



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:38 AM UTC

PDB ID : 1OU5 / pdb_00001ou5
Title : Crystal structure of human CCA-adding enzyme
Authors : Augustin, M.A.; Reichert, A.S.; Betat, H.; Huber, R.; Moerl, M.; Steegborn, C.
Deposited on : 2003-03-24
Resolution : 3.40 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 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

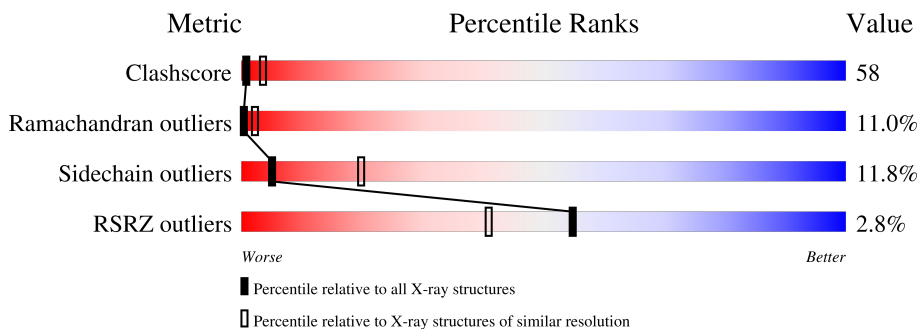
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

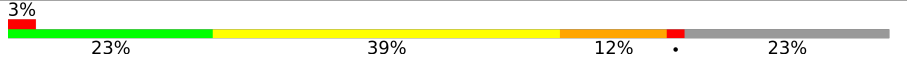
The reported resolution of this entry is 3.40 Å.

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))
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	448	
1	B	448	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5570 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 tRNA CCA-adding enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	266	0	0
			2785	1776	480	521	8			
1	B	344	Total	C	N	O	S	194	0	0
			2785	1776	480	521	8			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	cloning artifact	UNP Q96Q11
A	-41	HIS	-	cloning artifact	UNP Q96Q11
A	-40	HIS	-	cloning artifact	UNP Q96Q11
A	-39	HIS	-	cloning artifact	UNP Q96Q11
A	-38	HIS	-	cloning artifact	UNP Q96Q11
A	-37	HIS	-	cloning artifact	UNP Q96Q11
A	-36	HIS	-	cloning artifact	UNP Q96Q11
A	-35	SER	-	cloning artifact	UNP Q96Q11
A	-34	SER	-	cloning artifact	UNP Q96Q11
A	-33	GLY	-	cloning artifact	UNP Q96Q11
A	-32	LEU	-	cloning artifact	UNP Q96Q11
A	-31	VAL	-	cloning artifact	UNP Q96Q11
A	-30	PRO	-	cloning artifact	UNP Q96Q11
A	-29	ARG	-	cloning artifact	UNP Q96Q11
A	-28	GLY	-	cloning artifact	UNP Q96Q11
A	-27	SER	-	cloning artifact	UNP Q96Q11
A	-26	GLY	-	cloning artifact	UNP Q96Q11
A	-25	MET	-	cloning artifact	UNP Q96Q11
A	-24	LYS	-	cloning artifact	UNP Q96Q11
A	-23	GLU	-	cloning artifact	UNP Q96Q11
A	-22	THR	-	cloning artifact	UNP Q96Q11
A	-21	ALA	-	cloning artifact	UNP Q96Q11
A	-20	ALA	-	cloning artifact	UNP Q96Q11
A	-19	ALA	-	cloning artifact	UNP Q96Q11
A	-18	LYS	-	cloning artifact	UNP Q96Q11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	PHE	-	cloning artifact	UNP Q96Q11
A	-16	GLU	-	cloning artifact	UNP Q96Q11
A	-15	ARG	-	cloning artifact	UNP Q96Q11
A	-14	GLN	-	cloning artifact	UNP Q96Q11
A	-13	HIS	-	cloning artifact	UNP Q96Q11
A	-12	MET	-	cloning artifact	UNP Q96Q11
A	-11	ASP	-	cloning artifact	UNP Q96Q11
A	-10	SER	-	cloning artifact	UNP Q96Q11
A	-9	PRO	-	cloning artifact	UNP Q96Q11
A	-8	ASP	-	cloning artifact	UNP Q96Q11
A	-7	LEU	-	cloning artifact	UNP Q96Q11
A	-6	GLY	-	cloning artifact	UNP Q96Q11
A	-5	THR	-	cloning artifact	UNP Q96Q11
A	-4	ASP	-	cloning artifact	UNP Q96Q11
A	-3	ASP	-	cloning artifact	UNP Q96Q11
A	-2	ASP	-	cloning artifact	UNP Q96Q11
A	-1	ASP	-	cloning artifact	UNP Q96Q11
A	0	LYS	-	cloning artifact	UNP Q96Q11
B	-42	MET	-	cloning artifact	UNP Q96Q11
B	-41	HIS	-	cloning artifact	UNP Q96Q11
B	-40	HIS	-	cloning artifact	UNP Q96Q11
B	-39	HIS	-	cloning artifact	UNP Q96Q11
B	-38	HIS	-	cloning artifact	UNP Q96Q11
B	-37	HIS	-	cloning artifact	UNP Q96Q11
B	-36	HIS	-	cloning artifact	UNP Q96Q11
B	-35	SER	-	cloning artifact	UNP Q96Q11
B	-34	SER	-	cloning artifact	UNP Q96Q11
B	-33	GLY	-	cloning artifact	UNP Q96Q11
B	-32	LEU	-	cloning artifact	UNP Q96Q11
B	-31	VAL	-	cloning artifact	UNP Q96Q11
B	-30	PRO	-	cloning artifact	UNP Q96Q11
B	-29	ARG	-	cloning artifact	UNP Q96Q11
B	-28	GLY	-	cloning artifact	UNP Q96Q11
B	-27	SER	-	cloning artifact	UNP Q96Q11
B	-26	GLY	-	cloning artifact	UNP Q96Q11
B	-25	MET	-	cloning artifact	UNP Q96Q11
B	-24	LYS	-	cloning artifact	UNP Q96Q11
B	-23	GLU	-	cloning artifact	UNP Q96Q11
B	-22	THR	-	cloning artifact	UNP Q96Q11
B	-21	ALA	-	cloning artifact	UNP Q96Q11
B	-20	ALA	-	cloning artifact	UNP Q96Q11
B	-19	ALA	-	cloning artifact	UNP Q96Q11

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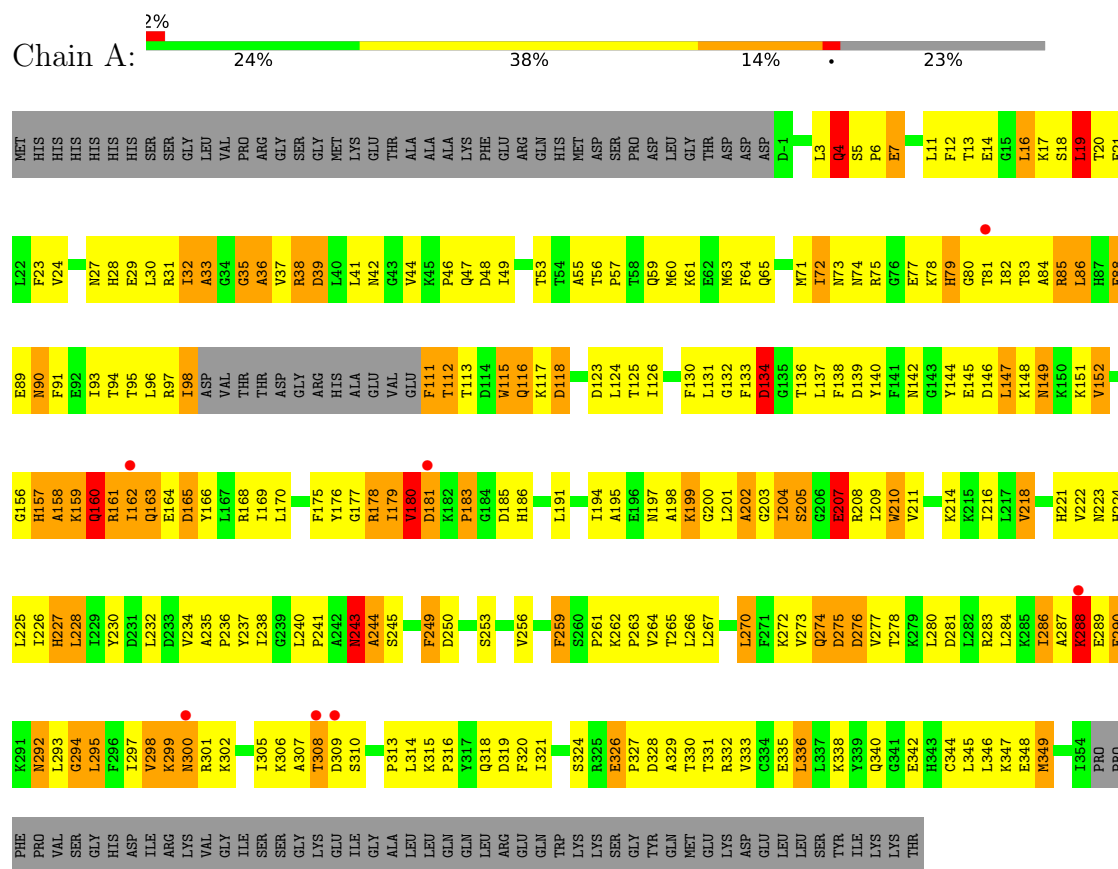
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	LYS	-	cloning artifact	UNP Q96Q11
B	-17	PHE	-	cloning artifact	UNP Q96Q11
B	-16	GLU	-	cloning artifact	UNP Q96Q11
B	-15	ARG	-	cloning artifact	UNP Q96Q11
B	-14	GLN	-	cloning artifact	UNP Q96Q11
B	-13	HIS	-	cloning artifact	UNP Q96Q11
B	-12	MET	-	cloning artifact	UNP Q96Q11
B	-11	ASP	-	cloning artifact	UNP Q96Q11
B	-10	SER	-	cloning artifact	UNP Q96Q11
B	-9	PRO	-	cloning artifact	UNP Q96Q11
B	-8	ASP	-	cloning artifact	UNP Q96Q11
B	-7	LEU	-	cloning artifact	UNP Q96Q11
B	-6	GLY	-	cloning artifact	UNP Q96Q11
B	-5	THR	-	cloning artifact	UNP Q96Q11
B	-4	ASP	-	cloning artifact	UNP Q96Q11
B	-3	ASP	-	cloning artifact	UNP Q96Q11
B	-2	ASP	-	cloning artifact	UNP Q96Q11
B	-1	ASP	-	cloning artifact	UNP Q96Q11
B	0	LYS	-	cloning artifact	UNP Q96Q11

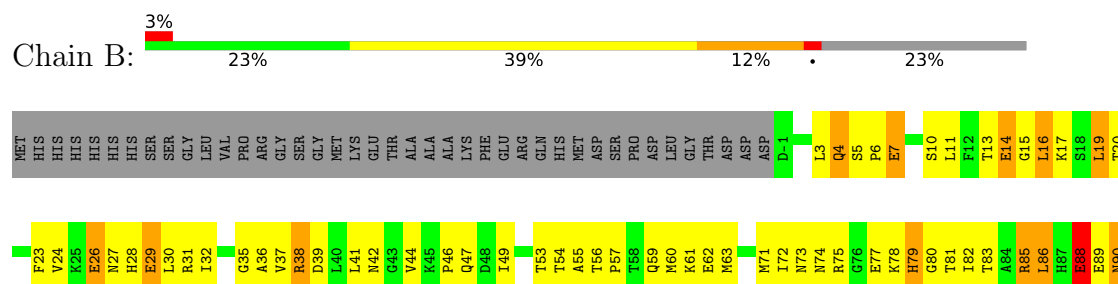
3 Residue-property plots

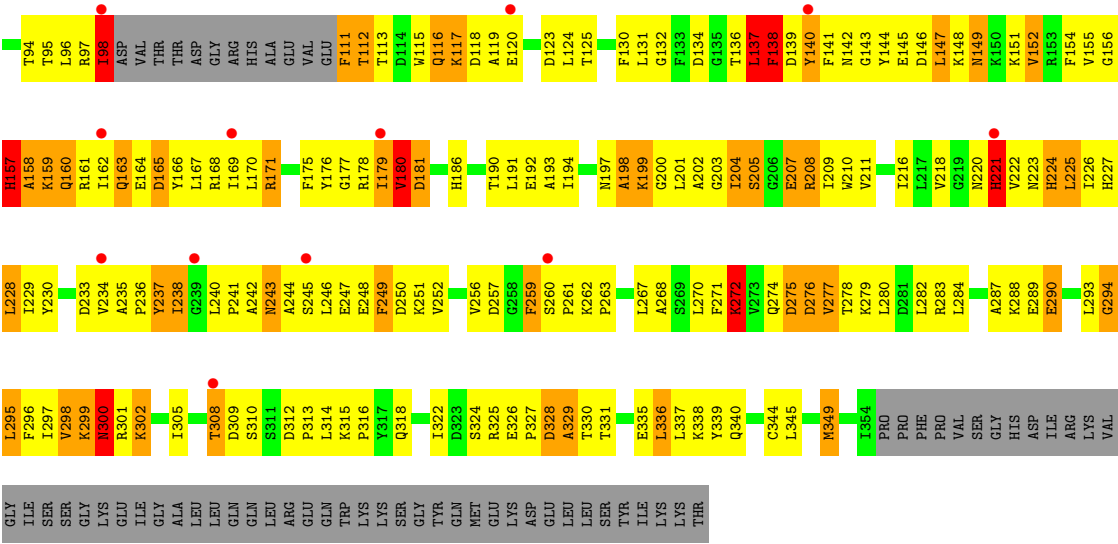
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: tRNA CCA-adding enzyme





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.52Å 102.52Å 206.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.40 20.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-3.40) 97.6 (20.00-3.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.278 , 0.318 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 5.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5570	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 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.12	6/2839 (0.2%)	1.36	41/3826 (1.1%)
1	B	0.78	4/2839 (0.1%)	1.22	30/3826 (0.8%)
All	All	0.96	10/5678 (0.2%)	1.29	71/7652 (0.9%)

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	B	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	ILE	C-N	37.86	1.86	1.33
1	A	98	ILE	CA-C	12.26	1.68	1.52
1	B	98	ILE	CB-CG2	11.44	1.90	1.52
1	A	98	ILE	CB-CG2	8.28	1.79	1.52
1	A	98	ILE	CB-CG1	-7.80	1.37	1.53
1	A	97	ARG	C-N	7.06	1.43	1.33
1	B	300	ASN	CA-CB	-6.01	1.43	1.53
1	B	137	LEU	CA-C	-5.88	1.47	1.52
1	B	111	PHE	N-CA	5.84	1.53	1.45
1	A	286	ILE	CA-C	-5.16	1.47	1.53

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	GLY	N-CA-C	-14.61	95.13	111.93
1	B	98	ILE	N-CA-C	-12.92	82.46	109.34
1	A	98	ILE	N-CA-C	-11.32	85.80	109.34
1	A	134	ASP	N-CA-C	-11.03	99.22	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	PHE	N-CA-CB	10.49	128.19	110.14
1	B	118	ASP	N-CA-C	-10.15	100.90	113.18
1	A	98	ILE	CA-C-N	-9.92	102.60	121.54
1	A	98	ILE	C-N-CA	-9.92	102.60	121.54
1	B	80	GLY	N-CA-C	-9.88	103.01	113.58
1	A	160	GLN	N-CA-C	-9.60	101.93	114.31
1	B	137	LEU	CB-CA-C	-9.22	96.27	110.83
1	A	118	ASP	N-CA-C	-9.21	100.83	112.90
1	A	98	ILE	O-C-N	-9.17	111.11	122.57
1	B	159	LYS	N-CA-C	-9.16	102.24	113.15
1	B	147	LEU	N-CA-C	-9.12	98.57	110.33
1	B	272	LYS	N-CA-C	9.10	123.70	112.59
1	A	259	PHE	N-CA-C	-8.36	99.74	110.53
1	A	98	ILE	CA-C-O	-8.12	110.64	120.78
1	A	324	SER	N-CA-C	8.08	121.11	111.33
1	A	207	GLU	N-CA-C	-7.92	103.62	113.28
1	B	199	LYS	N-CA-C	-7.82	102.83	112.38
1	A	159	LYS	N-CA-C	-7.71	101.76	112.25
1	A	98	ILE	CA-CB-CG1	7.63	123.37	110.40
1	B	149	ASN	N-CA-C	-7.58	103.87	113.72
1	A	199	LYS	N-CA-C	-7.57	103.15	112.38
1	A	300	ASN	N-CA-C	-7.32	104.09	112.87
1	A	97	ARG	CA-C-N	7.14	134.83	121.97
1	A	97	ARG	C-N-CA	7.14	134.83	121.97
1	B	276	ASP	N-CA-C	-7.13	104.67	113.15
1	A	274	GLN	N-CA-C	-7.07	101.17	110.43
1	B	120	GLU	N-CA-C	-7.04	95.80	110.80
1	B	207	GLU	N-CA-C	-6.97	104.52	113.16
1	B	97	ARG	N-CA-C	6.93	119.05	108.52
1	B	277	VAL	N-CA-C	-6.62	106.11	111.81
1	A	33	ALA	N-CA-C	6.62	117.01	108.34
1	B	98	ILE	CA-CB-CG2	-6.54	99.38	110.50
1	B	98	ILE	CG1-CB-CG2	-6.44	91.38	110.70
1	A	72	ILE	N-CA-C	6.41	119.31	108.86
1	A	98	ILE	CA-CB-CG2	-6.31	99.78	110.50
1	A	286	ILE	CB-CA-C	-6.27	104.43	111.45
1	A	98	ILE	CB-CA-C	6.26	121.56	111.29
1	A	161	ARG	N-CA-C	-6.24	104.39	111.07
1	A	276	ASP	N-CA-C	-6.13	105.89	113.19
1	B	290	GLU	N-CA-C	-5.92	104.01	111.11
1	B	247	GLU	N-CA-C	-5.89	104.50	111.03
1	B	98	ILE	CB-CA-C	5.86	120.90	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	PHE	N-CA-C	5.85	123.25	110.80
1	B	180	VAL	CB-CA-C	-5.74	101.88	111.29
1	A	132	GLY	N-CA-C	-5.66	105.30	112.54
1	B	4	GLN	N-CA-C	5.61	117.51	107.80
1	A	290	GLU	N-CA-C	-5.61	105.07	111.07
1	B	279	LYS	N-CA-C	-5.56	105.31	111.71
1	A	179	ILE	N-CA-C	5.56	116.12	107.28
1	B	98	ILE	CB-CG1-CD1	-5.49	102.28	113.80
1	A	227	HIS	N-CA-C	-5.37	105.33	111.07
1	A	19	LEU	N-CA-C	-5.36	105.13	110.97
1	B	208	ARG	N-CA-C	-5.36	106.59	113.23
1	B	272	LYS	CA-C-N	-5.30	115.07	122.75
1	B	272	LYS	C-N-CA	-5.30	115.07	122.75
1	A	288	LYS	N-CA-CB	-5.26	101.60	110.49
1	A	73	ASN	CA-CB-CG	-5.23	107.37	112.60
1	A	149	ASN	N-CA-C	-5.19	106.94	113.28
1	B	98	ILE	CA-CB-CG1	5.17	119.20	110.40
1	A	39	ASP	N-CA-C	-5.11	104.78	111.02
1	A	307	ALA	N-CA-C	5.08	116.51	109.54
1	A	278	THR	N-CA-C	-5.07	105.94	111.82
1	B	117	LYS	N-CA-C	-5.07	104.01	111.81
1	A	147	LEU	N-CA-C	-5.07	104.18	110.41
1	A	4	GLN	N-CA-C	5.06	115.80	107.20
1	A	115	TRP	CA-CB-CG	5.04	123.17	113.60
1	B	259	PHE	N-CA-C	-5.02	103.42	110.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	98	ILE	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	2785	0	2799	270	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2785	0	2803	309	1
All	All	5570	0	5602	577	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 58.

All (577) 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:B:199:LYS:HA	1:B:237:TYR:CE1	1.46	1.45
1:B:199:LYS:HA	1:B:237:TYR:CD1	1.69	1.24
1:B:241:PRO:HG3	1:B:271:PHE:HB3	1.35	1.06
1:B:209:ILE:HD11	1:B:284:LEU:HD11	1.34	1.05
1:B:199:LYS:CA	1:B:237:TYR:CE1	2.39	1.05
1:B:314:LEU:HD11	1:B:349:MET:HG2	1.42	1.01
1:A:308:THR:HG22	1:A:310:SER:H	1.25	0.98
1:B:308:THR:O	1:B:309:ASP:CG	2.06	0.97
1:B:131:LEU:HD23	1:B:136:THR:O	1.66	0.96
1:A:226:ILE:HG12	1:A:249:PHE:CZ	2.00	0.96
1:B:237:TYR:HD2	1:B:237:TYR:N	1.64	0.95
1:B:236:PRO:HG2	1:B:237:TYR:CD2	2.04	0.92
1:B:199:LYS:CA	1:B:237:TYR:HE1	1.80	0.91
1:B:119:ALA:O	1:B:141:PHE:CE2	2.24	0.90
1:A:230:TYR:CD2	1:A:243:ASN:HB3	2.06	0.90
1:A:209:ILE:HD11	1:A:284:LEU:HD11	1.52	0.90
1:B:272:LYS:HE2	1:B:299:LYS:H	1.35	0.90
1:B:199:LYS:HA	1:B:237:TYR:HE1	1.11	0.89
1:A:32:ILE:HD11	1:A:36:ALA:O	1.72	0.89
1:B:308:THR:HG22	1:B:310:SER:H	1.39	0.88
1:B:274:GLN:O	1:B:275:ASP:HB3	1.74	0.87
1:B:199:LYS:CA	1:B:237:TYR:CD1	2.57	0.87
1:B:267:LEU:O	1:B:270:LEU:HD23	1.75	0.86
1:A:336:LEU:HD22	1:A:340:GLN:HG3	1.55	0.86
1:B:119:ALA:O	1:B:141:PHE:HE2	1.56	0.85
1:B:226:ILE:HG12	1:B:249:PHE:CZ	2.12	0.84
1:B:237:TYR:N	1:B:237:TYR:CD2	2.39	0.83
1:B:179:ILE:O	1:B:180:VAL:HG13	1.77	0.83
1:B:275:ASP:H	1:B:277:VAL:HG12	1.43	0.83
1:B:146:ASP:HB3	1:B:151:LYS:HB3	1.59	0.82
1:A:20:THR:O	1:A:24:VAL:HG23	1.79	0.82
1:A:301:ARG:O	1:A:305:ILE:HG22	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LEU:HD22	1:B:340:GLN:HG3	1.61	0.81
1:B:165:ASP:HB3	1:B:168:ARG:HD3	1.63	0.80
1:B:280:LEU:HD11	1:B:284:LEU:HD22	1.64	0.80
1:A:280:LEU:HD11	1:A:284:LEU:HD22	1.64	0.79
1:A:39:ASP:HB3	1:A:44:VAL:HG23	1.65	0.79
1:B:46:PRO:HB2	1:B:49:ILE:HG12	1.64	0.79
1:B:197:ASN:O	1:B:198:ALA:HB3	1.81	0.78
1:B:272:LYS:HE2	1:B:299:LYS:N	1.98	0.78
1:B:236:PRO:HG2	1:B:237:TYR:CE2	2.18	0.78
1:B:11:LEU:HD11	1:B:46:PRO:HG3	1.65	0.77
1:B:199:LYS:CB	1:B:237:TYR:HE1	1.97	0.77
1:B:315:LYS:N	1:B:316:PRO:HD2	2.00	0.77
1:A:19:LEU:HD12	1:A:91:PHE:CD2	2.18	0.77
1:B:260:SER:H	1:B:338:LYS:HZ1	1.33	0.76
1:A:35:GLY:O	1:A:36:ALA:CB	2.30	0.76
1:B:165:ASP:HB3	1:B:168:ARG:CD	2.16	0.76
1:A:274:GLN:O	1:A:275:ASP:HB2	1.84	0.76
1:B:20:THR:O	1:B:24:VAL:HG23	1.86	0.76
1:A:46:PRO:HB2	1:A:49:ILE:HG12	1.68	0.75
1:A:230:TYR:CE2	1:A:243:ASN:HB3	2.22	0.74
1:A:160:GLN:HA	1:A:163:GLN:HB3	1.69	0.74
1:A:197:ASN:O	1:A:198:ALA:HB3	1.87	0.73
1:A:314:LEU:HD11	1:A:349:MET:HG2	1.69	0.73
1:B:157:HIS:C	1:B:159:LYS:H	1.96	0.73
1:B:298:VAL:O	1:B:300:ASN:N	2.20	0.73
1:A:160:GLN:HA	1:A:163:GLN:CB	2.19	0.73
1:B:274:GLN:O	1:B:275:ASP:CB	2.37	0.73
1:A:147:LEU:C	1:A:149:ASN:H	1.97	0.73
1:A:126:ILE:HD12	1:A:147:LEU:HB2	1.71	0.73
1:B:300:ASN:O	1:B:301:ARG:HD3	1.89	0.72
1:A:64:PHE:HB2	1:A:71:MET:HE2	1.70	0.72
1:B:260:SER:H	1:B:338:LYS:NZ	1.87	0.72
1:A:130:PHE:HB2	1:A:138:PHE:HB2	1.71	0.72
1:B:299:LYS:O	1:B:300:ASN:C	2.33	0.72
1:A:146:ASP:HB3	1:A:151:LYS:HB3	1.70	0.72
1:A:178:ARG:CG	1:A:178:ARG:HH21	2.02	0.71
1:A:147:LEU:O	1:A:148:LYS:HB3	1.90	0.71
1:B:145:GLU:O	1:B:149:ASN:HB2	1.91	0.71
1:A:287:ALA:O	1:A:290:GLU:HB2	1.89	0.71
1:B:11:LEU:HD22	1:B:49:ILE:HD11	1.72	0.71
1:A:170:LEU:HD11	1:A:238:ILE:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LEU:HD13	1:A:340:GLN:NE2	2.05	0.70
1:A:11:LEU:HD22	1:A:49:ILE:HD11	1.74	0.70
1:A:95:THR:HG21	1:A:112:THR:HG23	1.73	0.69
1:A:308:THR:HG22	1:A:310:SER:N	2.04	0.69
1:B:209:ILE:HD12	1:B:238:ILE:HG13	1.73	0.69
1:A:56:THR:OG1	1:A:59:GLN:HG2	1.91	0.69
1:A:165:ASP:O	1:A:168:ARG:HD3	1.92	0.69
1:A:41:LEU:HD13	1:A:144:TYR:HD1	1.56	0.69
1:B:61:LYS:C	1:B:63:MET:H	1.99	0.68
1:B:111:PHE:O	1:B:113:THR:N	2.27	0.68
1:B:95:THR:HG21	1:B:112:THR:HG23	1.75	0.68
1:A:288:LYS:O	1:A:290:GLU:N	2.24	0.67
1:B:205:SER:HB3	1:B:208:ARG:HB3	1.74	0.67
1:A:230:TYR:HD2	1:A:243:ASN:HB3	1.53	0.67
1:A:178:ARG:HH21	1:A:178:ARG:HG3	1.60	0.67
1:B:237:TYR:HD2	1:B:237:TYR:H	1.39	0.67
1:A:210:TRP:CE3	1:A:284:LEU:HD23	2.29	0.67
1:A:315:LYS:N	1:A:316:PRO:HD2	2.10	0.67
1:B:42:ASN:HD21	1:B:147:LEU:HD11	1.58	0.67
1:B:56:THR:OG1	1:B:59:GLN:HG2	1.95	0.67
1:A:299:LYS:HA	1:A:302:LYS:HB3	1.77	0.67
1:B:151:LYS:O	1:B:152:VAL:HB	1.93	0.66
1:B:130:PHE:O	1:B:137:LEU:O	2.14	0.66
1:B:305:ILE:HG23	1:B:305:ILE:O	1.94	0.66
1:A:305:ILE:HG23	1:A:305:ILE:O	1.94	0.66
1:A:158:ALA:C	1:A:160:GLN:H	2.01	0.66
1:B:30:LEU:C	1:B:30:LEU:HD23	2.20	0.66
1:B:328:ASP:O	1:B:329:ALA:C	2.37	0.66
1:A:89:GLU:O	1:A:90:ASN:HB2	1.96	0.65
1:A:11:LEU:HD11	1:A:46:PRO:HG3	1.78	0.65
1:B:31:ARG:CZ	1:B:116:GLN:OE1	2.44	0.65
1:A:139:ASP:O	1:A:140:TYR:HB2	1.97	0.65
1:A:273:VAL:O	1:A:276:ASP:HB3	1.97	0.65
1:B:301:ARG:O	1:B:305:ILE:HG22	1.96	0.65
1:B:147:LEU:C	1:B:149:ASN:H	2.04	0.65
1:A:11:LEU:O	1:A:16:LEU:HD12	1.97	0.65
1:B:160:GLN:O	1:B:163:GLN:HB3	1.97	0.65
1:A:145:GLU:O	1:A:149:ASN:HB2	1.97	0.65
1:B:226:ILE:HD12	1:B:227:HIS:N	2.11	0.65
1:A:273:VAL:HG12	1:A:274:GLN:N	2.12	0.64
1:A:328:ASP:O	1:A:329:ALA:C	2.40	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ARG:HG3	1:B:284:LEU:CD1	2.27	0.64
1:B:39:ASP:HB3	1:B:44:VAL:HG23	1.78	0.64
1:A:30:LEU:C	1:A:30:LEU:HD23	2.23	0.64
1:B:158:ALA:C	1:B:160:GLN:H	2.02	0.64
1:B:197:ASN:O	1:B:198:ALA:CB	2.45	0.64
1:A:115:TRP:O	1:A:117:LYS:N	2.30	0.64
1:B:31:ARG:HD3	1:B:116:GLN:HE22	1.61	0.64
1:A:134:ASP:OD2	1:A:136:THR:OG1	2.13	0.63
1:A:32:ILE:HG22	1:A:133:PHE:HE2	1.63	0.63
1:A:151:LYS:O	1:A:152:VAL:HB	1.98	0.63
1:A:259:PHE:N	1:A:259:PHE:CD1	2.66	0.63
1:B:180:VAL:O	1:B:181:ASP:CB	2.45	0.63
1:B:60:MET:O	1:B:63:MET:HB3	1.99	0.63
1:B:166:TYR:CD2	1:B:200:GLY:HA3	2.34	0.63
1:A:275:ASP:C	1:A:277:VAL:H	2.05	0.63
1:B:210:TRP:CE3	1:B:284:LEU:HD23	2.33	0.63
1:A:35:GLY:O	1:A:36:ALA:HB3	1.98	0.63
1:B:158:ALA:HB3	1:B:193:ALA:CB	2.29	0.63
1:B:165:ASP:O	1:B:168:ARG:HD3	1.98	0.62
1:B:78:LYS:O	1:B:79:HIS:O	2.16	0.62
1:B:205:SER:HB3	1:B:208:ARG:CB	2.28	0.62
1:A:111:PHE:O	1:A:113:THR:N	2.32	0.62
1:A:308:THR:O	1:A:309:ASP:HB2	1.99	0.62
1:B:280:LEU:CD1	1:B:284:LEU:HD22	2.30	0.62
1:B:53:THR:O	1:B:95:THR:HA	2.00	0.62
1:B:160:GLN:HA	1:B:163:GLN:HB3	1.81	0.62
1:B:124:LEU:HD23	1:B:154:PHE:HA	1.82	0.61
1:A:201:LEU:HD12	1:A:234:VAL:HG13	1.82	0.61
1:B:23:PHE:CD2	1:B:30:LEU:HD12	2.34	0.61
1:B:308:THR:HG22	1:B:310:SER:N	2.14	0.61
1:B:201:LEU:HD13	1:B:238:ILE:HD13	1.82	0.61
1:A:160:GLN:O	1:A:163:GLN:HB3	2.01	0.61
1:A:160:GLN:CA	1:A:163:GLN:HB3	2.31	0.61
1:B:275:ASP:N	1:B:277:VAL:HG12	2.14	0.61
1:A:126:ILE:CD1	1:A:147:LEU:HB2	2.29	0.61
1:A:61:LYS:C	1:A:63:MET:H	2.07	0.61
1:B:308:THR:OG1	1:B:313:PRO:HA	2.01	0.61
1:B:299:LYS:O	1:B:301:ARG:N	2.34	0.61
1:A:216:ILE:HG23	1:A:225:LEU:HD13	1.83	0.60
1:B:242:ALA:O	1:B:243:ASN:C	2.42	0.60
1:A:166:TYR:CD2	1:A:200:GLY:HA3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:PHE:CD2	1:A:30:LEU:HD12	2.37	0.60
1:A:280:LEU:CD1	1:A:284:LEU:HD22	2.30	0.60
1:A:294:GLY:O	1:A:298:VAL:HG23	2.02	0.60
1:A:125:THR:HG21	1:A:146:ASP:OD1	2.01	0.60
1:A:329:ALA:O	1:A:333:VAL:HG23	2.00	0.60
1:A:82:ILE:O	1:A:93:ILE:N	2.31	0.60
1:A:292:ASN:HA	1:A:295:LEU:HD21	1.84	0.60
1:A:336:LEU:HD22	1:A:340:GLN:CG	2.28	0.60
1:B:236:PRO:CG	1:B:237:TYR:CE2	2.85	0.59
1:A:11:LEU:HD21	1:A:46:PRO:HG2	1.84	0.59
1:A:209:ILE:HD12	1:A:238:ILE:CD1	2.31	0.59
1:B:11:LEU:HD21	1:B:46:PRO:HG2	1.84	0.59
1:B:308:THR:O	1:B:309:ASP:OD1	2.18	0.59
1:A:179:ILE:O	1:A:180:VAL:HG13	2.02	0.59
1:A:197:ASN:O	1:A:198:ALA:CB	2.51	0.59
1:A:201:LEU:HD13	1:A:238:ILE:HD13	1.84	0.59
1:A:61:LYS:HA	1:A:71:MET:HE1	1.85	0.59
1:A:72:ILE:HD11	1:A:90:ASN:ND2	2.18	0.59
1:B:26:GLU:HG2	1:B:63:MET:HE2	1.84	0.58
1:A:41:LEU:HD13	1:A:144:TYR:CD1	2.37	0.58
1:A:226:ILE:HD12	1:A:227:HIS:N	2.17	0.58
1:A:299:LYS:C	1:A:301:ARG:N	2.56	0.58
1:B:299:LYS:C	1:B:301:ARG:N	2.61	0.58
1:B:11:LEU:O	1:B:13:THR:HG23	2.04	0.58
1:B:82:ILE:HG22	1:B:83:THR:N	2.18	0.58
1:A:164:GLU:O	1:A:165:ASP:C	2.46	0.58
1:B:157:HIS:C	1:B:159:LYS:N	2.61	0.58
1:B:175:PHE:C	1:B:177:GLY:N	2.59	0.57
1:B:260:SER:N	1:B:338:LYS:HZ1	2.02	0.57
1:A:96:LEU:HD12	1:A:96:LEU:H	1.68	0.57
1:A:300:ASN:O	1:A:301:ARG:HD3	2.04	0.57
1:B:132:GLY:C	1:B:134:ASP:H	2.10	0.57
1:B:283:ARG:HG3	1:B:284:LEU:HD12	1.85	0.57
1:B:31:ARG:NH2	1:B:116:GLN:HE22	2.02	0.57
1:B:209:ILE:HD11	1:B:284:LEU:CD1	2.22	0.57
1:A:85:ARG:HG2	1:A:90:ASN:ND2	2.19	0.57
1:A:226:ILE:HD12	1:A:226:ILE:C	2.29	0.57
1:A:162:ILE:O	1:A:164:GLU:N	2.38	0.57
1:B:180:VAL:O	1:B:181:ASP:HB2	2.02	0.57
1:B:226:ILE:HD12	1:B:226:ILE:C	2.29	0.57
1:A:11:LEU:HD21	1:A:46:PRO:CG	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ALA:N	1:B:236:PRO:HD2	2.19	0.57
1:B:289:GLU:O	1:B:293:LEU:N	2.34	0.57
1:B:335:GLU:OE1	1:B:338:LYS:HE3	2.05	0.57
1:A:315:LYS:HA	1:A:318:GLN:HE21	1.70	0.57
1:B:199:LYS:HA	1:B:237:TYR:HD1	1.58	0.57
1:B:28:HIS:CG	1:B:55:ALA:HB2	2.39	0.57
1:B:132:GLY:C	1:B:134:ASP:N	2.63	0.57
1:B:256:VAL:HB	1:B:261:PRO:HB3	1.87	0.57
1:B:57:PRO:HA	1:B:60:MET:HE3	1.87	0.56
1:B:157:HIS:O	1:B:159:LYS:N	2.38	0.56
1:B:259:PHE:CD1	1:B:259:PHE:N	2.72	0.56
1:A:186:HIS:HB3	1:A:191:LEU:HD13	1.87	0.56
1:A:205:SER:HB3	1:A:208:ARG:CB	2.36	0.56
1:B:139:ASP:O	1:B:140:TYR:HB2	2.04	0.56
1:B:313:PRO:O	1:B:314:LEU:HB3	2.05	0.56
1:A:227:HIS:HE1	1:A:250:ASP:OD2	1.89	0.56
1:A:293:LEU:HD12	1:A:293:LEU:O	2.06	0.56
1:B:30:LEU:HD23	1:B:31:ARG:N	2.21	0.56
1:A:297:ILE:O	1:A:299:LYS:N	2.39	0.56
1:B:85:ARG:HD3	1:B:88:GLU:HA	1.88	0.55
1:A:78:LYS:O	1:A:79:HIS:CB	2.55	0.55
1:A:230:TYR:HE1	1:A:240:LEU:HD13	1.69	0.55
1:A:85:ARG:HE	1:A:90:ASN:ND2	2.05	0.55
1:B:96:LEU:HD12	1:B:96:LEU:H	1.71	0.55
1:B:216:ILE:HG23	1:B:225:LEU:HD13	1.89	0.55
1:B:275:ASP:C	1:B:277:VAL:H	2.13	0.55
1:A:199:LYS:HA	1:A:237:TYR:CE1	2.42	0.55
1:B:98:ILE:O	1:B:111:PHE:HD1	1.90	0.55
1:A:283:ARG:HG3	1:A:284:LEU:CD1	2.37	0.55
1:B:288:LYS:O	1:B:289:GLU:HB3	2.06	0.55
1:A:115:TRP:C	1:A:117:LYS:H	2.13	0.55
1:A:115:TRP:C	1:A:117:LYS:N	2.65	0.54
1:B:146:ASP:CB	1:B:151:LYS:HB3	2.33	0.54
1:B:158:ALA:C	1:B:160:GLN:N	2.65	0.54
1:B:274:GLN:HG3	1:B:295:LEU:HB3	1.90	0.54
1:A:160:GLN:HA	1:A:163:GLN:HB2	1.89	0.54
1:A:330:THR:O	1:A:331:THR:C	2.50	0.54
1:B:223:ASN:HA	1:B:249:PHE:HE2	1.71	0.54
1:A:275:ASP:C	1:A:277:VAL:N	2.66	0.54
1:B:315:LYS:N	1:B:316:PRO:CD	2.70	0.54
1:A:81:THR:HG23	1:A:94:THR:OG1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:C	1:A:149:ASN:N	2.60	0.54
1:B:160:GLN:HA	1:B:163:GLN:CB	2.37	0.54
1:B:241:PRO:HG3	1:B:271:PHE:CB	2.22	0.54
1:B:3:LEU:C	1:B:3:LEU:HD23	2.32	0.54
1:A:198:ALA:C	1:A:200:GLY:N	2.62	0.54
1:B:38:ARG:HG2	1:B:38:ARG:HH21	1.73	0.54
1:B:260:SER:N	1:B:338:LYS:NZ	2.55	0.54
1:A:299:LYS:C	1:A:301:ARG:H	2.16	0.53
1:B:287:ALA:C	1:B:288:LYS:O	2.49	0.53
1:B:146:ASP:C	1:B:147:LEU:O	2.47	0.53
1:B:163:GLN:O	1:B:163:GLN:HG2	2.08	0.53
1:B:222:VAL:O	1:B:223:ASN:C	2.51	0.53
1:B:336:LEU:HD22	1:B:340:GLN:HE21	1.74	0.53
1:B:119:ALA:O	1:B:141:PHE:CZ	2.62	0.53
1:A:210:TRP:NE1	1:A:286:ILE:HG22	2.24	0.53
1:A:137:LEU:HD13	1:A:137:LEU:C	2.34	0.53
1:A:175:PHE:C	1:A:177:GLY:N	2.65	0.53
1:A:175:PHE:C	1:A:177:GLY:H	2.16	0.53
1:A:180:VAL:O	1:A:181:ASP:CB	2.56	0.53
1:A:256:VAL:HB	1:A:261:PRO:HB3	1.91	0.53
1:A:30:LEU:HD23	1:A:31:ARG:N	2.24	0.53
1:A:84:ALA:O	1:A:90:ASN:HA	2.08	0.53
1:A:259:PHE:HD1	1:A:259:PHE:H	1.54	0.53
1:A:165:ASP:HB3	1:A:168:ARG:HD3	1.90	0.53
1:A:250:ASP:O	1:A:253:SER:HB3	2.08	0.53
1:A:288:LYS:O	1:A:289:GLU:HB3	2.08	0.53
1:B:61:LYS:C	1:B:63:MET:N	2.65	0.53
1:A:160:GLN:O	1:A:168:ARG:NH2	2.41	0.53
1:B:336:LEU:HD22	1:B:340:GLN:CG	2.35	0.53
1:B:199:LYS:CA	1:B:237:TYR:HD1	2.18	0.52
1:B:236:PRO:HG2	1:B:237:TYR:HD2	1.65	0.52
1:A:205:SER:HB3	1:A:208:ARG:HB2	1.91	0.52
1:A:13:THR:HG21	1:A:89:GLU:OE1	2.10	0.52
1:B:314:LEU:HD11	1:B:349:MET:CG	2.30	0.52
1:B:336:LEU:HD13	1:B:340:GLN:NE2	2.25	0.52
1:A:259:PHE:O	1:A:261:PRO:HD2	2.10	0.52
1:A:267:LEU:O	1:A:270:LEU:HD12	2.09	0.52
1:B:179:ILE:C	1:B:180:VAL:HG22	2.34	0.52
1:B:249:PHE:O	1:B:250:ASP:C	2.49	0.52
1:B:41:LEU:HD22	1:B:144:TYR:HE1	1.75	0.52
1:A:78:LYS:O	1:A:79:HIS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ILE:HD11	1:A:249:PHE:CE2	2.44	0.52
1:B:89:GLU:O	1:B:90:ASN:HB2	2.10	0.52
1:B:170:LEU:HD11	1:B:238:ILE:HD11	1.91	0.52
1:B:41:LEU:HD22	1:B:144:TYR:CE1	2.45	0.52
1:B:164:GLU:O	1:B:165:ASP:C	2.52	0.52
1:B:224:HIS:O	1:B:225:LEU:C	2.53	0.52
1:A:156:GLY:O	1:A:157:HIS:HB2	2.10	0.51
1:A:273:VAL:CG1	1:A:274:GLN:N	2.73	0.51
1:B:201:LEU:O	1:B:203:GLY:N	2.44	0.51
1:B:336:LEU:HD22	1:B:340:GLN:NE2	2.26	0.51
1:A:60:MET:O	1:A:63:MET:HB3	2.11	0.51
1:A:210:TRP:CE3	1:A:210:TRP:HA	2.46	0.51
1:B:131:LEU:CD2	1:B:136:THR:O	2.49	0.51
1:B:201:LEU:O	1:B:204:ILE:HD12	2.11	0.51
1:A:209:ILE:HD12	1:A:238:ILE:HD12	1.93	0.51
1:B:278:THR:O	1:B:282:LEU:HG	2.11	0.51
1:B:166:TYR:CE2	1:B:200:GLY:HA3	2.46	0.51
1:A:35:GLY:O	1:A:36:ALA:HB2	2.10	0.50
1:B:165:ASP:C	1:B:167:LEU:N	2.66	0.50
1:B:318:GLN:O	1:B:322:ILE:HG13	2.11	0.50
1:A:222:VAL:O	1:A:223:ASN:C	2.54	0.50
1:B:41:LEU:HD13	1:B:144:TYR:HD1	1.77	0.50
1:B:158:ALA:HB3	1:B:193:ALA:HB1	1.92	0.50
1:A:152:VAL:O	1:A:152:VAL:HG12	2.11	0.50
1:A:273:VAL:O	1:A:276:ASP:CB	2.59	0.50
1:A:344:CYS:SG	1:B:345:LEU:HD23	2.51	0.50
1:B:81:THR:HG23	1:B:94:THR:OG1	2.11	0.50
1:B:85:ARG:NH2	1:B:88:GLU:HB3	2.27	0.50
1:B:238:ILE:CG2	1:B:240:LEU:HG	2.42	0.50
1:A:160:GLN:C	1:A:163:GLN:HB3	2.37	0.50
1:B:272:LYS:HZ1	1:B:302:LYS:CB	2.25	0.50
1:A:79:HIS:O	1:A:81:THR:N	2.45	0.49
1:A:89:GLU:HB3	1:A:91:PHE:CE1	2.47	0.49
1:B:199:LYS:HB2	1:B:237:TYR:HE1	1.77	0.49
1:B:324:SER:O	1:B:325:ARG:C	2.54	0.49
1:A:61:LYS:C	1:A:63:MET:N	2.71	0.49
1:B:11:LEU:O	1:B:13:THR:N	2.43	0.49
1:A:38:ARG:HG2	1:A:38:ARG:HH21	1.78	0.49
1:A:210:TRP:CE2	1:A:286:ILE:HG22	2.48	0.49
1:B:229:ILE:O	1:B:229:ILE:HG22	2.12	0.49
1:A:194:ILE:O	1:A:195:ALA:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:MET:HA	1:B:83:THR:O	2.12	0.49
1:B:175:PHE:O	1:B:176:TYR:C	2.55	0.49
1:B:245:SER:O	1:B:246:LEU:HB2	2.12	0.49
1:A:5:SER:HB2	1:A:6:PRO:HD2	1.95	0.49
1:A:230:TYR:HE2	1:A:243:ASN:HA	1.78	0.49
1:A:3:LEU:O	1:A:4:GLN:CG	2.60	0.49
1:B:201:LEU:O	1:B:204:ILE:CD1	2.60	0.49
1:B:220:ASN:O	1:B:221:HIS:C	2.55	0.49
1:B:301:ARG:O	1:B:302:LYS:C	2.55	0.49
1:A:210:TRP:HA	1:A:210:TRP:HE3	1.78	0.49
1:B:3:LEU:HD13	1:B:131:LEU:HD11	1.93	0.49
1:A:226:ILE:CG1	1:A:249:PHE:CZ	2.86	0.49
1:B:28:HIS:O	1:B:29:GLU:C	2.55	0.49
1:B:124:LEU:O	1:B:125:THR:C	2.55	0.49
1:B:204:ILE:HD12	1:B:204:ILE:O	2.13	0.48
1:B:259:PHE:O	1:B:261:PRO:HD2	2.13	0.48
1:A:273:VAL:HG12	1:A:274:GLN:O	2.13	0.48
1:B:201:LEU:HD12	1:B:234:VAL:HG13	1.95	0.48
1:B:296:PHE:O	1:B:301:ARG:HG2	2.13	0.48
1:B:236:PRO:CG	1:B:237:TYR:CD2	2.89	0.48
1:A:301:ARG:O	1:A:302:LYS:C	2.57	0.48
1:B:56:THR:HB	1:B:57:PRO:HD2	1.95	0.48
1:B:78:LYS:O	1:B:79:HIS:C	2.56	0.48
1:B:300:ASN:C	1:B:301:ARG:HD3	2.39	0.48
1:A:281:ASP:HA	1:A:286:ILE:HG12	1.95	0.48
1:A:176:TYR:CE1	1:A:186:HIS:CE1	3.02	0.48
1:A:198:ALA:C	1:A:200:GLY:H	2.21	0.48
1:B:11:LEU:O	1:B:16:LEU:HD12	2.13	0.48
1:A:20:THR:O	1:A:21:GLU:C	2.54	0.48
1:B:224:HIS:O	1:B:227:HIS:N	2.45	0.48
1:B:36:ALA:HB1	1:B:49:ILE:HG23	1.95	0.48
1:A:297:ILE:O	1:A:302:LYS:HB2	2.14	0.48
1:B:175:PHE:C	1:B:177:GLY:H	2.22	0.48
1:B:201:LEU:C	1:B:203:GLY:H	2.22	0.48
1:B:209:ILE:HG13	1:B:210:TRP:N	2.28	0.48
1:A:156:GLY:O	1:A:157:HIS:CB	2.62	0.48
1:A:288:LYS:C	1:A:290:GLU:N	2.73	0.47
1:B:98:ILE:O	1:B:111:PHE:CD1	2.67	0.47
1:B:11:LEU:HD13	1:B:49:ILE:HD13	1.96	0.47
1:A:283:ARG:HG3	1:A:284:LEU:HD12	1.96	0.47
1:A:287:ALA:HB1	1:A:288:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:O	1:B:164:GLU:N	2.48	0.47
1:B:198:ALA:C	1:B:200:GLY:N	2.61	0.47
1:A:96:LEU:HD12	1:A:96:LEU:N	2.30	0.47
1:A:249:PHE:O	1:A:250:ASP:C	2.58	0.47
1:B:23:PHE:CE2	1:B:30:LEU:HD12	2.49	0.47
1:B:230:TYR:CE1	1:B:235:ALA:HB2	2.50	0.47
1:B:308:THR:HG22	1:B:309:ASP:N	2.29	0.47
1:A:19:LEU:HG	1:A:86:LEU:HD12	1.97	0.47
1:A:204:ILE:O	1:A:205:SER:C	2.58	0.47
1:B:176:TYR:CD1	1:B:180:VAL:HG11	2.50	0.47
1:B:299:LYS:HA	1:B:302:LYS:HB3	1.97	0.47
1:A:95:THR:CG2	1:A:112:THR:HG23	2.43	0.47
1:A:147:LEU:O	1:A:149:ASN:N	2.46	0.47
1:B:204:ILE:O	1:B:205:SER:C	2.58	0.47
1:B:211:VAL:HG12	1:B:211:VAL:O	2.13	0.47
1:A:235:ALA:N	1:A:236:PRO:HD2	2.31	0.46
1:B:162:ILE:HB	1:B:197:ASN:ND2	2.30	0.46
1:A:12:PHE:CD1	1:A:16:LEU:HD13	2.51	0.46
1:A:163:GLN:O	1:A:163:GLN:HG2	2.14	0.46
1:A:230:TYR:HE2	1:A:243:ASN:CA	2.29	0.46
1:B:201:LEU:C	1:B:203:GLY:N	2.71	0.46
1:A:205:SER:HB3	1:A:208:ARG:HB3	1.97	0.46
1:A:295:LEU:N	1:A:295:LEU:HD22	2.30	0.46
1:A:336:LEU:HD22	1:A:340:GLN:NE2	2.31	0.46
1:B:95:THR:HG21	1:B:112:THR:CG2	2.45	0.46
1:B:179:ILE:O	1:B:180:VAL:CG1	2.57	0.46
1:B:267:LEU:O	1:B:268:ALA:C	2.56	0.46
1:A:95:THR:HG22	1:A:96:LEU:N	2.31	0.46
1:A:157:HIS:O	1:A:158:ALA:HB2	2.15	0.46
1:A:293:LEU:O	1:A:297:ILE:HG13	2.16	0.46
1:B:94:THR:HG22	1:B:95:THR:O	2.16	0.46
1:B:275:ASP:C	1:B:277:VAL:N	2.73	0.46
1:A:318:GLN:O	1:A:319:ASP:C	2.57	0.46
1:B:205:SER:CB	1:B:208:ARG:HB2	2.46	0.46
1:A:139:ASP:O	1:A:140:TYR:CB	2.63	0.46
1:A:299:LYS:H	1:A:302:LYS:HB3	1.81	0.46
1:B:288:LYS:O	1:B:290:GLU:N	2.48	0.46
1:A:223:ASN:HA	1:A:249:PHE:HE2	1.81	0.46
1:B:297:ILE:O	1:B:298:VAL:C	2.59	0.46
1:B:298:VAL:C	1:B:300:ASN:H	2.16	0.46
1:B:335:GLU:OE1	1:B:338:LYS:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:CE2	1:A:200:GLY:HA3	2.50	0.46
1:B:335:GLU:OE1	1:B:338:LYS:CE	2.64	0.46
1:A:147:LEU:O	1:A:148:LYS:CB	2.57	0.46
1:B:31:ARG:NH2	1:B:116:GLN:NE2	2.63	0.46
1:B:175:PHE:O	1:B:177:GLY:N	2.49	0.46
1:A:28:HIS:CG	1:A:55:ALA:HB2	2.51	0.45
1:A:299:LYS:H	1:A:302:LYS:CB	2.29	0.45
1:A:30:LEU:C	1:A:30:LEU:CD2	2.88	0.45
1:A:180:VAL:O	1:A:181:ASP:HB2	2.15	0.45
1:A:238:ILE:O	1:A:238:ILE:HG23	2.16	0.45
1:A:275:ASP:H	1:A:277:VAL:HG12	1.81	0.45
1:A:313:PRO:O	1:A:314:LEU:HB3	2.15	0.45
1:B:147:LEU:C	1:B:149:ASN:N	2.72	0.45
1:A:38:ARG:O	1:A:39:ASP:C	2.59	0.45
1:A:179:ILE:O	1:A:179:ILE:HG13	2.15	0.45
1:B:85:ARG:HE	1:B:90:ASN:ND2	2.14	0.45
1:B:165:ASP:C	1:B:167:LEU:H	2.24	0.45
1:B:313:PRO:O	1:B:314:LEU:CB	2.63	0.45
1:A:315:LYS:N	1:A:316:PRO:CD	2.78	0.45
1:A:331:THR:O	1:A:332:ARG:C	2.59	0.45
1:B:186:HIS:NE2	1:B:228:LEU:HD11	2.32	0.45
1:B:248:GLU:O	1:B:249:PHE:C	2.60	0.45
1:B:262:LYS:O	1:B:263:PRO:C	2.60	0.45
1:B:276:ASP:OD2	1:B:276:ASP:C	2.58	0.45
1:B:305:ILE:O	1:B:305:ILE:CG2	2.65	0.45
1:A:165:ASP:HB3	1:A:168:ARG:CD	2.46	0.45
1:A:201:LEU:O	1:A:204:ILE:HD12	2.17	0.45
1:A:207:GLU:O	1:A:211:VAL:HG23	2.15	0.45
1:A:214:LYS:O	1:A:218:VAL:HG23	2.17	0.45
1:A:308:THR:HG22	1:A:309:ASP:N	2.32	0.45
1:B:75:ARG:C	1:B:77:GLU:H	2.25	0.45
1:B:111:PHE:O	1:B:112:THR:C	2.60	0.45
1:A:3:LEU:HD23	1:A:4:GLN:HA	1.99	0.45
1:A:13:THR:OG1	1:A:89:GLU:OE2	2.30	0.45
1:A:96:LEU:HD23	1:A:118:ASP:HB2	1.98	0.45
1:A:274:GLN:C	1:A:276:ASP:H	2.25	0.45
1:B:82:ILE:CG2	1:B:83:THR:N	2.80	0.45
1:A:201:LEU:O	1:A:204:ILE:CD1	2.66	0.45
1:B:156:GLY:O	1:B:157:HIS:O	2.34	0.45
1:A:56:THR:HB	1:A:57:PRO:HD2	1.99	0.44
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:THR:HG21	1:B:89:GLU:OE1	2.16	0.44
1:B:14:GLU:H	1:B:14:GLU:HG2	1.49	0.44
1:B:165:ASP:HB3	1:B:168:ARG:NE	2.33	0.44
1:A:259:PHE:O	1:A:261:PRO:CD	2.66	0.44
1:B:30:LEU:C	1:B:30:LEU:CD2	2.90	0.44
1:B:176:TYR:CE1	1:B:180:VAL:HG11	2.52	0.44
1:A:262:LYS:O	1:A:263:PRO:C	2.61	0.44
1:A:336:LEU:HD13	1:A:340:GLN:HE21	1.81	0.44
1:B:328:ASP:O	1:B:330:THR:N	2.50	0.44
1:A:235:ALA:O	1:A:238:ILE:HG22	2.18	0.44
1:A:243:ASN:HB2	1:A:244:ALA:H	1.28	0.44
1:B:85:ARG:O	1:B:86:LEU:O	2.34	0.44
1:B:123:ASP:O	1:B:155:VAL:HG22	2.18	0.44
1:B:297:ILE:O	1:B:299:LYS:N	2.51	0.44
1:A:201:LEU:C	1:A:203:GLY:N	2.76	0.44
1:B:175:PHE:O	1:B:178:ARG:N	2.50	0.44
1:B:95:THR:CG2	1:B:112:THR:HG23	2.44	0.44
1:B:230:TYR:CE2	1:B:243:ASN:HA	2.53	0.44
1:B:335:GLU:O	1:B:338:LYS:HB2	2.17	0.44
1:A:320:PHE:O	1:A:321:ILE:C	2.60	0.44
1:B:234:VAL:C	1:B:236:PRO:HD2	2.43	0.44
1:B:143:GLY:C	1:B:145:GLU:N	2.75	0.43
1:A:180:VAL:HG23	1:A:181:ASP:H	1.82	0.43
1:A:224:HIS:O	1:A:225:LEU:C	2.62	0.43
1:A:336:LEU:HD22	1:A:340:GLN:HE21	1.82	0.43
1:B:95:THR:HG22	1:B:96:LEU:N	2.33	0.43
1:B:294:GLY:O	1:B:295:LEU:C	2.61	0.43
1:B:328:ASP:O	1:B:331:THR:N	2.51	0.43
1:A:347:LYS:O	1:A:348:GLU:C	2.61	0.43
1:B:26:GLU:OE1	1:B:26:GLU:HA	2.18	0.43
1:B:137:LEU:O	1:B:138:PHE:CB	2.66	0.43
1:B:339:TYR:CD1	1:B:339:TYR:C	2.97	0.43
1:A:19:LEU:CD1	1:A:91:PHE:CD2	2.97	0.43
1:B:72:ILE:O	1:B:73:ASN:C	2.62	0.43
1:B:270:LEU:HD23	1:B:270:LEU:H	1.84	0.43
1:B:295:LEU:HA	1:B:298:VAL:HB	2.00	0.43
1:A:61:LYS:O	1:A:65:GLN:HB2	2.19	0.43
1:B:19:LEU:HD23	1:B:19:LEU:HA	1.90	0.43
1:B:190:THR:O	1:B:194:ILE:HG13	2.19	0.43
1:B:335:GLU:CD	1:B:338:LYS:HD2	2.44	0.43
1:A:3:LEU:O	1:A:4:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LYS:N	1:A:159:LYS:HD2	2.33	0.43
1:A:176:TYR:CD1	1:A:186:HIS:CE1	3.06	0.43
1:A:209:ILE:HD12	1:A:238:ILE:HG13	1.99	0.43
1:A:61:LYS:HA	1:A:71:MET:CE	2.49	0.43
1:A:201:LEU:C	1:A:203:GLY:H	2.27	0.43
1:A:299:LYS:HG2	1:A:302:LYS:HD2	2.00	0.43
1:B:35:GLY:C	1:B:37:VAL:N	2.75	0.43
1:B:96:LEU:HD21	1:B:116:GLN:OE1	2.18	0.43
1:B:256:VAL:O	1:B:257:ASP:C	2.62	0.43
1:A:6:PRO:HG2	1:A:7:GLU:H	1.84	0.43
1:B:7:GLU:O	1:B:10:SER:OG	2.35	0.43
1:B:271:PHE:CE1	1:B:277:VAL:HA	2.54	0.43
1:A:53:THR:O	1:A:95:THR:HA	2.19	0.42
1:A:288:LYS:HD3	1:A:288:LYS:H	1.84	0.42
1:B:5:SER:HB2	1:B:6:PRO:HD2	2.00	0.42
1:B:31:ARG:HH21	1:B:116:GLN:HE22	1.66	0.42
1:B:151:LYS:O	1:B:152:VAL:CB	2.59	0.42
1:B:229:ILE:O	1:B:229:ILE:CG2	2.67	0.42
1:A:169:ILE:CD1	1:A:198:ALA:HA	2.49	0.42
1:A:288:LYS:H	1:A:288:LYS:CD	2.27	0.42
1:A:326:GLU:HA	1:A:327:PRO:HD3	1.85	0.42
1:B:44:VAL:HG23	1:B:44:VAL:O	2.19	0.42
1:A:201:LEU:O	1:A:203:GLY:N	2.52	0.42
1:A:202:ALA:HB2	1:A:237:TYR:HD1	1.84	0.42
1:A:295:LEU:H	1:A:295:LEU:HD13	1.84	0.42
1:B:147:LEU:O	1:B:149:ASN:N	2.46	0.42
1:B:169:ILE:CD1	1:B:198:ALA:HA	2.49	0.42
1:B:298:VAL:C	1:B:300:ASN:N	2.75	0.42
1:B:337:LEU:O	1:B:338:LYS:C	2.61	0.42
1:B:147:LEU:O	1:B:148:LYS:HB3	2.19	0.42
1:A:61:LYS:CA	1:A:71:MET:HE1	2.50	0.42
1:B:225:LEU:O	1:B:229:ILE:HG13	2.19	0.42
1:A:41:LEU:HD22	1:A:144:TYR:HE1	1.85	0.42
1:B:227:HIS:HE1	1:B:250:ASP:OD2	2.03	0.42
1:B:61:LYS:O	1:B:63:MET:N	2.52	0.42
1:B:160:GLN:CA	1:B:163:GLN:HB3	2.47	0.42
1:B:330:THR:O	1:B:331:THR:C	2.61	0.42
1:A:83:THR:HA	1:A:91:PHE:O	2.20	0.42
1:B:36:ALA:CB	1:B:49:ILE:HG23	2.49	0.42
1:B:171:ARG:O	1:B:175:PHE:HD1	2.03	0.42
1:B:176:TYR:O	1:B:180:VAL:HG21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HD21	1:B:46:PRO:CG	2.49	0.42
1:B:176:TYR:O	1:B:180:VAL:CG2	2.68	0.42
1:B:230:TYR:CD1	1:B:235:ALA:HB2	2.54	0.41
1:B:277:VAL:O	1:B:280:LEU:HB3	2.20	0.41
1:A:39:ASP:O	1:A:42:ASN:N	2.53	0.41
1:A:72:ILE:CD1	1:A:90:ASN:ND2	2.82	0.41
1:A:117:LYS:HZ2	1:A:140:TYR:HD2	1.61	0.41
1:A:328:ASP:O	1:A:330:THR:N	2.52	0.41
1:B:138:PHE:N	1:B:138:PHE:CD2	2.87	0.41
1:B:230:TYR:HE2	1:B:243:ASN:HA	1.84	0.41
1:B:259:PHE:H	1:B:259:PHE:HD1	1.66	0.41
1:A:234:VAL:O	1:A:235:ALA:C	2.63	0.41
1:A:259:PHE:HB3	1:A:338:LYS:HZ3	1.85	0.41
1:B:238:ILE:O	1:B:238:ILE:HG23	2.20	0.41
1:A:315:LYS:O	1:A:316:PRO:C	2.63	0.41
1:B:13:THR:C	1:B:15:GLY:H	2.28	0.41
1:B:85:ARG:CD	1:B:88:GLU:HA	2.50	0.41
1:A:335:GLU:CD	1:A:338:LYS:HD2	2.45	0.41
1:B:198:ALA:C	1:B:200:GLY:H	2.27	0.41
1:A:313:PRO:O	1:A:314:LEU:CB	2.69	0.41
1:B:248:GLU:O	1:B:251:LYS:HB2	2.21	0.41
1:B:38:ARG:HG2	1:B:38:ARG:NH2	2.34	0.41
1:B:315:LYS:HA	1:B:318:GLN:HE21	1.85	0.41
1:A:115:TRP:O	1:A:116:GLN:C	2.64	0.41
1:A:147:LEU:HG	1:A:148:LYS:N	2.35	0.41
1:A:228:LEU:HD22	1:A:232:LEU:CD1	2.51	0.41
1:A:344:CYS:C	1:B:344:CYS:SG	3.04	0.41
1:A:33:ALA:HA	1:A:37:VAL:CG2	2.51	0.41
1:B:38:ARG:O	1:B:39:ASP:C	2.64	0.40
1:B:39:ASP:O	1:B:42:ASN:N	2.54	0.40
1:B:115:TRP:C	1:B:117:LYS:N	2.79	0.40
1:B:327:PRO:C	1:B:329:ALA:H	2.29	0.40
1:A:19:LEU:HD11	1:A:93:ILE:HD11	2.02	0.40
1:A:275:ASP:N	1:A:277:VAL:HG12	2.36	0.40
1:A:277:VAL:O	1:A:280:LEU:HB3	2.21	0.40
1:A:300:ASN:C	1:A:301:ARG:HD3	2.46	0.40
1:A:314:LEU:HD11	1:A:349:MET:CG	2.48	0.40
1:B:192:GLU:O	1:B:193:ALA:C	2.64	0.40
1:A:71:MET:HA	1:A:83:THR:O	2.20	0.40
1:A:85:ARG:HG2	1:A:90:ASN:HD21	1.86	0.40
1:A:124:LEU:O	1:A:125:THR:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:O	1:A:265:THR:C	2.62	0.40
1:B:54:THR:HA	1:B:96:LEU:CD1	2.52	0.40
1:B:252:VAL:HG11	1:B:339:TYR:CD2	2.56	0.40
1:A:266:LEU:O	1:A:267:LEU:C	2.64	0.40
1:A:342:GLU:HB3	1:A:345:LEU:HD12	2.04	0.40
1:B:155:VAL:O	1:B:155:VAL:HG23	2.22	0.40
1:B:180:VAL:HG23	1:B:181:ASP:H	1.87	0.40
1:A:38:ARG:HG2	1:A:38:ARG:NH2	2.37	0.40
1:A:205:SER:CB	1:A:208:ARG:HB2	2.51	0.40
1:A:228:LEU:HD22	1:A:232:LEU:HD11	2.04	0.40
1:B:115:TRP:C	1:B:117:LYS:H	2.30	0.40
1:B:205:SER:HB3	1:B:208:ARG:HB2	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:SER:OG	1:B:328:ASP:OD2[4_565]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/448 (76%)	229 (67%)	78 (23%)	35 (10%)	0	3
1	B	342/448 (76%)	227 (66%)	75 (22%)	40 (12%)	0	2
All	All	684/896 (76%)	456 (67%)	153 (22%)	75 (11%)	0	2

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	GLU

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Mol	Chain	Res	Type
1	A	79	HIS
1	A	80	GLY
1	A	86	LEU
1	A	112	THR
1	A	116	GLN
1	A	158	ALA
1	A	165	ASP
1	A	243	ASN
1	A	244	ALA
1	A	245	SER
1	A	298	VAL
1	B	79	HIS
1	B	86	LEU
1	B	112	THR
1	B	157	HIS
1	B	165	ASP
1	B	180	VAL
1	B	205	SER
1	B	221	HIS
1	B	243	ASN
1	B	298	VAL
1	A	36	ALA
1	A	123	ASP
1	A	157	HIS
1	A	163	GLN
1	A	180	VAL
1	A	183	PRO
1	A	205	SER
1	B	74	ASN
1	B	158	ALA
1	B	163	GLN
1	B	275	ASP
1	B	294	GLY
1	A	47	GLN
1	A	75	ARG
1	A	181	ASP
1	A	185	ASP
1	A	306	LYS
1	B	27	ASN
1	B	181	ASP
1	B	202	ALA
1	B	299	LYS

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Mol	Chain	Res	Type
1	B	328	ASP
1	A	88	GLU
1	A	202	ALA
1	A	308	THR
1	B	47	GLN
1	B	62	GLU
1	B	90	ASN
1	B	116	GLN
1	B	302	LYS
1	B	308	THR
1	B	329	ALA
1	A	27	ASN
1	A	90	ASN
1	A	152	VAL
1	A	241	PRO
1	A	299	LYS
1	B	88	GLU
1	B	98	ILE
1	B	138	PHE
1	B	140	TYR
1	B	198	ALA
1	B	249	PHE
1	B	300	ASN
1	A	98	ILE
1	A	249	PHE
1	B	224	HIS
1	B	225	LEU
1	B	233	ASP
1	B	244	ALA
1	B	152	VAL
1	B	312	ASP
1	A	294	GLY

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	304/393 (77%)	266 (88%)	38 (12%)	4	18
1	B	304/393 (77%)	270 (89%)	34 (11%)	6	21
All	All	608/786 (77%)	536 (88%)	72 (12%)	5	20

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	7	GLU
1	A	14	GLU
1	A	16	LEU
1	A	17	LYS
1	A	19	LEU
1	A	29	GLU
1	A	32	ILE
1	A	38	ARG
1	A	48	ASP
1	A	74	ASN
1	A	85	ARG
1	A	88	GLU
1	A	134	ASP
1	A	142	ASN
1	A	160	GLN
1	A	161	ARG
1	A	162	ILE
1	A	178	ARG
1	A	180	VAL
1	A	183	PRO
1	A	204	ILE
1	A	207	GLU
1	A	210	TRP
1	A	218	VAL
1	A	221	HIS
1	A	228	LEU
1	A	243	ASN
1	A	270	LEU
1	A	272	LYS
1	A	275	ASP
1	A	288	LYS
1	A	292	ASN
1	A	295	LEU
1	A	326	GLU

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Mol	Chain	Res	Type
1	A	336	LEU
1	A	346	LEU
1	A	349	MET
1	B	4	GLN
1	B	7	GLU
1	B	14	GLU
1	B	16	LEU
1	B	17	LYS
1	B	19	LEU
1	B	26	GLU
1	B	29	GLU
1	B	32	ILE
1	B	38	ARG
1	B	85	ARG
1	B	88	GLU
1	B	137	LEU
1	B	138	PHE
1	B	142	ASN
1	B	157	HIS
1	B	160	GLN
1	B	161	ARG
1	B	171	ARG
1	B	179	ILE
1	B	180	VAL
1	B	191	LEU
1	B	204	ILE
1	B	207	GLU
1	B	218	VAL
1	B	221	HIS
1	B	228	LEU
1	B	237	TYR
1	B	238	ILE
1	B	272	LYS
1	B	295	LEU
1	B	326	GLU
1	B	336	LEU
1	B	349	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN

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Mol	Chain	Res	Type
1	A	160	GLN
1	A	223	ASN
1	A	227	HIS
1	A	255	ASN
1	A	318	GLN
1	A	340	GLN
1	B	4	GLN
1	B	9	GLN
1	B	42	ASN
1	B	65	GLN
1	B	73	ASN
1	B	90	ASN
1	B	142	ASN
1	B	160	GLN
1	B	163	GLN
1	B	227	HIS
1	B	255	ASN
1	B	292	ASN
1	B	318	GLN
1	B	340	GLN
1	B	343	HIS
1	B	350	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

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	340/448 (75%)	0.27	7 (2%) 63 48	9, 26, 26, 26	56 (16%)
1	B	344/448 (76%)	0.29	12 (3%) 47 34	9, 26, 26, 26	47 (13%)
All	All	684/896 (76%)	0.28	19 (2%) 55 41	9, 26, 26, 26	103 (15%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	TYR	3.5
1	A	308	THR	3.4
1	A	162	ILE	3.4
1	B	162	ILE	3.0
1	B	245	SER	2.7
1	B	221	HIS	2.5
1	A	300	ASN	2.5
1	A	309	ASP	2.4
1	A	81	THR	2.4
1	A	288	LYS	2.4
1	B	98	ILE	2.4
1	B	179	ILE	2.3
1	B	234	VAL	2.3
1	B	260	SER	2.3
1	B	308	THR	2.2
1	B	120	GLU	2.2
1	B	239	GLY	2.2
1	A	181	ASP	2.1
1	B	169	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.