-	expression tag	UNP P07236
A	20	GLY	-	expression tag	UNP P07236
A	21	SER	-	expression tag	UNP P07236
A	22	HIS	-	expression tag	UNP P07236
A	23	MET	-	expression tag	UNP P07236

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	-	expression tag	UNP P07236
A	25	SER	-	expression tag	UNP P07236
B	3	MET	-	expression tag	UNP P07236
B	4	GLY	-	expression tag	UNP P07236
B	5	SER	-	expression tag	UNP P07236
B	6	SER	-	expression tag	UNP P07236
B	7	HIS	-	expression tag	UNP P07236
B	8	HIS	-	expression tag	UNP P07236
B	9	HIS	-	expression tag	UNP P07236
B	10	HIS	-	expression tag	UNP P07236
B	11	HIS	-	expression tag	UNP P07236
B	12	HIS	-	expression tag	UNP P07236
B	13	SER	-	expression tag	UNP P07236
B	14	SER	-	expression tag	UNP P07236
B	15	GLY	-	expression tag	UNP P07236
B	16	LEU	-	expression tag	UNP P07236
B	17	VAL	-	expression tag	UNP P07236
B	18	PRO	-	expression tag	UNP P07236
B	19	ARG	-	expression tag	UNP P07236
B	20	GLY	-	expression tag	UNP P07236
B	21	SER	-	expression tag	UNP P07236
B	22	HIS	-	expression tag	UNP P07236
B	23	MET	-	expression tag	UNP P07236
B	24	ALA	-	expression tag	UNP P07236
B	25	SER	-	expression tag	UNP P07236
C	3	MET	-	expression tag	UNP P07236
C	4	GLY	-	expression tag	UNP P07236
C	5	SER	-	expression tag	UNP P07236
C	6	SER	-	expression tag	UNP P07236
C	7	HIS	-	expression tag	UNP P07236
C	8	HIS	-	expression tag	UNP P07236
C	9	HIS	-	expression tag	UNP P07236
C	10	HIS	-	expression tag	UNP P07236
C	11	HIS	-	expression tag	UNP P07236
C	12	HIS	-	expression tag	UNP P07236
C	13	SER	-	expression tag	UNP P07236
C	14	SER	-	expression tag	UNP P07236
C	15	GLY	-	expression tag	UNP P07236
C	16	LEU	-	expression tag	UNP P07236
C	17	VAL	-	expression tag	UNP P07236
C	18	PRO	-	expression tag	UNP P07236
C	19	ARG	-	expression tag	UNP P07236

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	GLY	-	expression tag	UNP P07236
C	21	SER	-	expression tag	UNP P07236
C	22	HIS	-	expression tag	UNP P07236
C	23	MET	-	expression tag	UNP P07236
C	24	ALA	-	expression tag	UNP P07236
C	25	SER	-	expression tag	UNP P07236
D	3	MET	-	expression tag	UNP P07236
D	4	GLY	-	expression tag	UNP P07236
D	5	SER	-	expression tag	UNP P07236
D	6	SER	-	expression tag	UNP P07236
D	7	HIS	-	expression tag	UNP P07236
D	8	HIS	-	expression tag	UNP P07236
D	9	HIS	-	expression tag	UNP P07236
D	10	HIS	-	expression tag	UNP P07236
D	11	HIS	-	expression tag	UNP P07236
D	12	HIS	-	expression tag	UNP P07236
D	13	SER	-	expression tag	UNP P07236
D	14	SER	-	expression tag	UNP P07236
D	15	GLY	-	expression tag	UNP P07236
D	16	LEU	-	expression tag	UNP P07236
D	17	VAL	-	expression tag	UNP P07236
D	18	PRO	-	expression tag	UNP P07236
D	19	ARG	-	expression tag	UNP P07236
D	20	GLY	-	expression tag	UNP P07236
D	21	SER	-	expression tag	UNP P07236
D	22	HIS	-	expression tag	UNP P07236
D	23	MET	-	expression tag	UNP P07236
D	24	ALA	-	expression tag	UNP P07236
D	25	SER	-	expression tag	UNP P07236

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

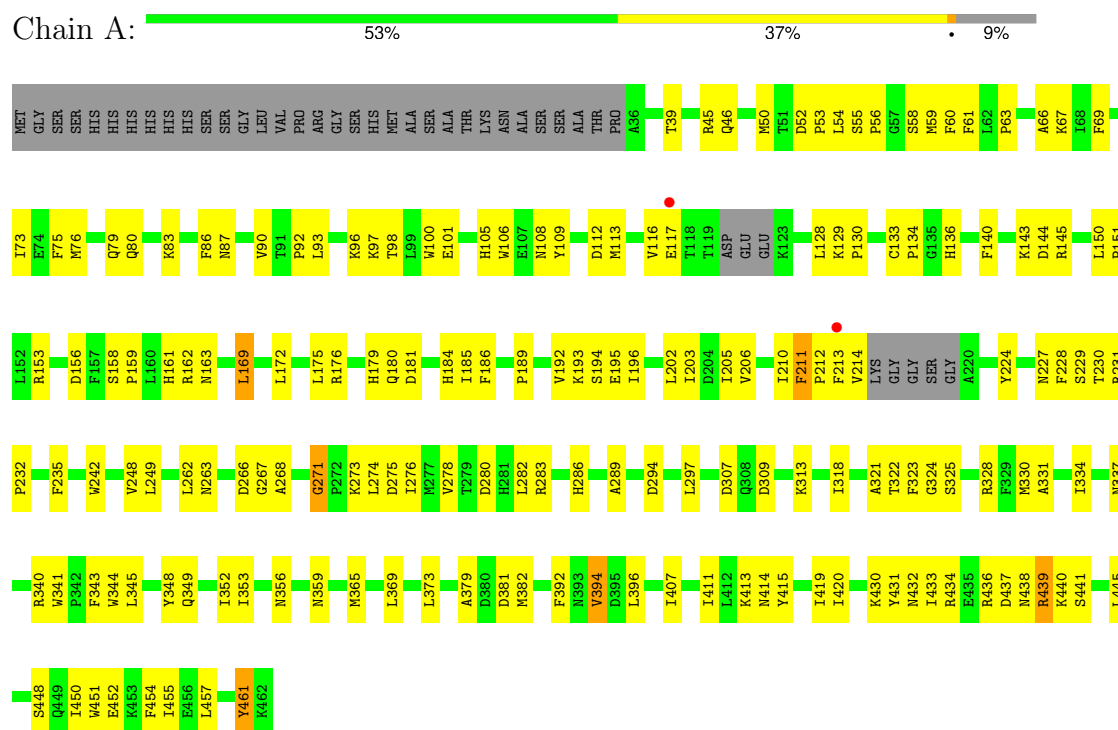
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total 18	O 18	0	0
3	B	7	Total 7	O 7	0	0
3	C	15	Total 15	O 15	0	0
3	D	6	Total 6	O 6	0	0

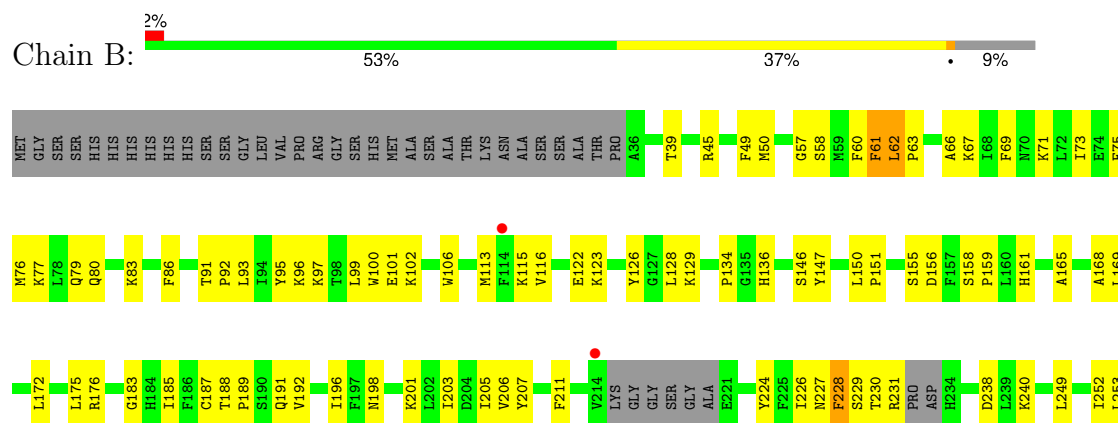
3 Residue-property plots

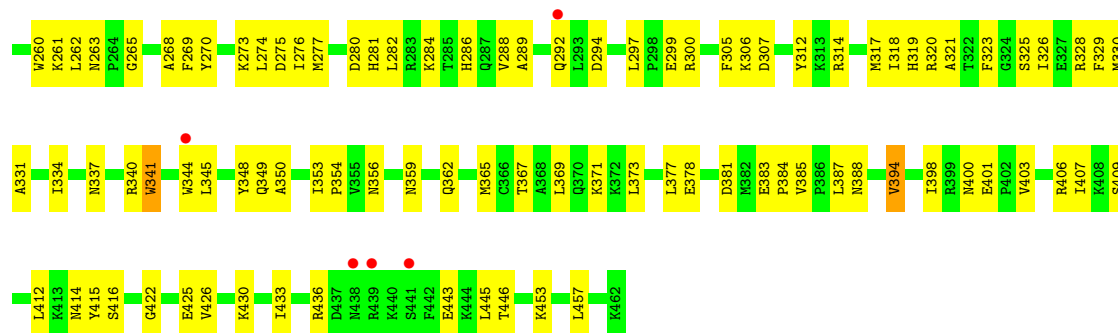
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Threonyl-tRNA synthetase, mitochondrial



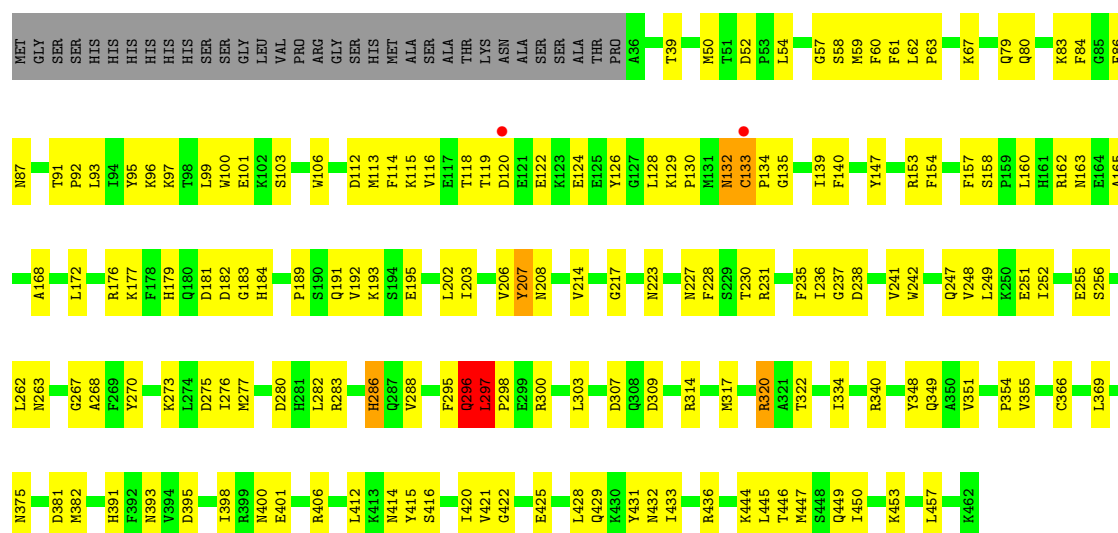
- Molecule 1: Threonyl-tRNA synthetase, mitochondrial





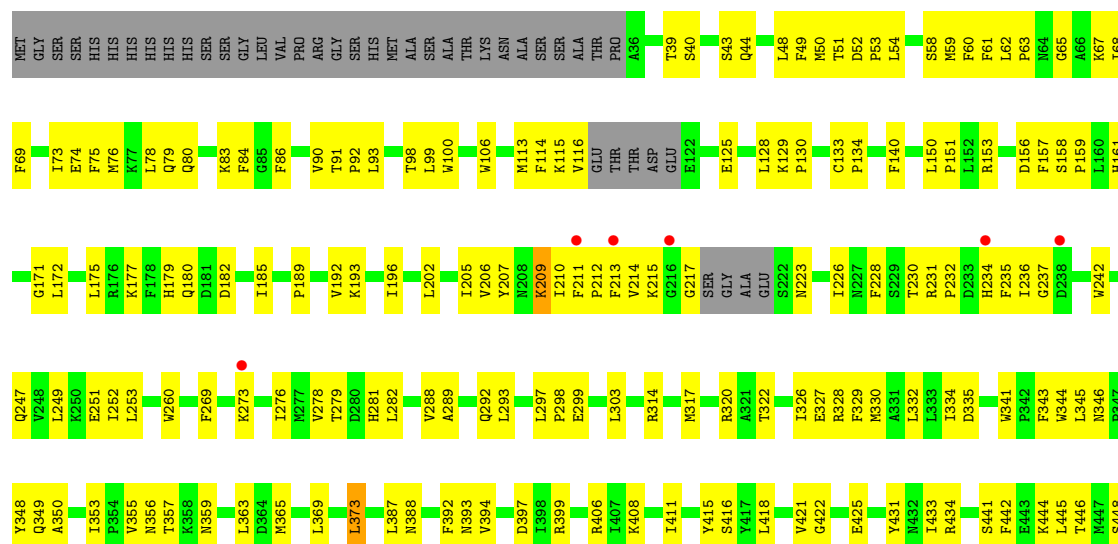
• Molecule 1: Threonyl-tRNA synthetase, mitochondrial

Chain C: 57% 34% 7%



• Molecule 1: Threonyl-tRNA synthetase, mitochondrial

Chain D: 53% 38% 9%



Q449	I450	W451	E452	K453	F454	I455	E456	L457	K462
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.08Å 157.94Å 237.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.11 – 3.60 35.11 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.11-3.60) 97.1 (35.11-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.237 , 0.275 0.231 , 0.271	Depositor DCC
R_{free} test set	1750 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	89.8	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13459	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.26	0/3494	0.77	5/4729 (0.1%)
1	B	0.27	0/3372	0.78	4/4574 (0.1%)
1	C	0.26	0/3529	0.77	6/4786 (0.1%)
1	D	0.26	0/3380	0.76	2/4590 (0.0%)
All	All	0.26	0/13775	0.77	17/18679 (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	1
1	B	0	1
1	C	0	3
All	All	0	5

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	PHE	CA-C-N	10.43	132.88	119.84
1	A	211	PHE	C-N-CA	10.43	132.88	119.84
1	A	271	GLY	CA-C-N	9.30	129.38	119.89
1	A	271	GLY	C-N-CA	9.30	129.38	119.89
1	B	263	ASN	CA-C-N	7.43	126.95	118.85
1	B	263	ASN	C-N-CA	7.43	126.95	118.85
1	B	228	PHE	N-CA-C	6.10	116.33	108.34
1	C	133	CYS	CA-C-N	5.90	125.28	118.85
1	C	133	CYS	C-N-CA	5.90	125.28	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	TYR	CB-CA-C	-5.66	110.06	116.63
1	C	296	GLN	N-CA-C	5.63	118.04	108.02
1	B	61	PHE	N-CA-C	5.37	118.84	112.72
1	D	91	THR	CA-C-N	5.12	125.13	119.90
1	D	91	THR	C-N-CA	5.12	125.13	119.90
1	C	207	TYR	N-CA-C	5.10	116.65	111.14
1	C	158	SER	CA-C-N	5.02	124.93	119.76
1	C	158	SER	C-N-CA	5.02	124.93	119.76

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	439	ARG	Peptide
1	B	62	LEU	Peptide
1	C	132	ASN	Peptide
1	C	296	GLN	Peptide
1	C	297	LEU	Peptide

5.2 Too-close contacts [i](#)

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	3397	0	3262	142	0
1	B	3285	0	3069	161	0
1	C	3432	0	3241	145	0
1	D	3295	0	3062	177	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	18	0	0	0	0
3	B	7	0	0	0	0
3	C	15	0	0	0	0
3	D	6	0	0	0	0
All	All	13459	0	12634	590	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 23.

All (590) 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:119:THR:H	1:C:120:ASP:HA	1.28	0.98
1:C:296:GLN:HA	1:C:298:PRO:HD2	1.46	0.97
1:B:269:PHE:HB2	1:B:270:TYR:HA	1.50	0.92
1:C:92:PRO:HB3	1:D:58:SER:HB3	1.53	0.90
1:D:40:SER:O	1:D:44:GLN:HB2	1.73	0.87
1:C:228:PHE:HE1	1:C:249:LEU:HB3	1.38	0.86
1:C:116:VAL:HG11	1:D:114:PHE:HB3	1.58	0.85
1:B:280:ASP:HB2	1:B:284:LYS:O	1.76	0.85
1:B:226:ILE:HG22	1:B:227:ASN:H	1.43	0.84
1:B:340:ARG:HA	1:B:436:ARG:HH21	1.41	0.83
1:C:118:THR:HB	1:C:119:THR:HA	1.59	0.83
1:B:299:GLU:HG2	1:B:314:ARG:HH21	1.44	0.83
1:C:58:SER:HB3	1:D:92:PRO:HB3	1.63	0.81
1:B:62:LEU:HB2	1:B:63:PRO:CD	2.13	0.78
1:B:414:ASN:HB3	1:B:436:ARG:HH22	1.45	0.78
1:A:161:HIS:HE1	1:B:93:LEU:HD12	1.48	0.78
1:A:242:TRP:CH2	1:A:271:GLY:HA2	2.19	0.78
1:C:119:THR:N	1:C:120:ASP:HA	1.91	0.77
1:D:93:LEU:HD21	1:D:159:PRO:HD2	1.66	0.77
1:C:92:PRO:HA	1:D:177:LYS:HE2	1.65	0.76
1:C:433:ILE:HD12	1:C:445:LEU:HD12	1.68	0.75
1:C:206:VAL:HG21	1:C:322:THR:HG21	1.69	0.75
1:C:400:ASN:O	1:C:401:GLU:HG2	1.87	0.74
1:B:229:SER:O	1:B:230:THR:HG22	1.88	0.74
1:D:153:ARG:HG2	1:D:185:ILE:HG12	1.69	0.74
1:A:58:SER:HB3	1:B:92:PRO:HB3	1.70	0.74
1:D:206:VAL:HG21	1:D:322:THR:HG21	1.70	0.74
1:B:369:LEU:O	1:B:373:LEU:HB2	1.88	0.74
1:D:422:GLY:H	1:D:425:GLU:HB2	1.53	0.74
1:C:420:ILE:HG22	1:C:432:ASN:HB3	1.68	0.73
1:D:434:ARG:HG2	1:D:441:SER:HA	1.70	0.73
1:A:46:GLN:HE22	1:A:341:TRP:HE1	1.36	0.73
1:D:202:LEU:HD23	1:D:320:ARG:HH22	1.54	0.72
1:B:340:ARG:HA	1:B:436:ARG:NH2	2.03	0.72
1:D:80:GLN:O	1:D:86:PHE:HB2	1.89	0.72
1:C:116:VAL:HG22	1:D:116:VAL:HG22	1.70	0.71
1:B:422:GLY:H	1:B:425:GLU:CG	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:LEU:HB3	1:D:63:PRO:HD2	1.71	0.71
1:D:365:MET:HG2	1:D:431:TYR:HE1	1.55	0.71
1:C:228:PHE:HE2	1:C:230:THR:HG22	1.56	0.70
1:D:226:ILE:HG22	1:D:276:ILE:HD13	1.72	0.69
1:D:206:VAL:HG13	1:D:211:PHE:CZ	2.28	0.69
1:D:59:MET:HE3	1:D:172:LEU:HG	1.75	0.69
1:C:112:ASP:HA	1:C:163:ASN:HB3	1.75	0.69
1:A:39:THR:HA	1:A:334:ILE:HG21	1.75	0.69
1:A:54:LEU:HA	1:B:96:LYS:HE2	1.73	0.69
1:C:228:PHE:CE2	1:C:230:THR:HG22	2.28	0.68
1:B:273:LYS:HG2	1:B:274:LEU:N	2.07	0.68
1:B:122:GLU:HA	1:B:123:LYS:CB	2.23	0.68
1:C:422:GLY:H	1:C:425:GLU:HB2	1.58	0.67
1:A:352:ILE:HD11	1:A:369:LEU:HD22	1.76	0.67
1:D:156:ASP:OD1	1:D:158:SER:HB3	1.94	0.67
1:B:203:ILE:HG21	1:B:276:ILE:HD13	1.76	0.67
1:A:242:TRP:CZ2	1:A:271:GLY:HA2	2.29	0.66
1:D:288:VAL:HG23	1:D:289:ALA:H	1.59	0.66
1:A:161:HIS:CE1	1:B:93:LEU:HD12	2.29	0.66
1:B:344:TRP:CE3	1:B:345:LEU:HG	2.31	0.66
1:B:39:THR:HA	1:B:334:ILE:HG21	1.77	0.65
1:C:133:CYS:N	1:C:134:PRO:HD2	2.10	0.65
1:A:61:PHE:HE1	1:A:330:MET:HE1	1.60	0.65
1:C:118:THR:HB	1:C:119:THR:CA	2.24	0.65
1:C:119:THR:H	1:C:120:ASP:CA	2.07	0.65
1:C:208:ASN:HB2	1:C:217:GLY:CA	2.26	0.65
1:C:227:ASN:HD22	1:C:277:MET:HE3	1.62	0.65
1:A:45:ARG:HH21	1:A:414:ASN:HD21	1.44	0.64
1:A:90:VAL:HB	1:B:61:PHE:HB2	1.80	0.64
1:C:147:TYR:HB3	1:C:307:ASP:HA	1.79	0.64
1:C:296:GLN:HA	1:C:298:PRO:CD	2.26	0.64
1:C:193:LYS:HB2	1:C:248:VAL:HB	1.80	0.63
1:A:213:PHE:O	1:A:214:VAL:HB	1.96	0.63
1:C:62:LEU:HB3	1:C:63:PRO:HD2	1.80	0.63
1:A:356:ASN:HB3	1:A:359:ASN:HB2	1.80	0.63
1:C:282:LEU:O	1:C:283:ARG:HB2	1.99	0.63
1:C:114:PHE:CE2	1:C:163:ASN:HB2	2.33	0.63
1:D:202:LEU:HD23	1:D:320:ARG:NH2	2.13	0.63
1:B:69:PHE:CZ	1:B:73:ILE:HD11	2.34	0.62
1:C:39:THR:HG21	1:C:172:LEU:HD23	1.82	0.62
1:B:128:LEU:HD23	1:B:129:LYS:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:HB2	1:D:54:LEU:HD23	1.81	0.62
1:B:161:HIS:HA	1:B:176:ARG:O	1.98	0.62
1:D:159:PRO:HA	1:D:179:HIS:HD2	1.64	0.62
1:A:325:SER:HB3	1:A:328:ARG:HB3	1.81	0.62
1:C:228:PHE:CE1	1:C:249:LEU:HB3	2.28	0.62
1:D:329:PHE:HA	1:D:332:LEU:HG	1.81	0.62
1:D:92:PRO:O	1:D:129:LYS:HE3	2.00	0.62
1:A:203:ILE:HD13	1:A:276:ILE:HG13	1.81	0.61
1:D:273:LYS:HG2	1:D:292:GLN:HG3	1.81	0.61
1:D:349:GLN:NE2	1:D:393:ASN:H	1.98	0.61
1:A:93:LEU:HD23	1:A:129:LYS:HE2	1.81	0.61
1:B:377:LEU:HD12	1:B:385:VAL:HG22	1.81	0.61
1:B:172:LEU:HB3	1:B:331:ALA:HB2	1.83	0.61
1:B:350:ALA:HB3	1:B:394:VAL:HG12	1.82	0.61
1:A:83:LYS:HE3	1:B:378:GLU:O	2.00	0.61
1:B:62:LEU:HB2	1:B:63:PRO:HD2	1.83	0.61
1:C:87:ASN:HB3	1:D:63:PRO:HB3	1.83	0.60
1:A:381:ASP:CG	1:A:382[A]:MET:H	2.08	0.60
1:C:428:LEU:O	1:C:429:GLN:HB2	2.01	0.60
1:D:206:VAL:HG13	1:D:211:PHE:CE2	2.36	0.60
1:B:367:THR:HB	1:B:371[A]:LYS:HE3	1.82	0.60
1:A:76:MET:HE3	1:A:80:GLN:HE21	1.65	0.60
1:C:208:ASN:HB2	1:C:217:GLY:HA2	1.81	0.60
1:D:50:MET:HE3	1:D:62:LEU:HD11	1.84	0.60
1:C:270:TYR:O	1:C:295:PHE:HB2	2.01	0.59
1:D:349:GLN:HE21	1:D:393:ASN:HD22	1.50	0.59
1:B:146:SER:HA	1:B:306:LYS:H	1.67	0.59
1:B:344:TRP:HE3	1:B:345:LEU:HG	1.67	0.59
1:B:93:LEU:HD23	1:B:129:LYS:HE2	1.85	0.59
1:C:93:LEU:O	1:C:128:LEU:HD12	2.03	0.59
1:A:419:ILE:HG12	1:A:433:ILE:HG13	1.85	0.59
1:D:249:LEU:O	1:D:253:LEU:HG	2.03	0.59
1:A:59:MET:HE3	1:A:172:LEU:HD23	1.83	0.59
1:A:373:LEU:HB3	1:A:394:VAL:HG21	1.85	0.59
1:D:113:MET:HG2	1:D:114:PHE:H	1.68	0.58
1:B:453:LYS:O	1:B:457:LEU:HG	2.03	0.58
1:C:92:PRO:HB3	1:D:58:SER:CB	2.29	0.58
1:A:87:ASN:HB3	1:B:63:PRO:HB3	1.84	0.58
1:D:217:GLY:HA2	1:D:223:ASN:HD21	1.68	0.58
1:B:129:LYS:O	1:B:129:LYS:HG3	2.02	0.58
1:C:95:TYR:HB3	1:C:99:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:GLN:HB2	1:C:393:ASN:O	2.04	0.58
1:D:211:PHE:N	1:D:212:PRO:HD3	2.18	0.58
1:B:207:TYR:HE1	1:B:329:PHE:HE1	1.51	0.58
1:B:289:ALA:HB1	1:B:321:ALA:O	2.04	0.58
1:A:63:PRO:O	1:A:66:ALA:HB3	2.04	0.58
1:D:86:PHE:HZ	1:D:320:ARG:HD3	1.68	0.58
1:D:212:PRO:HA	1:D:213:PHE:CB	2.34	0.58
1:D:373:LEU:HD23	1:D:394:VAL:HG21	1.86	0.57
1:B:433:ILE:HG12	1:B:443:GLU:O	2.04	0.57
1:B:422:GLY:H	1:B:425:GLU:HG3	1.69	0.57
1:B:230:THR:O	1:B:230:THR:HG23	2.04	0.57
1:B:292:GLN:HB2	1:B:319:HIS:HB2	1.87	0.57
1:D:303:LEU:O	1:D:314:ARG:HD3	2.04	0.57
1:A:75:PHE:O	1:A:79:GLN:HG2	2.05	0.57
1:A:348:TYR:HB3	1:A:415:TYR:CD1	2.40	0.57
1:C:93:LEU:HA	1:C:129:LYS:HE2	1.87	0.57
1:A:224:TYR:HB3	1:A:278:VAL:HG12	1.85	0.57
1:A:337:ASN:HB2	1:A:340:ARG:O	2.05	0.57
1:B:348:TYR:HB3	1:B:415:TYR:CE1	2.40	0.57
1:B:409:SER:HB3	1:B:412:LEU:HD23	1.87	0.56
1:B:228:PHE:HB2	1:B:262:LEU:HA	1.87	0.56
1:D:172:LEU:HA	1:D:175:LEU:HD11	1.87	0.56
1:D:356:ASN:HB2	1:D:359:ASN:HB2	1.85	0.56
1:A:228:PHE:HE1	1:A:249:LEU:HD13	1.70	0.56
1:C:133:CYS:N	1:C:134:PRO:CD	2.68	0.56
1:C:297:LEU:N	1:C:298:PRO:CD	2.69	0.56
1:C:348:TYR:HB3	1:C:415:TYR:CE1	2.40	0.56
1:D:281:HIS:HE1	1:D:335:ASP:HB3	1.70	0.56
1:B:93:LEU:HA	1:B:129:LYS:HE2	1.87	0.56
1:B:354:PRO:C	1:B:406:ARG:HH22	2.14	0.56
1:D:343:PHE:CZ	1:D:454:PHE:HD1	2.24	0.56
1:A:92:PRO:HB3	1:B:58:SER:HB3	1.88	0.56
1:A:348:TYR:HB3	1:A:415:TYR:CE1	2.41	0.56
1:C:203:ILE:HD13	1:C:276:ILE:HG13	1.88	0.56
1:C:416:SER:HA	1:C:436:ARG:HH11	1.70	0.56
1:C:433:ILE:HD11	1:C:450:ILE:HG12	1.86	0.56
1:D:69:PHE:CZ	1:D:73:ILE:HD11	2.41	0.56
1:D:348:TYR:HB3	1:D:415:TYR:CE1	2.41	0.56
1:A:153:ARG:HG2	1:A:185:ILE:HG12	1.88	0.56
1:B:227:ASN:HB2	1:B:275:ASP:HB2	1.88	0.56
1:C:93:LEU:HD13	1:D:177:LYS:HD2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:LEU:HG	1:D:161:HIS:HB2	1.86	0.56
1:A:307:ASP:HB3	1:A:309[A]:ASP:OD1	2.06	0.56
1:B:57:GLY:O	1:B:175:LEU:HB3	2.06	0.56
1:B:188:THR:HB	1:B:189:PRO:HD2	1.88	0.56
1:B:231:ARG:HB2	1:B:265:GLY:HA2	1.88	0.56
1:B:276:ILE:HG22	1:B:289:ALA:O	2.05	0.56
1:B:433:ILE:HD13	1:B:445:LEU:HD12	1.86	0.56
1:A:93:LEU:HD12	1:B:161:HIS:HE1	1.71	0.56
1:D:159:PRO:HA	1:D:179:HIS:CD2	2.40	0.56
1:A:439:ARG:O	1:A:439:ARG:HG2	2.06	0.55
1:B:96:LYS:HG2	1:B:126:TYR:CE1	2.41	0.55
1:C:62:LEU:HB3	1:C:63:PRO:CD	2.36	0.55
1:D:387:LEU:O	1:D:388:ASN:HB2	2.06	0.55
1:C:298:PRO:HB2	1:C:314:ARG:HD2	1.87	0.55
1:D:52:ASP:CG	1:D:53:PRO:HD2	2.32	0.55
1:A:205:ILE:O	1:A:210:ILE:HG12	2.07	0.55
1:C:247:GLN:O	1:C:251:GLU:HB2	2.06	0.55
1:A:352:ILE:O	1:A:396:LEU:HD12	2.06	0.55
1:B:128:LEU:CD2	1:B:161:HIS:HB2	2.37	0.55
1:D:326:ILE:O	1:D:330:MET:HG3	2.07	0.55
1:C:58:SER:HB3	1:D:92:PRO:CB	2.36	0.55
1:D:62:LEU:CB	1:D:63:PRO:HD2	2.37	0.54
1:A:231:ARG:HB2	1:A:242:TRP:CZ3	2.41	0.54
1:D:40:SER:O	1:D:44:GLN:CB	2.52	0.54
1:D:357:THR:O	1:D:363:LEU:HD11	2.08	0.54
1:A:229:SER:HB2	1:A:273:LYS:HB2	1.89	0.54
1:C:106:TRP:CZ2	1:C:115:LYS:HD3	2.43	0.54
1:A:231:ARG:HD2	1:A:235:PHE:CD2	2.43	0.54
1:A:180:GLN:HG3	1:A:324:GLY:O	2.07	0.54
1:C:208:ASN:HB2	1:C:217:GLY:HA3	1.89	0.54
1:C:236:ILE:HG13	1:C:237:GLY:H	1.73	0.54
1:B:73:ILE:O	1:B:77:LYS:HG2	2.07	0.54
1:C:382:MET:HA	1:D:205:ILE:HD11	1.90	0.54
1:B:100:TRP:CD1	1:B:113:MET:HE1	2.43	0.54
1:B:433:ILE:O	1:B:433:ILE:HG13	2.08	0.54
1:B:203:ILE:HG21	1:B:276:ILE:CD1	2.37	0.53
1:B:49:PHE:CE1	1:B:172:LEU:HD21	2.42	0.53
1:C:381:ASP:C	1:D:83:LYS:HZ1	2.16	0.53
1:C:58:SER:CB	1:D:92:PRO:HB3	2.36	0.53
1:C:191:GLN:O	1:C:195:GLU:HG2	2.08	0.53
1:D:281:HIS:CD2	1:D:282:LEU:H	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:MET:O	1:B:60:PHE:HB2	2.09	0.53
1:D:210:ILE:C	1:D:212:PRO:HD3	2.34	0.53
1:D:288:VAL:HG12	1:D:328:ARG:NH1	2.23	0.53
1:C:135:GLY:O	1:C:139:ILE:HG13	2.09	0.53
1:C:189:PRO:HA	1:C:192:VAL:HG23	1.91	0.53
1:A:436:ARG:HG2	1:A:437:ASP:N	2.23	0.53
1:B:276:ILE:HG23	1:B:288:VAL:HG23	1.90	0.53
1:C:231:ARG:HD2	1:C:235:PHE:CD2	2.44	0.53
1:D:228:PHE:HD1	1:D:253:LEU:HD11	1.74	0.53
1:D:450:ILE:HG23	1:D:454:PHE:CE2	2.44	0.53
1:A:451:TRP:NE1	1:A:455:ILE:HD11	2.24	0.52
1:B:155:SER:HA	1:B:183:GLY:HA2	1.90	0.52
1:C:39:THR:HA	1:C:334:ILE:HG21	1.91	0.52
1:B:294:ASP:OD2	1:B:297:LEU:HD13	2.10	0.52
1:C:307:ASP:HB3	1:C:309:ASP:OD2	2.09	0.52
1:D:86:PHE:CD1	1:D:153:ARG:HB3	2.45	0.52
1:A:212:PRO:O	1:A:213:PHE:CG	2.62	0.52
1:A:328:ARG:O	1:A:331:ALA:HB3	2.09	0.52
1:B:277:MET:HA	1:B:286:HIS:O	2.10	0.52
1:A:282:LEU:O	1:A:283:ARG:HB2	2.10	0.52
1:A:461:TYR:CZ	1:B:387:LEU:HD11	2.45	0.52
1:B:416:SER:O	1:B:436:ARG:HB2	2.09	0.52
1:C:351:VAL:HA	1:C:395:ASP:O	2.10	0.52
1:B:228:PHE:HD2	1:B:261:LYS:O	1.93	0.52
1:D:43:SER:HB2	1:D:49:PHE:HD2	1.74	0.51
1:D:171:GLY:O	1:D:172:LEU:HB2	2.09	0.51
1:B:398:ILE:HG22	1:B:398:ILE:O	2.09	0.51
1:C:97:LYS:HE3	1:C:106:TRP:NE1	2.25	0.51
1:B:75:PHE:O	1:B:79:GLN:HG2	2.10	0.51
1:B:422:GLY:H	1:B:425:GLU:HG2	1.75	0.51
1:B:341:TRP:H	1:B:341:TRP:CD1	2.28	0.51
1:C:61:PHE:HB2	1:D:90:VAL:HB	1.92	0.51
1:D:442:PHE:O	1:D:444:LYS:HG2	2.10	0.51
1:A:69:PHE:O	1:A:73:ILE:HG12	2.10	0.51
1:A:116:VAL:HG22	1:B:116:VAL:HG22	1.93	0.51
1:A:413:LYS:O	1:A:414:ASN:HB2	2.09	0.51
1:B:49:PHE:HZ	1:B:330:MET:SD	2.34	0.51
1:D:93:LEU:HA	1:D:129:LYS:HG2	1.93	0.51
1:C:54:LEU:HD22	1:D:98:THR:OG1	2.11	0.51
1:D:113:MET:HG2	1:D:114:PHE:N	2.25	0.51
1:A:50:MET:O	1:A:60:PHE:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:ASN:HD22	1:D:416:SER:HB2	1.76	0.51
1:D:408:LYS:O	1:D:411:ILE:HG22	2.10	0.51
1:B:39:THR:HG23	1:B:334:ILE:HD12	1.92	0.51
1:D:365:MET:HG2	1:D:431:TYR:CE1	2.40	0.51
1:B:128:LEU:HD21	1:B:161:HIS:HB2	1.91	0.50
1:B:201:LYS:O	1:B:205:ILE:HG12	2.11	0.50
1:B:226:ILE:HG22	1:B:227:ASN:N	2.18	0.50
1:B:99:LEU:HD11	1:B:134:PRO:HB2	1.92	0.50
1:A:76:MET:HE1	1:A:202:LEU:HD21	1.93	0.50
1:A:407:ILE:O	1:A:411:ILE:HG13	2.11	0.50
1:B:79:GLN:O	1:B:83:LYS:HB3	2.11	0.50
1:A:150:LEU:HA	1:A:151:PRO:C	2.37	0.50
1:B:62:LEU:HD13	1:B:63:PRO:HD2	1.93	0.50
1:D:299:GLU:HA	1:D:314:ARG:NH1	2.27	0.50
1:D:329:PHE:O	1:D:329:PHE:CG	2.64	0.50
1:D:75:PHE:O	1:D:79:GLN:HG2	2.12	0.50
1:D:205:ILE:O	1:D:209:LYS:HB2	2.12	0.50
1:D:278:VAL:HG12	1:D:279:THR:N	2.27	0.50
1:A:61:PHE:CE1	1:A:330:MET:HE1	2.43	0.50
1:A:92:PRO:HB3	1:B:58:SER:CB	2.41	0.50
1:A:330:MET:O	1:A:334:ILE:HG12	2.12	0.49
1:B:282:LEU:O	1:B:282:LEU:HD12	2.12	0.49
1:A:181:ASP:OD2	1:A:323:PHE:HB2	2.12	0.49
1:B:45:ARG:HH21	1:B:414:ASN:HD21	1.60	0.49
1:B:96:LYS:HG2	1:B:126:TYR:CD1	2.47	0.49
1:C:236:ILE:HG13	1:C:237:GLY:N	2.27	0.49
1:D:392:PHE:HZ	1:D:455:ILE:HD13	1.76	0.49
1:B:97:LYS:O	1:B:101:GLU:HG3	2.11	0.49
1:D:288:VAL:HA	1:D:328:ARG:HH12	1.76	0.49
1:D:348:TYR:HB3	1:D:415:TYR:CD1	2.46	0.49
1:C:80:GLN:HB3	1:C:86:PHE:HB2	1.94	0.49
1:D:212:PRO:HG2	1:D:215:LYS:HA	1.93	0.49
1:D:226:ILE:HG13	1:D:260:TRP:HB3	1.94	0.49
1:D:346:ASN:ND2	1:D:416:SER:HB2	2.27	0.49
1:A:100:TRP:CH2	1:A:130:PRO:HD2	2.48	0.49
1:A:369:LEU:HD12	1:A:431:TYR:CE2	2.48	0.49
1:B:354:PRO:HD2	1:B:406:ARG:HH21	1.76	0.49
1:C:63:PRO:O	1:C:67:LYS:HG3	2.12	0.49
1:D:327:GLU:O	1:D:330:MET:HB2	2.13	0.49
1:D:343:PHE:CE1	1:D:349:GLN:HB3	2.48	0.49
1:C:86:PHE:CE2	1:C:320:ARG:NE	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LYS:HA	1:C:126:TYR:CD1	2.48	0.49
1:B:325:SER:HB3	1:B:328:ARG:HB3	1.95	0.49
1:B:400:ASN:C	1:B:401:GLU:HG2	2.37	0.49
1:B:231:ARG:HD3	1:B:265:GLY:HA2	1.95	0.48
1:B:381:ASP:HB3	1:B:383:GLU:H	1.77	0.48
1:C:57:GLY:HA3	1:C:176:ARG:CG	2.43	0.48
1:D:328:ARG:O	1:D:329:PHE:HB3	2.13	0.48
1:D:369:LEU:HD13	1:D:431:TYR:HE2	1.77	0.48
1:B:136:HIS:CE1	1:B:156:ASP:HB2	2.48	0.48
1:A:45:ARG:NH2	1:A:414:ASN:HD21	2.07	0.48
1:D:193:LYS:HA	1:D:252:ILE:HD11	1.95	0.48
1:A:90:VAL:HB	1:B:61:PHE:CB	2.43	0.48
1:B:39:THR:HG21	1:B:172:LEU:HD22	1.94	0.48
1:D:397:ASP:OD1	1:D:399:ARG:HG2	2.13	0.48
1:A:189:PRO:HA	1:A:192:VAL:HG23	1.95	0.48
1:A:369:LEU:HD11	1:A:450:ILE:HD12	1.95	0.48
1:A:440:LYS:HA	1:C:214:VAL:O	2.14	0.48
1:B:150:LEU:HA	1:B:151:PRO:C	2.38	0.48
1:D:86:PHE:CE1	1:D:153:ARG:HB3	2.48	0.48
1:A:143:LYS:HG2	1:A:144:ASP:N	2.27	0.48
1:B:136:HIS:NE2	1:B:156:ASP:HB2	2.29	0.48
1:C:118:THR:OG1	1:C:124:GLU:HB2	2.13	0.48
1:D:236:ILE:HG12	1:D:269:PHE:HD1	1.78	0.48
1:C:52:ASP:OD1	1:C:54:LEU:HG	2.14	0.48
1:C:114:PHE:HE2	1:C:163:ASN:ND2	2.11	0.48
1:A:365:MET:HG2	1:A:431:TYR:CZ	2.49	0.48
1:B:365:MET:HE1	1:B:426:VAL:HA	1.96	0.48
1:C:177:LYS:HE2	1:C:179:HIS:HE1	1.78	0.48
1:A:169:LEU:HD22	1:A:169:LEU:O	2.14	0.47
1:B:305:PHE:O	1:B:312:TYR:HA	2.13	0.47
1:C:59[A]:MET:HE3	1:C:172:LEU:HD13	1.96	0.47
1:C:54:LEU:HD13	1:D:99:LEU:HB2	1.96	0.47
1:C:139:ILE:HA	1:D:50:MET:HE1	1.95	0.47
1:C:428:LEU:O	1:C:428:LEU:HD23	2.14	0.47
1:C:280:ASP:HB2	1:C:286:HIS:NE2	2.30	0.47
1:B:353:ILE:HG21	1:B:403:VAL:HG23	1.95	0.47
1:B:430:LYS:HE2	1:B:446:THR:HG23	1.95	0.47
1:C:140:PHE:HD2	1:C:303:LEU:HD22	1.79	0.47
1:A:105:HIS:HA	1:A:108:ASN:HB3	1.96	0.47
1:D:332:LEU:HD12	1:D:332:LEU:C	2.39	0.47
1:B:63:PRO:O	1:B:67:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ILE:O	1:B:317:MET:HA	2.15	0.47
1:B:253:LEU:HD11	1:B:274:LEU:HD22	1.95	0.47
1:A:213:PHE:O	1:A:214:VAL:CB	2.63	0.47
1:A:461:TYR:CE1	1:B:387:LEU:HD11	2.49	0.47
1:C:59[B]:MET:HE3	1:C:172:LEU:HD13	1.96	0.47
1:C:122:GLU:H	1:C:122:GLU:CD	2.23	0.47
1:C:412:LEU:HD12	1:C:412:LEU:H	1.80	0.47
1:D:75:PHE:CZ	1:D:210:ILE:HD11	2.50	0.47
1:D:288:VAL:HG23	1:D:289:ALA:N	2.28	0.47
1:A:116:VAL:HG12	1:A:117:GLU:N	2.29	0.47
1:A:231:ARG:HD2	1:A:235:PHE:CG	2.50	0.47
1:B:337:ASN:O	1:B:340:ARG:HB2	2.14	0.47
1:C:154:PHE:O	1:C:183:GLY:HA2	2.14	0.47
1:D:434:ARG:CG	1:D:441:SER:HA	2.42	0.47
1:C:103:SER:C	1:C:300:ARG:HD3	2.40	0.47
1:C:400:ASN:O	1:C:401:GLU:CG	2.61	0.47
1:A:340:ARG:HB3	1:A:436:ARG:NH2	2.30	0.47
1:B:80:GLN:HB3	1:B:86:PHE:HB2	1.95	0.46
1:D:232:PRO:HG2	1:D:234:HIS:O	2.15	0.46
1:A:433:ILE:HG21	1:A:445:LEU:HD12	1.96	0.46
1:B:106:TRP:HH2	1:B:115:LYS:HD2	1.80	0.46
1:B:187:CYS:HB2	1:B:191:GLN:HG3	1.97	0.46
1:B:231:ARG:HB3	1:B:268:ALA:HA	1.96	0.46
1:C:119:THR:N	1:C:120:ASP:CA	2.71	0.46
1:D:100:TRP:HB2	1:D:106:TRP:HE3	1.80	0.46
1:D:231:ARG:HD2	1:D:235:PHE:CG	2.50	0.46
1:D:228:PHE:HE2	1:D:230:THR:HG22	1.80	0.46
1:A:133:CYS:N	1:A:134:PRO:HD2	2.30	0.46
1:B:299:GLU:HA	1:B:314:ARG:HD3	1.98	0.46
1:D:63:PRO:O	1:D:67:LYS:HG3	2.16	0.46
1:A:80:GLN:HB3	1:A:86:PHE:HB2	1.97	0.46
1:C:86:PHE:HE2	1:C:320:ARG:HE	1.61	0.46
1:C:130:PRO:O	1:C:160:LEU:HB3	2.15	0.46
1:C:165:ALA:HB3	1:C:168:ALA:HB3	1.97	0.46
1:D:206:VAL:HG13	1:D:211:PHE:HZ	1.75	0.46
1:B:281:HIS:ND1	1:B:282:LEU:HD23	2.31	0.46
1:C:446:THR:HG22	1:C:449:GLN:CD	2.39	0.46
1:D:113:MET:HE2	1:D:130:PRO:HG3	1.98	0.46
1:D:212:PRO:CB	1:D:215:LYS:HA	2.46	0.46
1:A:56:PRO:O	1:A:176:ARG:HD2	2.15	0.46
1:B:299:GLU:HG2	1:B:314:ARG:NH2	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:HIS:HA	1:A:318:ILE:O	2.16	0.46
1:C:184:HIS:CD2	1:C:317:MET:HE2	2.50	0.46
1:C:369:LEU:HD13	1:C:447:MET:HG3	1.98	0.46
1:A:100:TRP:CZ2	1:A:129:LYS:HA	2.51	0.46
1:D:185:ILE:O	1:D:317:MET:HA	2.16	0.46
1:D:445:LEU:HB2	1:D:450:ILE:HG13	1.98	0.46
1:D:453:LYS:O	1:D:457:LEU:HG	2.15	0.46
1:A:151:PRO:HB2	1:A:153:ARG:NH1	2.31	0.45
1:D:418:LEU:O	1:D:433:ILE:HA	2.16	0.45
1:C:251:GLU:O	1:C:255:GLU:HG2	2.16	0.45
1:D:434:ARG:HD3	1:D:441:SER:HA	1.98	0.45
1:A:54:LEU:O	1:B:96:LYS:HG3	2.17	0.45
1:A:109:TYR:HE1	1:A:162:ARG:NH1	2.15	0.45
1:A:206:VAL:O	1:A:211:PHE:HD2	2.00	0.45
1:A:434:ARG:HA	1:A:441:SER:OG	2.17	0.45
1:B:188:THR:OG1	1:B:191:GLN:HG2	2.16	0.45
1:B:326:ILE:O	1:B:330:MET:HB2	2.17	0.45
1:B:359:ASN:ND2	1:B:362:GLN:HG3	2.32	0.45
1:D:365:MET:HE2	1:D:431:TYR:CE1	2.52	0.45
1:C:97:LYS:HE3	1:C:106:TRP:CE2	2.51	0.45
1:C:238:ASP:O	1:C:242:TRP:HD1	1.99	0.45
1:D:212:PRO:HB3	1:D:213:PHE:O	2.15	0.45
1:B:61:PHE:O	1:B:66:ALA:HB2	2.17	0.45
1:B:175:LEU:N	1:B:175:LEU:HD12	2.31	0.45
1:C:86:PHE:CE1	1:C:153:ARG:HB3	2.52	0.45
1:D:93:LEU:O	1:D:128:LEU:HD12	2.16	0.45
1:D:116:VAL:O	1:D:125:GLU:HA	2.16	0.45
1:D:450:ILE:HG23	1:D:454:PHE:HE2	1.81	0.45
1:A:369:LEU:C	1:A:369:LEU:HD23	2.42	0.45
1:B:147:TYR:HB3	1:B:307:ASP:HA	1.99	0.45
1:B:192:VAL:O	1:B:196:ILE:HG12	2.17	0.45
1:B:348:TYR:HB3	1:B:415:TYR:CD1	2.52	0.45
1:A:206:VAL:HG21	1:A:322:THR:HG21	1.99	0.45
1:A:228:PHE:CE2	1:A:230:THR:HG22	2.52	0.45
1:C:84:PHE:CE2	1:C:202:LEU:HD13	2.51	0.45
1:C:252:ILE:O	1:C:256:SER:HB3	2.17	0.45
1:A:419:ILE:HA	1:A:432:ASN:O	2.17	0.45
1:C:103:SER:HA	1:C:300:ARG:HD3	1.98	0.45
1:C:298:PRO:O	1:C:303:LEU:N	2.45	0.45
1:C:401:GLU:HB2	1:C:406:ARG:HD2	1.99	0.45
1:A:55:SER:OG	1:A:58:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:PHE:O	1:A:213:PHE:CD1	2.70	0.45
1:B:165:ALA:HB3	1:B:168:ALA:HB2	1.99	0.45
1:B:353:ILE:N	1:B:353:ILE:HD12	2.31	0.45
1:C:208:ASN:HA	1:C:223:ASN:OD1	2.17	0.45
1:C:238:ASP:HB2	1:C:241:VAL:HG23	1.98	0.45
1:D:281:HIS:CG	1:D:282:LEU:H	2.35	0.45
1:C:50:MET:O	1:C:60:PHE:HB2	2.18	0.44
1:C:97:LYS:HE2	1:C:101:GLU:OE2	2.17	0.44
1:D:62:LEU:HB3	1:D:63:PRO:CD	2.42	0.44
1:D:86:PHE:CZ	1:D:320:ARG:HD3	2.49	0.44
1:D:231:ARG:HD2	1:D:235:PHE:CD2	2.53	0.44
1:A:227:ASN:HB2	1:A:275:ASP:HB2	2.00	0.44
1:A:228:PHE:O	1:A:262:LEU:O	2.36	0.44
1:B:76:MET:HB2	1:B:323:PHE:CE2	2.52	0.44
1:D:61:PHE:HZ	1:D:327:GLU:HG3	1.81	0.44
1:D:74:GLU:O	1:D:78:LEU:HD23	2.16	0.44
1:A:213:PHE:O	1:A:213:PHE:HD1	2.01	0.44
1:B:62:LEU:HB2	1:B:63:PRO:HD3	1.97	0.44
1:B:249:LEU:HA	1:B:252:ILE:HG22	1.99	0.44
1:A:159:PRO:HG3	1:A:179:HIS:NE2	2.32	0.44
1:B:91:THR:HB	1:B:95:TYR:OH	2.17	0.44
1:C:100:TRP:CD1	1:C:113:MET:HE1	2.53	0.44
1:D:133:CYS:N	1:D:134:PRO:HD2	2.33	0.44
1:D:344:TRP:CE2	1:D:345:LEU:HG	2.53	0.44
1:A:185:ILE:HB	1:A:318:ILE:HB	2.00	0.44
1:B:102:LYS:O	1:B:300:ARG:HD3	2.17	0.44
1:D:39:THR:O	1:D:43:SER:HB3	2.18	0.44
1:D:100:TRP:HB3	1:D:106:TRP:HB2	2.00	0.44
1:D:106:TRP:CD1	1:D:106:TRP:C	2.96	0.44
1:D:355:VAL:HG23	1:D:421:VAL:O	2.18	0.44
1:A:262:LEU:O	1:A:263:ASN:C	2.60	0.44
1:B:383:GLU:HA	1:B:384:PRO:HD3	1.85	0.44
1:B:238:ASP:OD2	1:B:240:LYS:HB2	2.18	0.44
1:C:267:GLY:HA2	1:C:268:ALA:HA	1.76	0.44
1:D:61:PHE:HE1	1:D:330:MET:HE1	1.83	0.44
1:D:369:LEU:HD22	1:D:431:TYR:CE2	2.52	0.44
1:A:96:LYS:HB3	1:A:98:THR:HG22	2.00	0.44
1:D:293:LEU:N	1:D:293:LEU:HD12	2.33	0.44
1:A:50:MET:HE2	1:A:60:PHE:CG	2.53	0.43
1:A:280:ASP:HB3	1:A:282:LEU:H	1.83	0.43
1:C:297:LEU:HD12	1:C:297:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:ILE:O	1:C:398:ILE:HG22	2.18	0.43
1:D:349:GLN:HB2	1:D:393:ASN:O	2.18	0.43
1:C:355:VAL:HG23	1:C:421:VAL:O	2.18	0.43
1:D:69:PHE:CE2	1:D:73:ILE:HD11	2.53	0.43
1:A:63:PRO:O	1:A:67:LYS:HG3	2.18	0.43
1:B:189:PRO:HA	1:B:192:VAL:HG23	2.00	0.43
1:C:114:PHE:HZ	1:C:176:ARG:HD2	1.82	0.43
1:D:68:ILE:HD13	1:D:341:TRP:CZ2	2.54	0.43
1:B:387:LEU:O	1:B:388:ASN:HB2	2.19	0.43
1:C:354:PRO:HG3	1:C:366:CYS:SG	2.58	0.43
1:A:228:PHE:HA	1:A:274:LEU:HD23	2.01	0.43
1:D:129:LYS:HA	1:D:130:PRO:HD2	1.88	0.43
1:D:329:PHE:CA	1:D:332:LEU:HG	2.46	0.43
1:A:136:HIS:CE1	1:A:156:ASP:HB2	2.54	0.43
1:B:400:ASN:O	1:B:401:GLU:HG2	2.18	0.43
1:C:184:HIS:HD2	1:C:317:MET:HE2	1.84	0.43
1:C:340:ARG:HG2	1:C:414:ASN:OD1	2.18	0.43
1:A:100:TRP:CD1	1:A:113:MET:HE1	2.54	0.43
1:C:262:LEU:O	1:C:263:ASN:C	2.62	0.43
1:D:140:PHE:HD2	1:D:303:LEU:HD22	1.84	0.43
1:B:249:LEU:O	1:B:252:ILE:HG22	2.19	0.43
1:B:409:SER:HA	1:B:412:LEU:HB3	1.99	0.43
1:B:414:ASN:C	1:B:436:ARG:HH12	2.27	0.43
1:C:453:LYS:O	1:C:457:LEU:HD13	2.18	0.43
1:D:236:ILE:HG12	1:D:269:PHE:CD1	2.54	0.43
1:D:343:PHE:CZ	1:D:454:PHE:CD1	3.07	0.43
1:A:45:ARG:HH21	1:A:414:ASN:ND2	2.15	0.43
1:B:403:VAL:O	1:B:407:ILE:HG13	2.19	0.43
1:C:86:PHE:HE2	1:C:320:ARG:NE	2.17	0.43
1:D:276:ILE:HG13	1:D:289:ALA:HB3	2.01	0.43
1:A:267:GLY:HA2	1:A:268:ALA:HA	1.81	0.42
1:C:91:THR:HB	1:C:92:PRO:HD2	2.01	0.42
1:C:182:ASP:HB3	1:C:183:GLY:H	1.62	0.42
1:C:431:TYR:O	1:C:444:LYS:HA	2.20	0.42
1:D:150:LEU:HA	1:D:151:PRO:C	2.44	0.42
1:D:192:VAL:O	1:D:196:ILE:HG12	2.19	0.42
1:A:231:ARG:HG2	1:A:232:PRO:O	2.19	0.42
1:B:373:LEU:CD2	1:B:394:VAL:HG11	2.49	0.42
1:C:97:LYS:HG3	1:C:106:TRP:CD2	2.54	0.42
1:D:206:VAL:HG12	1:D:207:TYR:N	2.33	0.42
1:D:247:GLN:O	1:D:251:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:LEU:HB2	1:D:298:PRO:HD3	2.01	0.42
1:D:349:GLN:NE2	1:D:393:ASN:HD22	2.14	0.42
1:A:212:PRO:O	1:A:213:PHE:CD2	2.72	0.42
1:C:416:SER:HA	1:C:436:ARG:NH1	2.34	0.42
1:D:76:MET:HG3	1:D:157:PHE:HZ	1.85	0.42
1:D:330:MET:O	1:D:334:ILE:HG13	2.18	0.42
1:B:49:PHE:HE1	1:B:172:LEU:HD21	1.83	0.42
1:D:140:PHE:CE2	1:D:303:LEU:HB3	2.54	0.42
1:A:193:LYS:O	1:A:194:SER:C	2.63	0.42
1:A:448:SER:O	1:A:452:GLU:HG2	2.19	0.42
1:B:387:LEU:N	1:B:387:LEU:HD12	2.35	0.42
1:C:207:TYR:OH	1:C:288:VAL:HB	2.20	0.42
1:D:214:VAL:HB	1:D:223:ASN:OD1	2.19	0.42
1:A:97:LYS:HE2	1:A:101:GLU:OE2	2.19	0.42
1:B:330:MET:O	1:B:334:ILE:HG13	2.19	0.42
1:A:294:ASP:OD2	1:A:297:LEU:HD13	2.20	0.42
1:B:340:ARG:O	1:B:341:TRP:C	2.62	0.42
1:D:205:ILE:O	1:D:209:LYS:CB	2.68	0.42
1:D:343:PHE:CE1	1:D:454:PHE:HD1	2.37	0.42
1:D:450:ILE:CG2	1:D:454:PHE:HE2	2.33	0.42
1:A:100:TRP:CZ3	1:A:134:PRO:HG3	2.55	0.42
1:A:229:SER:HB3	1:A:266:ASP:O	2.20	0.42
1:D:180:GLN:HG2	1:D:182:ASP:H	1.84	0.42
1:A:113:MET:HE3	1:A:128:LEU:O	2.20	0.42
1:D:50:MET:O	1:D:60:PHE:HB2	2.20	0.42
1:A:150:LEU:HD22	1:A:186:PHE:O	2.19	0.41
1:B:71:LYS:HE3	1:B:71:LYS:HB2	1.93	0.41
1:C:340:ARG:HB3	1:C:436:ARG:HH21	1.85	0.41
1:C:375:ASN:HD22	1:C:391:HIS:CE1	2.37	0.41
1:D:349:GLN:O	1:D:350:ALA:HB2	2.21	0.41
1:A:454:PHE:O	1:A:457:LEU:HB2	2.20	0.41
1:B:196:ILE:CD1	1:B:318:ILE:HD13	2.50	0.41
1:B:320:ARG:HB3	1:B:320:ARG:NH1	2.35	0.41
1:C:446:THR:HG22	1:C:449:GLN:CG	2.50	0.41
1:D:48:LEU:O	1:D:65:GLY:HA3	2.20	0.41
1:A:344:TRP:CE2	1:A:345:LEU:HG	2.54	0.41
1:A:438:ASN:OD1	1:A:440:LYS:O	2.38	0.41
1:B:356:ASN:OD1	1:B:359:ASN:HB2	2.19	0.41
1:C:273:LYS:HE3	1:C:275:ASP:OD1	2.20	0.41
1:D:448:SER:O	1:D:452:GLU:HG2	2.19	0.41
1:A:112:ASP:HA	1:A:163:ASN:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:PHE:CZ	1:B:253:LEU:HD12	2.55	0.41
1:C:132:ASN:HA	1:C:134:PRO:HD2	2.02	0.41
1:C:297:LEU:N	1:C:298:PRO:HD3	2.34	0.41
1:C:351:VAL:HB	1:C:415:TYR:CE1	2.55	0.41
1:A:289:ALA:HB2	1:A:322:THR:O	2.20	0.41
1:A:349:GLN:OE1	1:A:392:PHE:HD1	2.03	0.41
1:B:165:ALA:O	1:B:169:LEU:HD13	2.21	0.41
1:A:181:ASP:O	1:A:181:ASP:CG	2.64	0.41
1:A:210:ILE:HG22	1:A:210:ILE:O	2.20	0.41
1:A:289:ALA:HB1	1:A:321:ALA:O	2.21	0.41
1:A:341:TRP:N	1:A:436:ARG:HH22	2.18	0.41
1:D:43:SER:HA	1:D:48:LEU:HB2	2.01	0.41
1:D:343:PHE:HE1	1:D:349:GLN:HB3	1.85	0.41
1:C:116:VAL:HG13	1:D:115:LYS:O	2.21	0.41
1:D:226:ILE:C	1:D:226:ILE:HD12	2.46	0.41
1:D:236:ILE:HG22	1:D:237:GLY:N	2.35	0.41
1:D:329:PHE:O	1:D:329:PHE:CD2	2.74	0.41
1:D:369:LEU:HD13	1:D:431:TYR:CE2	2.54	0.41
1:A:59:MET:HB2	1:A:175:LEU:HD21	2.01	0.41
1:A:365:MET:HE1	1:A:430:LYS:N	2.36	0.41
1:B:353:ILE:HA	1:B:354:PRO:HD3	1.81	0.41
1:C:297:LEU:H	1:C:298:PRO:HD3	1.85	0.41
1:D:353:ILE:HD12	1:D:353:ILE:N	2.35	0.41
1:D:399:ARG:O	1:D:406:ARG:HD3	2.21	0.41
1:A:140:PHE:CZ	1:A:145:ARG:HG3	2.56	0.41
1:A:195:GLU:O	1:A:196:ILE:C	2.63	0.41
1:A:379:ALA:HB1	1:B:198:ASN:HB3	2.02	0.41
1:B:349:GLN:O	1:B:350:ALA:HB2	2.21	0.41
1:D:50:MET:HG2	1:D:51:THR:N	2.36	0.41
1:B:224:TYR:CD1	1:B:276:ILE:HD11	2.56	0.41
1:B:226:ILE:CG2	1:B:227:ASN:H	2.23	0.41
1:C:79:GLN:O	1:C:83:LYS:HB3	2.21	0.41
1:D:408:LYS:HA	1:D:411:ILE:HG22	2.03	0.41
1:A:343:PHE:CG	1:A:457:LEU:HD13	2.55	0.40
1:B:206:VAL:O	1:B:211:PHE:HD2	2.03	0.40
1:B:269:PHE:CB	1:B:270:TYR:HA	2.25	0.40
1:D:67:LYS:HE2	1:D:393:ASN:OD1	2.21	0.40
1:D:189:PRO:HA	1:D:192:VAL:HG23	2.03	0.40
1:A:52:ASP:HA	1:A:53:PRO:HD3	1.97	0.40
1:C:86:PHE:CD1	1:C:153:ARG:HB3	2.56	0.40
1:C:86:PHE:HE1	1:C:153:ARG:HD3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:PRO:HD2	1:C:406:ARG:NH2	2.37	0.40
1:A:106:TRP:O	1:A:109:TYR:O	2.40	0.40
1:B:158:SER:HA	1:B:159:PRO:HD3	1.93	0.40
1:C:162:ARG:HG2	1:C:163:ASN:N	2.35	0.40
1:C:348:TYR:HB3	1:C:415:TYR:CD1	2.55	0.40
1:D:84:PHE:CE2	1:D:202:LEU:HD13	2.56	0.40
1:D:231:ARG:HB2	1:D:242:TRP:CE3	2.55	0.40
1:D:446:THR:HB	1:D:449:GLN:HG3	2.02	0.40
1:A:158:SER:HA	1:A:159:PRO:HD3	1.91	0.40
1:A:353:ILE:HB	1:A:420:ILE:HG22	2.03	0.40
1:C:157:PHE:CD2	1:C:181:ASP:HA	2.57	0.40
1:A:286:HIS:HB3	1:A:328:ARG:NH2	2.36	0.40
1:A:307:ASP:OD1	1:A:313:LYS:HD2	2.22	0.40
1:B:62:LEU:CB	1:B:63:PRO:CD	2.94	0.40
1:B:416:SER:HA	1:B:436:ARG:HH11	1.86	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	415/460 (90%)	377 (91%)	37 (9%)	1 (0%)	43	72
1	B	415/460 (90%)	368 (89%)	46 (11%)	1 (0%)	43	72
1	C	426/460 (93%)	390 (92%)	36 (8%)	0	100	100
1	D	412/460 (90%)	370 (90%)	42 (10%)	0	100	100
All	All	1668/1840 (91%)	1505 (90%)	161 (10%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	394	VAL
1	A	394	VAL

5.3.2 Protein sidechains [i](#)

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	362/416 (87%)	360 (99%)	2 (1%)	78	79
1	B	335/416 (80%)	334 (100%)	1 (0%)	86	83
1	C	364/416 (88%)	361 (99%)	3 (1%)	73	77
1	D	338/416 (81%)	336 (99%)	2 (1%)	78	79
All	All	1399/1664 (84%)	1391 (99%)	8 (1%)	78	79

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	LEU
1	A	248	VAL
1	B	341	TRP
1	C	286	HIS
1	C	297	LEU
1	C	320	ARG
1	D	209	LYS
1	D	373	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	70	ASN
1	A	80	GLN
1	A	136	HIS
1	A	161	HIS
1	A	179	HIS
1	A	184	HIS

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Mol	Chain	Res	Type
1	A	292	GLN
1	A	319	HIS
1	A	414	ASN
1	A	432	ASN
1	B	161	HIS
1	B	391	HIS
1	B	414	ASN
1	B	429[A]	GLN
1	C	105	HIS
1	C	132	ASN
1	C	184	HIS
1	C	234	HIS
1	C	391	HIS
1	C	393	ASN
1	C	432	ASN
1	D	184	HIS
1	D	223	ASN
1	D	244	HIS
1	D	281	HIS
1	D	292	GLN
1	D	349	GLN
1	D	370	GLN
1	D	391	HIS
1	D	414	ASN
1	D	449	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	419/460 (91%)	-0.02	2 (0%)	87 66	63, 83, 110, 132	2 (0%)
1	B	419/460 (91%)	0.23	7 (1%)	69 41	49, 98, 138, 149	3 (0%)
1	C	427/460 (92%)	0.04	2 (0%)	87 66	55, 79, 105, 115	3 (0%)
1	D	418/460 (90%)	0.19	6 (1%)	73 46	64, 93, 126, 137	1 (0%)
All	All	1683/1840 (91%)	0.11	17 (1%)	79 54	49, 88, 125, 149	9 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	344	TRP	3.6
1	D	213	PHE	3.0
1	D	211	PHE	2.7
1	A	117	GLU	2.5
1	B	438	ASN	2.5
1	B	439	ARG	2.5
1	A	213	PHE	2.4
1	B	292	GLN	2.3
1	B	114	PHE	2.2
1	D	273	LYS	2.2
1	D	234	HIS	2.2
1	B	214	VAL	2.1
1	B	441	SER	2.1
1	C	133	CYS	2.1
1	D	216	GLY	2.0
1	C	120	ASP	2.0
1	D	238	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	D	463	1/1	0.93	0.08	103,103,103,103	0
2	ZN	B	2	1/1	0.96	0.10	92,92,92,92	0
2	ZN	C	463	1/1	0.97	0.08	59,59,59,59	0
2	ZN	A	1	1/1	0.97	0.06	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.