



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:42 PM UTC

PDB ID : 4E85 / pdb_00004e85
Title : crystal STRUCTURE OF HAT DOMAIN OF RNA14
Authors : Paulson, A.R.; Tong, L.
Deposited on : 2012-03-19
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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
Xtrriage (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

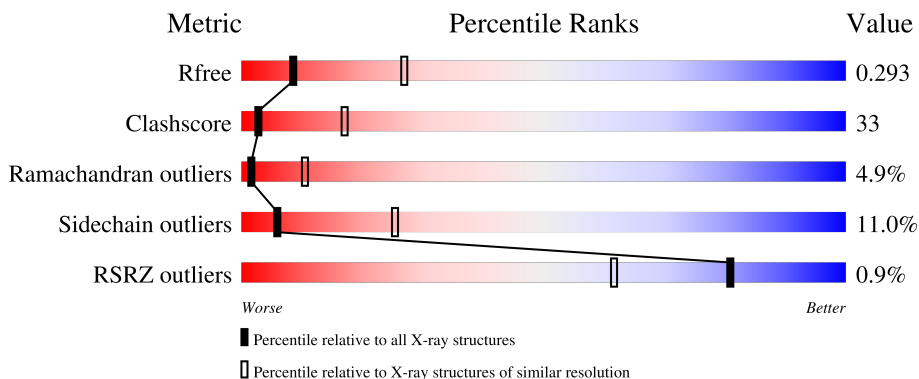
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	678	<div style="display: flex; align-items: center;"> <div style="width: 20px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 34%; height: 100%; background-color: green;"></div> <div style="width: 37%; height: 100%; background-color: yellow;"></div> <div style="width: 11%; height: 100%; background-color: orange;"></div> <div style="width: 18%; height: 100%; background-color: grey;"></div> </div> </div> <p style="margin-top: 5px;">34% 37% 11% 18%</p>
1	B	678	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 34%; height: 100%; background-color: green;"></div> <div style="width: 37%; height: 100%; background-color: yellow;"></div> <div style="width: 9%; height: 100%; background-color: orange;"></div> <div style="width: 19%; height: 100%; background-color: grey;"></div> </div> </div> <p style="margin-top: 5px;">34% 37% 9% 19%</p>

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 9221 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 mRNA 3'-end-processing protein RNA14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	555	4623	2976	765	856	26	0	0	0
1	B	552	4598	2962	760	851	25	0	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	UNP Q6CII8
A	-15	GLY	-	expression tag	UNP Q6CII8
A	-14	SER	-	expression tag	UNP Q6CII8
A	-13	SER	-	expression tag	UNP Q6CII8
A	-12	HIS	-	expression tag	UNP Q6CII8
A	-11	HIS	-	expression tag	UNP Q6CII8
A	-10	HIS	-	expression tag	UNP Q6CII8
A	-9	HIS	-	expression tag	UNP Q6CII8
A	-8	HIS	-	expression tag	UNP Q6CII8
A	-7	HIS	-	expression tag	UNP Q6CII8
A	-6	SER	-	expression tag	UNP Q6CII8
A	-5	SER	-	expression tag	UNP Q6CII8
A	-4	GLY	-	expression tag	UNP Q6CII8
A	-3	LEU	-	expression tag	UNP Q6CII8
A	-2	VAL	-	expression tag	UNP Q6CII8
A	-1	PRO	-	expression tag	UNP Q6CII8
A	0	ARG	-	expression tag	UNP Q6CII8
A	1	GLY	-	expression tag	UNP Q6CII8
A	2	SER	-	expression tag	UNP Q6CII8
A	3	HIS	-	expression tag	UNP Q6CII8
A	4	MET	-	expression tag	UNP Q6CII8
A	5	ALA	-	expression tag	UNP Q6CII8
A	6	SER	-	expression tag	UNP Q6CII8
A	7	MET	-	expression tag	UNP Q6CII8
A	8	THR	-	expression tag	UNP Q6CII8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLY	-	expression tag	UNP Q6CII8
A	10	GLY	-	expression tag	UNP Q6CII8
A	11	GLN	-	expression tag	UNP Q6CII8
A	12	GLN	-	expression tag	UNP Q6CII8
A	13	MET	-	expression tag	UNP Q6CII8
A	14	GLY	-	expression tag	UNP Q6CII8
A	15	ARG	-	expression tag	UNP Q6CII8
A	16	GLY	-	expression tag	UNP Q6CII8
A	17	MET	-	expression tag	UNP Q6CII8
B	-16	MET	-	expression tag	UNP Q6CII8
B	-15	GLY	-	expression tag	UNP Q6CII8
B	-14	SER	-	expression tag	UNP Q6CII8
B	-13	SER	-	expression tag	UNP Q6CII8
B	-12	HIS	-	expression tag	UNP Q6CII8
B	-11	HIS	-	expression tag	UNP Q6CII8
B	-10	HIS	-	expression tag	UNP Q6CII8
B	-9	HIS	-	expression tag	UNP Q6CII8
B	-8	HIS	-	expression tag	UNP Q6CII8
B	-7	HIS	-	expression tag	UNP Q6CII8
B	-6	SER	-	expression tag	UNP Q6CII8
B	-5	SER	-	expression tag	UNP Q6CII8
B	-4	GLY	-	expression tag	UNP Q6CII8
B	-3	LEU	-	expression tag	UNP Q6CII8
B	-2	VAL	-	expression tag	UNP Q6CII8
B	-1	PRO	-	expression tag	UNP Q6CII8
B	0	ARG	-	expression tag	UNP Q6CII8
B	1	GLY	-	expression tag	UNP Q6CII8
B	2	SER	-	expression tag	UNP Q6CII8
B	3	HIS	-	expression tag	UNP Q6CII8
B	4	MET	-	expression tag	UNP Q6CII8
B	5	ALA	-	expression tag	UNP Q6CII8
B	6	SER	-	expression tag	UNP Q6CII8
B	7	MET	-	expression tag	UNP Q6CII8
B	8	THR	-	expression tag	UNP Q6CII8
B	9	GLY	-	expression tag	UNP Q6CII8
B	10	GLY	-	expression tag	UNP Q6CII8
B	11	GLN	-	expression tag	UNP Q6CII8
B	12	GLN	-	expression tag	UNP Q6CII8
B	13	MET	-	expression tag	UNP Q6CII8
B	14	GLY	-	expression tag	UNP Q6CII8
B	15	ARG	-	expression tag	UNP Q6CII8
B	16	GLY	-	expression tag	UNP Q6CII8

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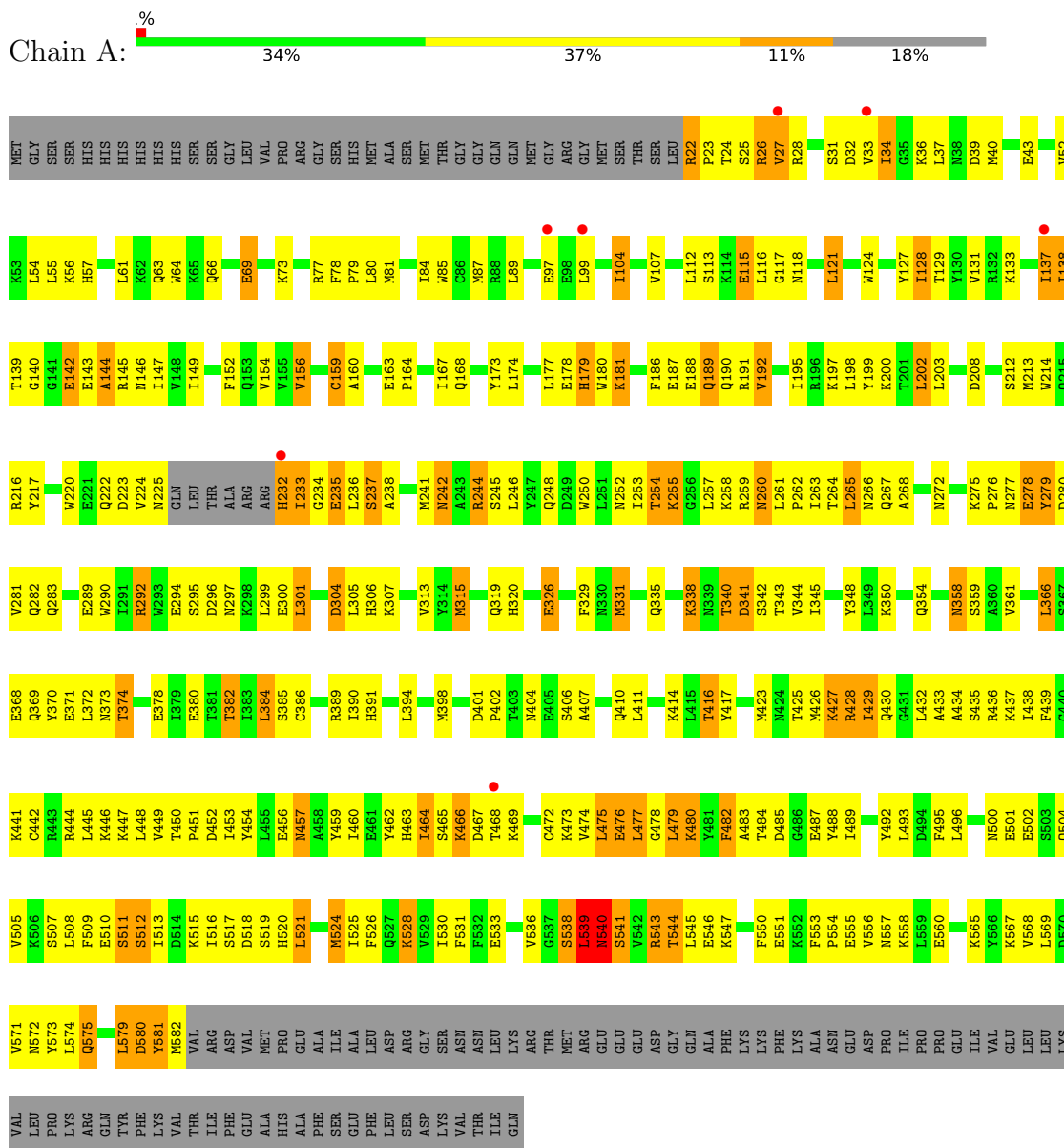
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Chain	Residue	Modelled	Actual	Comment	Reference
B	17	MET	-	expression tag	UNP Q6CII8

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: mRNA 3'-end-processing protein RNA14



- Molecule 1: mRNA 3'-end-processing protein RNA14



MET	L54	Y197	T203	M266	K356	K437	I516	VAL	THR
GLY	L55	I128	L202	Q267	I357	K446	S517	ARG	ILE
SER	R56	T129	L203	A268	P357	K447	D518	ASP	PHE
HIS	L61	K133	M207	L273	S359	L448	S519	VAL	GLU
HIS	K62	I137	D208	P274	S366	V449	H520	ALA	HIS
HIS	Q63	I138	C209	K275	S367	T450	L521	ALA	ALA
HIS	R64	I139	S212	P276	E368	P451	L522	ALA	PHE
HIS	R65	T139	S213	E278	E369	D452	K523	ALA	PHE
HIS	Q66	G140	W214	Y279	Q370	E456	I525	LEU	GLU
SER	V67	G141	Q215	D280	E371	E460	F526	LEU	PHE
SER	Y68	E142	Q216	W281	E372	I460	Q527	ASP	LEU
GLY	E69	E143	Y217	Q282	N373	E461	K528	ARG	SER
LEU	T70	A144	W220	Q283	K375	H462	V529	ASP	ASP
VAL	F71	R145	E221	L288	E378	H463	I530	SER	LYS
PRO	R73	M146	Q222	E289	E379	I464	F531	ASN	VAL
ARG	K74	F152	D223	W290	I379	K466	F532	ASN	THR
GLY	L74	Q153	W224	W291	E380	D467	E533	LEU	ILE
SER	R77	V154	M225	E292	E381	T468	S538	LEU	GLN
HIS	F78	V155	M226	Q226	T382	A471	L539	THR	
MET	P79	V156	Q227	R292	I383	C472	S540	THR	
ALA	L80	C159	L228	W293	L384	L475	S541	ARG	
SER	M81	A160	T228	W296	S385	L476	V542	ARG	
MET		I161	A229	D296	C386	E476	F543	GLU	
THR		R162	R230	W297	E386	F477	T544	GLU	
GLY		F162	R231	K298	I390	G478	L545	GLU	
GLY		E163	H232	L299	T390	L479	L546	ASP	
GLN		P164	Q233	L300	H391	K480	K547	ASP	
GLN		K165	G234	E301	E391	F481	F550	GLY	
MET		S166	E235	L301	L394	K482	S551	GLY	
GLY		L167	L236	R304	L397	F483	K552	PHE	
ARG		Q168	S237	K307	M398	A483	R553	LYS	
GLY		F169	Q239	R309	E399	T484	F554	LYS	
SER		L173	Y240	D400	D401	I489	E555	ALA	
LEU		Y103	W241	V313	M404	Y492	K558	ASN	
ARG		I104	N242	Y314	E405	L493	L559	GLU	
PRO		E105	A243	Q319	S406	D494	L560	ASP	
THR		P106	R244	S245	S406	F495	T563	PRO	
SER		V107	L246	H320	Q410	L496	N564	ILE	
ARG		L108	D249	A324	L411	N500	K565	PRO	
VAL		C111	W250	F326	K412	E501	Y566	GLU	
ARG		L112	L251	E326	T416	E502	K567	ILE	
ASP		S113	M252	I327	Y417	S503	V568	VAL	
E30		K114	L253	W328	Y417	Q504	L569	GLU	
S31		E115	T254	E337	M426	V505	D570	LEU	
D32		G117	G256	K338	K427	S507	V571	LEU	
K36		M118	L257	R339	R428	L574	N572	LYS	
L37		N119	G256	N339	S507	L575	Y573	VAL	
M38		D120	R259	T340	L508	Q575	V574	LEU	
D39		Y194	R259	F509	L508	R576	L574	LEU	
M40		L121	N260	Q430	F509	E510	Q575	PRO	
F49		S122	L263	G431	G431	E511	L577	ARG	
L50		L123	P262	L432	L432	S511	E578	ARG	
Y51		M124	L263	A433	A433	S512	L579	GLN	
S126		L125	T264	A434	A434	I513	D580	TYR	
		K200	T264	S435	S435	I513	L581	PHE	
			L349	R436	R436	K515	MET	LYS	
								VAL	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.87Å 241.73Å 49.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.77 – 3.00 46.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.8 (46.77-3.00) 87.8 (46.77-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.01Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.233 , 0.293 0.233 , 0.293	Depositor DCC
R_{free} test set	1280 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtrriage
Anisotropy	0.474	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9221	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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

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	0.82	2/4724 (0.0%)	1.17	31/6385 (0.5%)
1	B	0.82	0/4699	1.15	32/6353 (0.5%)
All	All	0.82	2/9423 (0.0%)	1.16	63/12738 (0.5%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	MET	SD-CE	6.22	1.95	1.79
1	A	27	VAL	CA-CB	5.59	1.62	1.54

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ILE	N-CA-C	10.36	121.24	110.36
1	B	186	PHE	N-CA-C	-8.85	102.39	113.01
1	B	104	ILE	N-CA-C	8.49	118.54	110.30
1	A	186	PHE	N-CA-C	-8.27	103.18	113.18
1	B	540	ASN	N-CA-C	-8.17	103.45	113.50
1	B	292	ARG	N-CA-C	-7.69	102.49	111.03
1	B	85	TRP	N-CA-C	-7.59	103.02	111.82
1	A	85	TRP	N-CA-C	-7.47	103.22	111.36
1	A	567	LYS	N-CA-C	-7.44	99.47	110.48
1	B	193	GLN	N-CA-C	-7.42	103.28	111.36
1	A	540	ASN	N-CA-C	-7.23	104.61	113.50
1	A	320	HIS	N-CA-C	7.22	121.92	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	430	GLN	N-CA-C	7.02	119.86	110.88
1	A	344	VAL	N-CA-C	6.93	117.44	110.23
1	B	446	LYS	CB-CA-C	-6.92	107.82	117.23
1	B	541	SER	N-CA-C	-6.92	102.96	111.40
1	A	69	GLU	N-CA-C	-6.55	104.07	111.14
1	A	331	MET	N-CA-C	-6.53	104.16	111.28
1	B	89	LEU	N-CA-C	-6.35	104.28	111.14
1	A	512	SER	N-CA-C	6.34	120.65	112.41
1	B	31	SER	N-CA-C	6.26	118.43	110.61
1	B	229	ALA	N-CA-C	-6.22	103.80	112.45
1	A	442	CYS	N-CA-C	-6.22	104.58	111.36
1	A	22	ARG	CA-C-N	-6.17	112.13	119.84
1	A	22	ARG	C-N-CA	-6.17	112.13	119.84
1	B	477	LEU	N-CA-C	-6.17	104.25	110.97
1	B	61	LEU	N-CA-C	-5.96	105.32	113.30
1	B	275	LYS	N-CA-C	-5.92	101.59	110.24
1	A	27	VAL	N-CA-C	-5.88	97.10	109.34
1	A	410	GLN	N-CA-C	-5.87	104.79	111.07
1	B	545	LEU	N-CA-C	-5.70	104.27	111.11
1	B	249	ASP	N-CA-C	-5.69	105.00	111.14
1	B	375	LYS	N-CA-C	-5.68	99.11	108.49
1	B	126	SER	N-CA-C	-5.64	104.52	111.40
1	A	73	LYS	N-CA-C	-5.60	105.18	111.28
1	B	410	GLN	N-CA-C	-5.58	105.20	111.28
1	B	246	LEU	N-CA-C	-5.56	105.37	111.82
1	B	304	ASP	N-CA-C	-5.56	106.63	113.41
1	A	460	ILE	N-CA-C	-5.56	107.03	111.81
1	A	64	TRP	N-CA-C	5.55	118.86	111.75
1	B	554	PRO	N-CA-C	-5.52	103.43	111.33
1	A	541	SER	N-CA-C	-5.52	104.67	111.40
1	B	277	ASN	N-CA-C	5.47	119.78	113.38
1	A	575	GLN	N-CA-C	5.46	118.40	111.69
1	A	581	TYR	N-CA-C	-5.44	106.01	113.30
1	A	459	TYR	N-CA-C	5.42	119.38	112.34
1	B	227	LEU	N-CA-C	-5.38	106.56	113.23
1	A	457	ASN	N-CA-C	-5.27	104.97	111.40
1	B	240	TYR	N-CA-C	-5.25	105.45	111.07
1	B	214	TRP	N-CA-C	-5.24	104.49	112.04
1	B	207	MET	N-CA-C	5.22	117.00	109.07
1	B	482	PHE	N-CA-C	5.22	117.56	110.88
1	A	163	GLU	CA-C-N	-5.18	113.30	119.05
1	A	163	GLU	C-N-CA	-5.18	113.30	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	530	ILE	N-CA-C	-5.16	105.68	110.53
1	A	260	ASN	N-CA-C	5.15	119.13	111.87
1	A	159	CYS	N-CA-C	5.10	121.66	110.80
1	A	246	LEU	N-CA-C	-5.08	106.18	112.38
1	B	359	SER	N-CA-C	5.08	116.59	108.41
1	A	476	GLU	N-CA-C	-5.07	105.65	111.07
1	A	482	PHE	N-CA-C	5.06	118.53	111.30
1	B	320	HIS	N-CA-C	5.01	119.44	113.23
1	B	349	LEU	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	348	TYR	Sidechain

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	4623	0	4620	311	0
1	B	4598	0	4598	312	0
All	All	9221	0	9218	608	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 33.

All (608) 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:200:LYS:HD3	1:B:236:LEU:HD21	1.27	1.14
1:B:61:LEU:HD12	1:B:63:GLN:NE2	1.70	1.06
1:B:264:THR:HB	1:B:267:GLN:HG3	1.43	1.00
1:B:533:GLU:HG3	1:B:545:LEU:HD11	1.40	0.98
1:B:244:ARG:HH11	1:B:244:ARG:HB3	1.27	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:LEU:HD12	1:A:475:LEU:H	1.25	0.97
1:A:428:ARG:HH11	1:A:428:ARG:HG2	1.26	0.97
1:A:264:THR:HB	1:A:267:GLN:HG3	1.43	0.96
1:B:475:LEU:HD12	1:B:475:LEU:H	1.31	0.94
1:A:307:LYS:HD3	1:A:338:LYS:HD2	1.50	0.94
1:A:546:GLU:O	1:A:550:PHE:HD1	1.51	0.92
1:A:341:ASP:OD2	1:A:343:THR:HG22	1.72	0.89
1:A:61:LEU:HD12	1:A:63:GLN:NE2	1.88	0.89
1:B:61:LEU:HD12	1:B:63:GLN:HE21	1.34	0.88
1:B:307:LYS:HD3	1:B:338:LYS:HD2	1.54	0.88
1:B:115:GLU:H	1:B:115:GLU:CD	1.82	0.88
1:B:81:MET:HE1	1:B:319:GLN:HA	1.57	0.85
1:A:480:LYS:HA	1:A:480:LYS:HE2	1.59	0.84
1:B:299:LEU:HB3	1:B:301:LEU:HD21	1.61	0.83
1:A:115:GLU:HG2	1:A:116:LEU:H	1.45	0.82
1:A:428:ARG:HH11	1:A:428:ARG:CG	1.92	0.82
1:A:191:ARG:O	1:A:195:ILE:HG13	1.80	0.81
1:B:137:ILE:HD12	1:B:138:ILE:HG13	1.63	0.81
1:B:386:CYS:O	1:B:390:ILE:HG13	1.80	0.81
1:B:231:ARG:HD2	1:B:231:ARG:O	1.81	0.80
1:B:341:ASP:OD2	1:B:343:THR:HG22	1.80	0.80
1:A:386:CYS:O	1:A:390:ILE:HG13	1.81	0.80
1:A:202:LEU:HD21	1:A:213:MET:HG2	1.62	0.79
1:B:546:GLU:O	1:B:550:PHE:HD1	1.63	0.79
1:A:81:MET:HE1	1:A:319:GLN:HA	1.64	0.79
1:B:480:LYS:HE2	1:B:480:LYS:HA	1.62	0.79
1:A:61:LEU:HD12	1:A:63:GLN:HE21	1.46	0.79
1:A:560:GLU:HA	1:A:582:MET:CE	2.13	0.79
1:A:378:GLU:O	1:A:382:THR:HG22	1.83	0.78
1:B:307:LYS:NZ	1:B:338:LYS:HG3	1.98	0.78
1:B:258:LYS:H	1:B:283:GLN:HE22	1.30	0.77
1:A:538:SER:C	1:A:540:ASN:H	1.92	0.77
1:A:26:ARG:HH11	1:A:26:ARG:HG2	1.51	0.76
1:A:99:LEU:CD1	1:A:133:LYS:HD3	2.15	0.76
1:A:520:HIS:HE1	1:A:524:MET:HE3	1.51	0.76
1:A:427:LYS:HB2	1:A:435:SER:OG	1.87	0.75
1:B:230:ARG:HB3	1:B:230:ARG:NH1	2.01	0.75
1:B:254:THR:O	1:B:256:GLY:N	2.19	0.75
1:A:550:PHE:CE2	1:A:558:LYS:HD3	2.22	0.75
1:A:237:SER:O	1:A:241:MET:HG2	1.86	0.75
1:B:80:LEU:HA	1:B:118:ASN:HD21	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LYS:HD3	1:A:236:LEU:HD21	1.68	0.75
1:B:394:LEU:HG	1:B:398:MET:HE3	1.69	0.74
1:A:258:LYS:H	1:A:283:GLN:HE22	1.36	0.74
1:A:536:VAL:HG12	1:A:536:VAL:O	1.87	0.74
1:A:423:MET:HA	1:A:438:ILE:HD12	1.69	0.73
1:B:231:ARG:HG3	1:B:232:HIS:HD2	1.54	0.73
1:A:358:ASN:C	1:A:358:ASN:HD22	1.96	0.72
1:B:128:ILE:HD11	1:B:152:PHE:HA	1.70	0.72
1:B:224:VAL:O	1:B:225:ASN:HB2	1.87	0.72
1:B:538:SER:C	1:B:540:ASN:H	1.98	0.72
1:B:230:ARG:HB3	1:B:230:ARG:HH11	1.53	0.72
1:B:238:ALA:HB3	1:B:239:GLN:NE2	2.04	0.72
1:B:227:LEU:HD23	1:B:228:THR:HG23	1.71	0.72
1:B:533:GLU:HG3	1:B:545:LEU:CD1	2.19	0.72
1:B:358:ASN:C	1:B:358:ASN:HD22	1.98	0.71
1:B:278:GLU:O	1:B:279:TYR:HB3	1.88	0.71
1:A:140:GLY:HA3	1:A:144:ALA:HB2	1.72	0.71
1:B:115:GLU:HG2	1:B:116:LEU:H	1.55	0.70
1:A:394:LEU:HG	1:A:398:MET:HE3	1.73	0.70
1:B:299:LEU:HB3	1:B:301:LEU:CD2	2.22	0.70
1:A:520:HIS:CE1	1:A:524:MET:HE3	2.26	0.70
1:A:546:GLU:O	1:A:550:PHE:CD1	2.40	0.70
1:B:426:MET:HE2	1:B:426:MET:HA	1.73	0.70
1:A:394:LEU:CG	1:A:398:MET:HE3	2.21	0.69
1:B:511:SER:O	1:B:515:LYS:HE2	1.92	0.69
1:A:99:LEU:HD11	1:A:133:LYS:HD3	1.74	0.69
1:B:167:ILE:HG23	1:B:168:GLN:N	2.08	0.69
1:B:520:HIS:CE1	1:B:524:MET:HE3	2.27	0.69
1:A:167:ILE:HG23	1:A:168:GLN:N	2.08	0.69
1:A:292:ARG:HH11	1:A:292:ARG:HB3	1.56	0.69
1:A:501:GLU:O	1:A:504:GLN:HB2	1.92	0.69
1:A:380:GLU:O	1:A:384:LEU:HB2	1.93	0.69
1:A:342:SER:HB2	1:A:373:ASN:OD1	1.92	0.69
1:A:569:LEU:HD12	1:B:452:ASP:OD2	1.93	0.68
1:A:214:TRP:CH2	1:A:233:ILE:HG23	2.29	0.68
1:B:202:LEU:HD21	1:B:213:MET:HG2	1.74	0.68
1:A:462:TYR:O	1:A:464:ILE:N	2.26	0.68
1:B:428:ARG:HG2	1:B:428:ARG:HH11	1.58	0.68
1:B:378:GLU:O	1:B:382:THR:HG22	1.94	0.68
1:A:468:THR:HG22	1:A:468:THR:O	1.94	0.68
1:B:521:LEU:O	1:B:525:ILE:HG13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:HIS:HE1	1:B:524:MET:HE3	1.58	0.67
1:A:350:LYS:NZ	1:A:354:GLN:HE21	1.92	0.67
1:B:244:ARG:HB3	1:B:244:ARG:NH1	2.06	0.67
1:A:115:GLU:CD	1:A:115:GLU:H	2.03	0.67
1:B:533:GLU:CG	1:B:545:LEU:HD11	2.22	0.66
1:A:78:PHE:HB3	1:A:81:MET:HG2	1.77	0.66
1:B:156:VAL:HA	1:B:160:ALA:HB3	1.77	0.66
1:A:371:GLU:OE1	1:B:539:LEU:HD22	1.94	0.66
1:B:99:LEU:HD11	1:B:133:LYS:HD3	1.77	0.66
1:B:290:TRP:HD1	1:B:290:TRP:O	1.79	0.66
1:A:36:LYS:O	1:A:40:MET:HG3	1.96	0.66
1:B:237:SER:O	1:B:241:MET:HG2	1.96	0.66
1:A:278:GLU:O	1:A:279:TYR:HB3	1.96	0.66
1:A:282:GLN:HE21	1:A:282:GLN:HA	1.60	0.65
1:A:428:ARG:CG	1:A:428:ARG:NH1	2.57	0.65
1:A:560:GLU:HA	1:A:582:MET:HE1	1.77	0.65
1:A:398:MET:O	1:A:402:PRO:HB3	1.97	0.65
1:A:22:ARG:HA	1:A:22:ARG:NE	2.12	0.64
1:B:78:PHE:HB3	1:B:81:MET:HG2	1.79	0.64
1:A:178:GLU:C	1:A:180:TRP:H	2.05	0.64
1:B:138:ILE:HG22	1:B:139:THR:N	2.13	0.63
1:B:307:LYS:HZ1	1:B:338:LYS:HG3	1.62	0.63
1:A:560:GLU:HA	1:A:582:MET:HE3	1.80	0.63
1:B:554:PRO:O	1:B:555:GLU:HB3	1.97	0.63
1:A:299:LEU:HB3	1:A:301:LEU:HD21	1.81	0.63
1:B:543:ARG:HA	1:B:543:ARG:HH11	1.63	0.63
1:B:546:GLU:O	1:B:550:PHE:CD1	2.50	0.63
1:A:477:LEU:O	1:A:480:LYS:HB2	1.99	0.62
1:B:61:LEU:HD12	1:B:63:GLN:HE22	1.62	0.62
1:B:99:LEU:CD1	1:B:133:LYS:HD3	2.29	0.62
1:A:456:GLU:CG	1:B:568:VAL:HG13	2.29	0.62
1:A:480:LYS:HA	1:A:480:LYS:CE	2.29	0.62
1:B:145:ARG:HG2	1:B:145:ARG:O	1.98	0.62
1:A:80:LEU:HA	1:A:118:ASN:HD21	1.64	0.62
1:A:178:GLU:O	1:A:180:TRP:N	2.32	0.62
1:A:137:ILE:HD12	1:A:138:ILE:HG13	1.82	0.62
1:A:275:LYS:O	1:A:278:GLU:HB2	2.00	0.62
1:B:36:LYS:O	1:B:40:MET:HG3	1.99	0.62
1:A:394:LEU:CD1	1:A:398:MET:HE3	2.29	0.62
1:B:37:LEU:HD23	1:B:54:LEU:HA	1.82	0.61
1:B:366:LEU:HD22	1:B:370:TYR:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:HIS:HA	1:A:235:GLU:OE1	1.99	0.61
1:A:472:CYS:O	1:A:476:GLU:HG3	2.00	0.61
1:A:489:ILE:HD12	1:A:508:LEU:HD11	1.81	0.61
1:B:162:PHE:CD2	1:B:309:ARG:HG3	2.36	0.61
1:A:465:SER:O	1:A:467:ASP:N	2.34	0.60
1:A:543:ARG:HH11	1:A:543:ARG:HA	1.66	0.60
1:B:142:GLU:HG3	1:B:143:GLU:N	2.15	0.60
1:B:394:LEU:CG	1:B:398:MET:HE3	2.30	0.60
1:A:394:LEU:HD11	1:A:398:MET:HE3	1.82	0.60
1:B:264:THR:HG22	1:B:266:ASN:H	1.66	0.60
1:A:282:GLN:HA	1:A:282:GLN:NE2	2.16	0.60
1:B:61:LEU:CD1	1:B:63:GLN:HE21	2.10	0.60
1:B:290:TRP:O	1:B:290:TRP:CD1	2.54	0.60
1:A:167:ILE:HB	1:A:208:ASP:OD1	2.02	0.60
1:A:202:LEU:C	1:A:202:LEU:HD12	2.27	0.60
1:B:559:LEU:HD21	1:B:579:LEU:HD11	1.84	0.60
1:B:275:LYS:O	1:B:278:GLU:HB2	2.01	0.59
1:A:254:THR:HG23	1:A:257:LEU:HB2	1.84	0.59
1:A:368:GLU:O	1:A:372:LEU:HD13	2.01	0.59
1:B:538:SER:O	1:B:540:ASN:N	2.35	0.59
1:B:178:GLU:C	1:B:180:TRP:H	2.10	0.59
1:A:23:PRO:O	1:A:25:SER:N	2.34	0.59
1:B:37:LEU:HD12	1:B:40:MET:HE3	1.82	0.59
1:A:173:TYR:CE2	1:A:198:LEU:HD13	2.38	0.59
1:A:427:LYS:HE2	1:A:427:LYS:O	2.02	0.59
1:B:254:THR:HG23	1:B:257:LEU:HB2	1.84	0.59
1:B:140:GLY:HA3	1:B:144:ALA:HB2	1.85	0.59
1:B:528:LYS:HB2	1:B:528:LYS:NZ	2.17	0.59
1:B:37:LEU:HD23	1:B:54:LEU:CA	2.33	0.59
1:B:167:ILE:HB	1:B:208:ASP:OD1	2.02	0.59
1:A:479:LEU:CD1	1:A:483:ALA:HA	2.33	0.58
1:B:401:ASP:OD2	1:B:404:ASN:HB2	2.02	0.58
1:A:138:ILE:HG22	1:A:139:THR:N	2.19	0.58
1:A:189:GLN:HE21	1:A:190:GLN:N	2.01	0.58
1:A:280:ASP:OD1	1:A:282:GLN:HB3	2.04	0.58
1:B:65:LYS:O	1:B:69:GLU:HG3	2.03	0.58
1:A:224:VAL:O	1:A:225:ASN:HB2	2.02	0.58
1:A:533:GLU:HG3	1:A:545:LEU:HD11	1.86	0.58
1:B:538:SER:HB2	1:B:541:SER:OG	2.04	0.58
1:A:429:ILE:HG22	1:A:430:GLN:HG3	1.84	0.57
1:B:232:HIS:O	1:B:234:GLY:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:O	1:A:238:ALA:N	2.37	0.57
1:B:202:LEU:HD12	1:B:202:LEU:C	2.29	0.57
1:B:264:THR:HB	1:B:267:GLN:CG	2.24	0.57
1:A:518:ASP:CG	1:A:519:SER:H	2.12	0.57
1:A:531:PHE:CD1	1:A:531:PHE:C	2.82	0.57
1:B:191:ARG:O	1:B:195:ILE:HG13	2.04	0.57
1:B:199:TYR:CD1	1:B:217:TYR:HB2	2.40	0.57
1:A:429:ILE:CG2	1:A:430:GLN:HG3	2.34	0.57
1:A:538:SER:O	1:A:540:ASN:N	2.37	0.57
1:A:417:TYR:CD1	1:B:573:TYR:HB2	2.38	0.57
1:B:55:LEU:HD21	1:B:70:THR:HB	1.87	0.57
1:A:26:ARG:HG2	1:A:26:ARG:NH1	2.16	0.57
1:B:292:ARG:HH11	1:B:292:ARG:HB3	1.70	0.57
1:A:361:VAL:HG21	1:B:579:LEU:HD21	1.86	0.57
1:A:433:ALA:O	1:A:437:LYS:HG3	2.04	0.57
1:A:475:LEU:HD12	1:A:475:LEU:N	2.07	0.57
1:A:401:ASP:O	1:A:401:ASP:CG	2.47	0.57
1:A:520:HIS:HE1	1:A:524:MET:CE	2.18	0.57
1:A:142:GLU:HG3	1:A:143:GLU:N	2.20	0.57
1:B:531:PHE:CD1	1:B:531:PHE:C	2.83	0.57
1:B:432:LEU:C	1:B:432:LEU:HD23	2.30	0.56
1:A:143:GLU:HA	1:A:146:ASN:HB3	1.86	0.56
1:B:299:LEU:CB	1:B:301:LEU:HD21	2.34	0.56
1:A:521:LEU:O	1:A:525:ILE:HG13	2.05	0.56
1:B:559:LEU:HD21	1:B:579:LEU:CD1	2.35	0.56
1:A:482:PHE:HB2	1:A:488:TYR:CD2	2.40	0.56
1:B:30:GLU:N	1:B:36:LYS:HZ1	2.02	0.56
1:B:489:ILE:HD12	1:B:508:LEU:HD11	1.85	0.56
1:A:479:LEU:HD12	1:A:483:ALA:HA	1.88	0.56
1:A:432:LEU:HD23	1:A:436:ARG:HD3	1.88	0.56
1:B:220:TRP:O	1:B:224:VAL:HG23	2.06	0.56
1:A:167:ILE:HG23	1:A:168:GLN:H	1.70	0.55
1:A:579:LEU:C	1:A:581:TYR:H	2.12	0.55
1:B:450:THR:HG23	1:B:452:ASP:H	1.72	0.55
1:A:224:VAL:O	1:A:224:VAL:HG12	2.07	0.55
1:B:61:LEU:CD1	1:B:63:GLN:NE2	2.56	0.55
1:A:307:LYS:NZ	1:A:338:LYS:HG3	2.21	0.55
1:A:539:LEU:HD22	1:B:371:GLU:OE1	2.06	0.55
1:A:189:GLN:NE2	1:A:189:GLN:C	2.65	0.55
1:A:259:ARG:C	1:A:260:ASN:HD22	2.13	0.55
1:B:178:GLU:O	1:B:180:TRP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:TRP:CD1	1:B:290:TRP:C	2.84	0.55
1:B:520:HIS:HE1	1:B:524:MET:CE	2.19	0.55
1:A:78:PHE:HB3	1:A:81:MET:CG	2.37	0.54
1:A:299:LEU:CB	1:A:301:LEU:HD21	2.37	0.54
1:A:489:ILE:HG21	1:A:516:ILE:HD11	1.88	0.54
1:A:66:GLN:HA	1:A:69:GLU:HG3	1.90	0.54
1:A:232:HIS:O	1:A:234:GLY:N	2.40	0.54
1:A:26:ARG:O	1:A:28:ARG:N	2.40	0.54
1:B:230:ARG:HH11	1:B:230:ARG:CB	2.20	0.54
1:A:456:GLU:HG3	1:B:568:VAL:HG13	1.89	0.54
1:A:181:LYS:NZ	1:A:181:LYS:H	2.06	0.54
1:B:173:TYR:CE2	1:B:198:LEU:HD13	2.43	0.54
1:B:493:LEU:O	1:B:494:ASP:C	2.50	0.54
1:A:345:ILE:HB	1:A:369:GLN:OE1	2.08	0.54
1:B:291:ILE:HD13	1:B:314:TYR:CE1	2.42	0.54
1:B:463:HIS:HD2	1:B:466:LYS:HE2	1.72	0.54
1:B:468:THR:O	1:B:472:CYS:HB2	2.08	0.54
1:A:489:ILE:HG13	1:A:516:ILE:HD11	1.90	0.53
1:B:428:ARG:HG2	1:B:428:ARG:NH1	2.23	0.53
1:A:99:LEU:HD13	1:A:133:LYS:HD3	1.89	0.53
1:A:371:GLU:CD	1:B:539:LEU:HD22	2.33	0.53
1:A:538:SER:HB2	1:A:541:SER:OG	2.08	0.53
1:A:568:VAL:O	1:A:569:LEU:HB2	2.08	0.53
1:B:342:SER:HB2	1:B:373:ASN:OD1	2.08	0.53
1:A:531:PHE:CD1	1:A:531:PHE:O	2.61	0.53
1:A:199:TYR:CD1	1:A:217:TYR:HB2	2.43	0.53
1:B:292:ARG:O	1:B:293:TRP:C	2.50	0.53
1:B:551:GLU:O	1:B:554:PRO:HD3	2.09	0.53
1:A:245:SER:O	1:A:248:GLN:HB2	2.09	0.53
1:A:432:LEU:CD2	1:A:436:ARG:HD3	2.39	0.53
1:A:511:SER:O	1:A:515:LYS:HE2	2.09	0.53
1:B:202:LEU:HD12	1:B:203:LEU:N	2.24	0.53
1:A:220:TRP:O	1:A:224:VAL:HG23	2.09	0.52
1:B:304:ASP:N	1:B:304:ASP:OD2	2.42	0.52
1:A:140:GLY:CA	1:A:144:ALA:HB2	2.40	0.52
1:A:254:THR:HG23	1:A:257:LEU:CB	2.39	0.52
1:A:232:HIS:CD2	1:A:232:HIS:N	2.77	0.52
1:A:299:LEU:O	1:A:300:GLU:HB2	2.09	0.52
1:A:340:THR:O	1:A:341:ASP:HB3	2.09	0.52
1:A:307:LYS:HE3	1:A:335:GLN:HE22	1.74	0.52
1:B:238:ALA:HB3	1:B:239:GLN:HE21	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:PHE:O	1:B:513:ILE:HG13	2.09	0.52
1:B:538:SER:C	1:B:540:ASN:N	2.66	0.52
1:B:137:ILE:CD1	1:B:138:ILE:HG13	2.37	0.52
1:B:225:ASN:C	1:B:227:LEU:H	2.18	0.52
1:B:468:THR:O	1:B:468:THR:HG22	2.10	0.52
1:A:156:VAL:HA	1:A:160:ALA:HB3	1.92	0.52
1:A:264:THR:HG22	1:A:265:LEU:N	2.24	0.52
1:B:518:ASP:CG	1:B:519:SER:H	2.17	0.52
1:A:462:TYR:C	1:A:464:ILE:H	2.17	0.52
1:B:433:ALA:O	1:B:437:LYS:HG3	2.10	0.52
1:A:372:LEU:C	1:A:374:THR:H	2.17	0.51
1:B:37:LEU:HD23	1:B:54:LEU:HB2	1.92	0.51
1:B:222:GLN:C	1:B:224:VAL:H	2.18	0.51
1:B:231:ARG:HG3	1:B:232:HIS:CD2	2.39	0.51
1:B:115:GLU:CD	1:B:115:GLU:N	2.60	0.51
1:A:307:LYS:HE3	1:A:335:GLN:NE2	2.26	0.51
1:A:553:PHE:C	1:A:554:PRO:O	2.50	0.51
1:B:543:ARG:HA	1:B:543:ARG:NH1	2.25	0.51
1:B:167:ILE:CG2	1:B:168:GLN:N	2.72	0.51
1:A:192:VAL:HG12	1:A:220:TRP:HZ2	1.75	0.51
1:A:350:LYS:HZ1	1:A:354:GLN:HE21	1.56	0.51
1:A:547:LYS:O	1:A:551:GLU:HG3	2.10	0.51
1:B:162:PHE:HD2	1:B:309:ARG:HG3	1.75	0.51
1:B:565:LYS:HZ3	1:B:565:LYS:HB3	1.75	0.51
1:A:304:ASP:OD2	1:A:304:ASP:N	2.44	0.51
1:B:77:ARG:C	1:B:79:PRO:HD3	2.36	0.50
1:B:68:TYR:N	1:B:68:TYR:CD2	2.78	0.50
1:B:307:LYS:HZ2	1:B:338:LYS:HG3	1.76	0.50
1:B:202:LEU:HD21	1:B:213:MET:CG	2.42	0.50
1:A:292:ARG:O	1:A:295:SER:OG	2.23	0.50
1:A:452:ASP:O	1:A:456:GLU:HB2	2.11	0.50
1:B:173:TYR:CD2	1:B:198:LEU:HD13	2.46	0.50
1:B:56:LYS:HG3	1:B:265:LEU:HD23	1.94	0.50
1:B:192:VAL:HG12	1:B:220:TRP:HZ2	1.76	0.50
1:A:89:LEU:HD21	1:A:107:VAL:CG1	2.41	0.50
1:A:538:SER:OG	1:A:541:SER:HB2	2.12	0.50
1:B:189:GLN:HE21	1:B:190:GLN:N	2.08	0.50
1:B:509:PHE:CE2	1:B:513:ILE:HD11	2.47	0.50
1:B:544:THR:O	1:B:547:LYS:N	2.45	0.50
1:B:432:LEU:HD23	1:B:436:ARG:HD3	1.94	0.50
1:A:262:PRO:HG3	1:A:272:ASN:ND2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:LEU:HD23	1:A:496:LEU:HD12	1.93	0.50
1:A:315:MET:HG3	1:A:331:MET:CE	2.42	0.49
1:B:282:GLN:HE21	1:B:282:GLN:HA	1.77	0.49
1:B:144:ALA:C	1:B:146:ASN:H	2.19	0.49
1:A:236:LEU:O	1:A:237:SER:C	2.55	0.49
1:A:554:PRO:O	1:A:555:GLU:HB3	2.11	0.49
1:B:72:ASP:OD1	1:B:88:ARG:NH1	2.43	0.49
1:A:426:MET:HG3	1:A:438:ILE:HD11	1.93	0.49
1:A:573:TYR:O	1:A:574:LEU:C	2.56	0.49
1:B:280:ASP:OD1	1:B:282:GLN:HB3	2.13	0.49
1:A:167:ILE:CG2	1:A:168:GLN:N	2.75	0.49
1:B:192:VAL:HG12	1:B:220:TRP:CZ2	2.47	0.49
1:B:429:ILE:HG22	1:B:430:GLN:HG3	1.92	0.49
1:B:236:LEU:O	1:B:238:ALA:N	2.46	0.49
1:B:436:ARG:O	1:B:437:LYS:C	2.55	0.49
1:A:22:ARG:HA	1:A:22:ARG:CZ	2.43	0.49
1:A:550:PHE:HE2	1:A:558:LYS:HA	1.78	0.49
1:B:258:LYS:H	1:B:283:GLN:NE2	2.04	0.49
1:B:401:ASP:CG	1:B:401:ASP:O	2.55	0.49
1:A:22:ARG:CB	1:A:23:PRO:HD3	2.43	0.49
1:B:489:ILE:HG21	1:B:516:ILE:HD11	1.94	0.49
1:A:294:GLU:HG3	1:A:313:VAL:HG21	1.95	0.49
1:B:282:GLN:HA	1:B:282:GLN:NE2	2.27	0.49
1:B:299:LEU:O	1:B:300:GLU:HB2	2.13	0.49
1:A:350:LYS:HZ2	1:A:354:GLN:HE21	1.61	0.48
1:A:366:LEU:O	1:A:369:GLN:N	2.46	0.48
1:A:315:MET:HG3	1:A:331:MET:HE3	1.95	0.48
1:A:338:LYS:HE2	1:A:338:LYS:HA	1.95	0.48
1:A:414:LYS:HB2	1:B:577:LEU:HD13	1.95	0.48
1:B:309:ARG:O	1:B:313:VAL:HG23	2.13	0.48
1:B:563:THR:HB	1:B:572:ASN:HD21	1.78	0.48
1:A:61:LEU:HB2	1:A:63:GLN:HG3	1.95	0.48
1:A:472:CYS:SG	1:A:504:GLN:NE2	2.87	0.48
1:A:485:ASP:CG	1:A:487:GLU:HB3	2.38	0.48
1:B:214:TRP:CH2	1:B:233:ILE:HG23	2.48	0.48
1:B:542:VAL:HG12	1:B:546:GLU:HG3	1.95	0.48
1:B:214:TRP:O	1:B:215:GLN:C	2.57	0.48
1:B:264:THR:HG22	1:B:265:LEU:N	2.28	0.48
1:B:501:GLU:O	1:B:504:GLN:HB2	2.12	0.48
1:A:145:ARG:O	1:A:145:ARG:HG2	2.12	0.48
1:A:428:ARG:NH2	1:B:539:LEU:HD13	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:PHE:CE2	1:B:558:LYS:HD3	2.48	0.48
1:A:89:LEU:HD21	1:A:107:VAL:HG12	1.95	0.48
1:A:180:TRP:CE3	1:A:191:ARG:HG3	2.48	0.48
1:A:474:VAL:O	1:A:477:LEU:HB2	2.13	0.48
1:B:55:LEU:HD22	1:B:67:VAL:HG13	1.94	0.48
1:A:52:VAL:HG11	1:A:268:ALA:HB3	1.95	0.48
1:A:187:GLU:C	1:A:189:GLN:N	2.70	0.48
1:A:359:SER:HA	1:B:578:GLU:OE2	2.13	0.48
1:A:553:PHE:HB3	1:A:556:VAL:CG2	2.44	0.48
1:A:277:ASN:ND2	1:A:358:ASN:OD1	2.45	0.48
1:A:401:ASP:OD2	1:A:404:ASN:HB2	2.14	0.48
1:A:385:SER:O	1:A:386:CYS:C	2.56	0.48
1:B:189:GLN:NE2	1:B:190:GLN:N	2.62	0.48
1:B:140:GLY:C	1:B:144:ALA:HB2	2.38	0.47
1:B:224:VAL:O	1:B:224:VAL:HG12	2.14	0.47
1:B:539:LEU:HA	1:B:542:VAL:CG2	2.43	0.47
1:A:192:VAL:HG12	1:A:220:TRP:CZ2	2.49	0.47
1:B:259:ARG:C	1:B:260:ASN:HD22	2.21	0.47
1:A:512:SER:HB2	1:A:516:ILE:HG13	1.96	0.47
1:B:565:LYS:NZ	1:B:565:LYS:CB	2.77	0.47
1:A:326:GLU:O	1:A:326:GLU:HG3	2.09	0.47
1:B:55:LEU:CD2	1:B:70:THR:HB	2.44	0.47
1:B:366:LEU:O	1:B:367:SER:C	2.57	0.47
1:B:432:LEU:CD2	1:B:436:ARG:HD3	2.44	0.47
1:B:90:SER:O	1:B:91:LEU:C	2.58	0.47
1:A:37:LEU:HD12	1:A:40:MET:HE3	1.97	0.47
1:A:180:TRP:CD1	1:A:180:TRP:C	2.91	0.47
1:A:297:ASN:CG	1:A:297:ASN:O	2.56	0.47
1:B:121:LEU:HD21	1:B:169:PHE:HB2	1.96	0.47
1:B:232:HIS:C	1:B:234:GLY:N	2.72	0.47
1:B:246:LEU:HD22	1:B:293:TRP:CZ2	2.50	0.47
1:A:212:SER:O	1:A:216:ARG:HG3	2.14	0.47
1:A:426:MET:HE2	1:A:426:MET:HA	1.95	0.47
1:B:293:TRP:NE1	1:B:298:LYS:HD2	2.29	0.47
1:B:479:LEU:HD12	1:B:483:ALA:HA	1.97	0.47
1:B:479:LEU:HD22	1:B:492:TYR:HE2	1.80	0.47
1:A:445:LEU:O	1:A:446:LYS:HB2	2.14	0.47
1:A:297:ASN:HB2	1:A:306:HIS:CD2	2.50	0.46
1:B:155:VAL:HG11	1:B:169:PHE:CE1	2.50	0.46
1:B:489:ILE:HG13	1:B:516:ILE:HD11	1.96	0.46
1:A:329:PHE:CG	1:B:559:LEU:HD13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:HD12	1:A:483:ALA:CA	2.44	0.46
1:A:509:PHE:HZ	1:A:526:PHE:CE2	2.34	0.46
1:B:112:LEU:HD22	1:B:124:TRP:CH2	2.51	0.46
1:B:231:ARG:HD2	1:B:231:ARG:C	2.40	0.46
1:B:307:LYS:CD	1:B:338:LYS:HD2	2.38	0.46
1:B:460:ILE:C	1:B:462:TYR:N	2.73	0.46
1:A:236:LEU:C	1:A:238:ALA:N	2.71	0.46
1:A:543:ARG:HA	1:A:543:ARG:NH1	2.30	0.46
1:A:407:ALA:O	1:A:411:LEU:HD13	2.15	0.46
1:B:144:ALA:C	1:B:146:ASN:N	2.74	0.46
1:B:568:VAL:O	1:B:569:LEU:HB2	2.15	0.46
1:B:372:LEU:C	1:B:374:THR:H	2.22	0.46
1:A:439:PHE:CD2	1:A:457:ASN:OD1	2.69	0.46
1:B:181:LYS:H	1:B:181:LYS:HZ3	1.62	0.46
1:B:249:ASP:O	1:B:250:TRP:C	2.59	0.46
1:B:284:LEU:O	1:B:288:LEU:HG	2.15	0.46
1:A:189:GLN:NE2	1:A:190:GLN:N	2.63	0.46
1:A:307:LYS:CE	1:A:335:GLN:HE22	2.28	0.46
1:A:350:LYS:HZ1	1:A:354:GLN:NE2	2.14	0.46
1:A:454:TYR:CE1	1:A:482:PHE:HE1	2.34	0.46
1:A:509:PHE:CE2	1:A:513:ILE:HD11	2.51	0.46
1:B:448:LEU:HD12	1:B:448:LEU:HA	1.75	0.46
1:B:107:VAL:HG12	1:B:108:LEU:N	2.31	0.45
1:B:244:ARG:HH11	1:B:244:ARG:CB	2.14	0.45
1:B:569:LEU:O	1:B:571:VAL:HG23	2.16	0.45
1:A:142:GLU:O	1:A:146:ASN:HB2	2.16	0.45
1:B:555:GLU:CD	1:B:555:GLU:C	2.84	0.45
1:B:209:CYS:O	1:B:213:MET:HB2	2.16	0.45
1:B:452:ASP:O	1:B:456:GLU:HB2	2.17	0.45
1:B:484:THR:O	1:B:484:THR:HG22	2.16	0.45
1:A:550:PHE:CD2	1:A:558:LYS:HD3	2.52	0.45
1:A:569:LEU:O	1:A:571:VAL:HG23	2.16	0.45
1:B:125:LEU:HD23	1:B:125:LEU:HA	1.53	0.45
1:B:221:GLU:HA	1:B:221:GLU:OE1	2.15	0.45
1:B:416:THR:HG21	1:B:450:THR:HG22	1.99	0.45
1:B:564:ASN:O	1:B:567:LYS:HG3	2.16	0.45
1:A:37:LEU:HD23	1:A:54:LEU:HA	1.98	0.45
1:A:264:THR:HG22	1:A:266:ASN:H	1.81	0.45
1:A:484:THR:HG22	1:A:484:THR:O	2.16	0.45
1:B:528:LYS:HB2	1:B:528:LYS:HZ3	1.81	0.45
1:B:380:GLU:O	1:B:384:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ARG:C	1:A:79:PRO:HD3	2.42	0.45
1:A:115:GLU:HG2	1:A:116:LEU:N	2.23	0.45
1:A:128:ILE:HD11	1:A:152:PHE:HA	1.99	0.45
1:A:275:LYS:O	1:A:276:PRO:C	2.59	0.45
1:A:475:LEU:H	1:A:475:LEU:CD1	2.04	0.45
1:B:49:PHE:HD1	1:B:273:LEU:HD12	1.82	0.45
1:B:523:LYS:HB2	1:B:553:PHE:CE2	2.52	0.45
1:A:178:GLU:C	1:A:180:TRP:N	2.72	0.45
1:A:358:ASN:C	1:A:358:ASN:ND2	2.66	0.45
1:B:78:PHE:HB3	1:B:81:MET:CG	2.45	0.45
1:B:547:LYS:O	1:B:551:GLU:HG3	2.17	0.45
1:A:241:MET:O	1:A:242:ASN:C	2.60	0.44
1:B:125:LEU:CD1	1:B:168:GLN:NE2	2.80	0.44
1:B:142:GLU:C	1:B:144:ALA:H	2.25	0.44
1:B:182:PRO:HG2	1:B:188:GLU:HA	1.98	0.44
1:B:519:SER:O	1:B:521:LEU:N	2.50	0.44
1:B:565:LYS:HB3	1:B:565:LYS:NZ	2.32	0.44
1:B:115:GLU:HG2	1:B:116:LEU:N	2.27	0.44
1:B:200:LYS:HD3	1:B:236:LEU:CD2	2.20	0.44
1:B:520:HIS:O	1:B:520:HIS:ND1	2.49	0.44
1:A:244:ARG:HH11	1:A:244:ARG:HB3	1.81	0.44
1:A:428:ARG:HD2	1:A:428:ARG:O	2.17	0.44
1:B:142:GLU:C	1:B:144:ALA:N	2.74	0.44
1:B:337:GLU:O	1:B:338:LYS:O	2.35	0.44
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.77	0.44
1:B:254:THR:HG23	1:B:257:LEU:CB	2.48	0.44
1:B:565:LYS:HD2	1:B:566:TYR:CE1	2.53	0.44
1:A:508:LEU:O	1:A:508:LEU:HD12	2.17	0.44
1:A:519:SER:OG	1:A:520:HIS:N	2.49	0.44
1:B:212:SER:O	1:B:216:ARG:HG3	2.17	0.44
1:A:61:LEU:CD1	1:A:63:GLN:NE2	2.72	0.44
1:A:572:ASN:HD21	1:A:574:LEU:HB2	1.83	0.44
1:B:140:GLY:CA	1:B:144:ALA:HB2	2.46	0.44
1:A:189:GLN:HE21	1:A:189:GLN:C	2.25	0.44
1:B:79:PRO:HB3	1:B:116:LEU:HD13	1.99	0.44
1:B:174:LEU:HA	1:B:174:LEU:HD23	1.77	0.44
1:B:493:LEU:HD22	1:B:505:VAL:HG13	1.99	0.44
1:A:32:ASP:O	1:A:33:VAL:C	2.60	0.44
1:A:181:LYS:H	1:A:181:LYS:HZ3	1.65	0.44
1:A:454:TYR:HE1	1:A:482:PHE:HE1	1.64	0.44
1:B:519:SER:C	1:B:521:LEU:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:THR:O	1:B:545:LEU:C	2.61	0.44
1:A:438:ILE:O	1:A:441:LYS:HG2	2.18	0.44
1:A:468:THR:O	1:A:468:THR:CG2	2.65	0.44
1:A:579:LEU:N	1:A:579:LEU:HD23	2.32	0.44
1:A:25:SER:O	1:A:27:VAL:N	2.46	0.43
1:A:140:GLY:C	1:A:144:ALA:HB2	2.43	0.43
1:A:579:LEU:C	1:A:581:TYR:N	2.75	0.43
1:B:508:LEU:HD12	1:B:508:LEU:O	2.17	0.43
1:A:173:TYR:CD2	1:A:198:LEU:HD13	2.54	0.43
1:A:425:THR:O	1:A:429:ILE:HB	2.17	0.43
1:A:478:GLY:C	1:A:480:LYS:N	2.76	0.43
1:A:52:VAL:HG11	1:A:268:ALA:CB	2.48	0.43
1:A:197:LYS:O	1:A:197:LYS:HG2	2.19	0.43
1:A:477:LEU:HD13	1:A:477:LEU:HA	1.87	0.43
1:A:528:LYS:HB2	1:A:528:LYS:NZ	2.33	0.43
1:B:225:ASN:O	1:B:227:LEU:N	2.51	0.43
1:A:22:ARG:HB3	1:A:23:PRO:HD3	2.00	0.43
1:A:115:GLU:CD	1:A:115:GLU:N	2.75	0.43
1:A:456:GLU:HG3	1:B:568:VAL:CG1	2.48	0.43
1:A:84:ILE:HA	1:A:87:MET:CE	2.49	0.43
1:A:544:THR:O	1:A:545:LEU:C	2.60	0.43
1:B:137:ILE:HD12	1:B:138:ILE:N	2.33	0.43
1:A:121:LEU:HD23	1:A:121:LEU:O	2.19	0.43
1:A:441:LYS:O	1:A:444:ARG:HB3	2.19	0.43
1:B:115:GLU:HB2	1:B:347:LYS:NZ	2.33	0.43
1:B:180:TRP:CD1	1:B:180:TRP:C	2.97	0.43
1:B:539:LEU:HA	1:B:542:VAL:HG23	2.00	0.43
1:A:281:VAL:O	1:A:282:GLN:C	2.62	0.43
1:B:462:TYR:O	1:B:464:ILE:N	2.52	0.43
1:B:492:TYR:O	1:B:495:PHE:HB3	2.19	0.43
1:B:37:LEU:CD2	1:B:54:LEU:HA	2.48	0.43
1:B:89:LEU:O	1:B:90:SER:C	2.59	0.43
1:B:358:ASN:C	1:B:358:ASN:ND2	2.66	0.43
1:B:56:LYS:CG	1:B:265:LEU:HD23	2.48	0.43
1:B:143:GLU:HA	1:B:146:ASN:HB3	2.01	0.43
1:B:207:MET:HE2	1:B:207:MET:HB3	1.68	0.43
1:B:495:PHE:O	1:B:496:LEU:C	2.62	0.43
1:B:289:GLU:OE2	1:B:289:GLU:HA	2.19	0.43
1:A:299:LEU:HB3	1:A:301:LEU:CD2	2.49	0.42
1:A:451:PRO:HG3	1:A:482:PHE:CG	2.54	0.42
1:B:37:LEU:HD23	1:B:54:LEU:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LEU:O	1:B:369:GLN:N	2.52	0.42
1:A:430:GLN:O	1:A:434:ALA:HB2	2.19	0.42
1:A:492:TYR:O	1:A:495:PHE:HB3	2.19	0.42
1:B:128:ILE:CD1	1:B:152:PHE:CD1	3.03	0.42
1:B:327:ILE:HG23	1:B:328:TRP:N	2.35	0.42
1:B:460:ILE:C	1:B:462:TYR:H	2.27	0.42
1:A:55:LEU:O	1:A:56:LYS:C	2.62	0.42
1:B:165:LYS:HE3	1:B:208:ASP:HB3	2.02	0.42
1:B:368:GLU:O	1:B:372:LEU:HD13	2.20	0.42
1:B:471:ALA:O	1:B:475:LEU:HD11	2.19	0.42
1:A:436:ARG:HG2	1:A:436:ARG:HH11	1.85	0.42
1:A:575:GLN:O	1:A:580:ASP:HA	2.19	0.42
1:B:137:ILE:HG22	1:B:145:ARG:HB2	2.01	0.42
1:A:479:LEU:HD12	1:A:479:LEU:HA	1.78	0.42
1:B:181:LYS:H	1:B:181:LYS:NZ	2.16	0.42
1:A:232:HIS:O	1:A:235:GLU:OE1	2.37	0.42
1:B:103:VAL:O	1:B:106:PRO:HG2	2.20	0.42
1:B:120:ASP:OD2	1:B:122:SER:HB2	2.19	0.42
1:B:531:PHE:CD1	1:B:531:PHE:O	2.72	0.42
1:A:560:GLU:CA	1:A:582:MET:HE3	2.48	0.42
1:B:262:PRO:HG2	1:B:268:ALA:HA	2.02	0.42
1:B:279:TYR:CE2	1:B:324:ALA:HA	2.54	0.42
1:B:573:TYR:C	1:B:575:GLN:N	2.76	0.42
1:A:493:LEU:HD23	1:A:493:LEU:HA	1.89	0.42
1:B:77:ARG:O	1:B:79:PRO:HD3	2.20	0.42
1:B:263:ILE:H	1:B:263:ILE:HG13	1.80	0.42
1:B:512:SER:HB2	1:B:516:ILE:HG13	2.01	0.42
1:A:112:LEU:HD22	1:A:124:TRP:CH2	2.54	0.41
1:A:187:GLU:O	1:A:188:GLU:C	2.62	0.41
1:B:51:TYR:CD2	1:B:74:LEU:HD21	2.55	0.41
1:B:191:ARG:O	1:B:191:ARG:HG2	2.18	0.41
1:B:324:ALA:O	1:B:327:ILE:HG22	2.19	0.41
1:B:394:LEU:HD13	1:B:411:LEU:HB3	2.02	0.41
1:B:412:LYS:NZ	1:B:447:LYS:O	2.39	0.41
1:A:37:LEU:HD23	1:A:54:LEU:CA	2.50	0.41
1:A:77:ARG:HG2	1:A:78:PHE:CD1	2.54	0.41
1:A:80:LEU:HA	1:A:118:ASN:ND2	2.32	0.41
1:A:550:PHE:CE2	1:A:558:LYS:HA	2.55	0.41
1:B:119:ASN:OD1	1:B:159:CYS:HB2	2.19	0.41
1:B:202:LEU:HD11	1:B:213:MET:HG2	2.02	0.41
1:A:177:LEU:HA	1:A:177:LEU:HD23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LYS:HB3	1:A:447:LYS:H	1.45	0.41
1:A:539:LEU:HD23	1:B:372:LEU:HD11	2.01	0.41
1:B:164:PRO:HG2	1:B:250:TRP:CZ2	2.55	0.41
1:B:189:GLN:NE2	1:B:189:GLN:C	2.79	0.41
1:A:195:ILE:HG22	1:A:195:ILE:O	2.21	0.41
1:A:290:TRP:CD1	1:A:290:TRP:C	2.97	0.41
1:A:138:ILE:HG22	1:A:139:THR:HG23	2.02	0.41
1:A:164:PRO:HG3	1:A:250:TRP:CE2	2.55	0.41
1:A:261:LEU:HA	1:A:262:PRO:HD3	1.87	0.41
1:A:574:LEU:HA	1:A:574:LEU:HD23	1.64	0.41
1:B:125:LEU:HD21	1:B:169:PHE:HD1	1.85	0.41
1:A:84:ILE:HA	1:A:87:MET:HE3	2.02	0.41
1:A:115:GLU:C	1:A:117:GLY:H	2.28	0.41
1:A:187:GLU:O	1:A:189:GLN:N	2.54	0.41
1:A:253:ILE:HG23	1:A:289:GLU:HG3	2.02	0.41
1:A:479:LEU:HD11	1:A:483:ALA:HA	2.01	0.41
1:B:232:HIS:C	1:B:234:GLY:H	2.28	0.41
1:B:526:PHE:O	1:B:530:ILE:HG13	2.21	0.41
1:A:464:ILE:HB	1:A:465:SER:H	1.65	0.41
1:A:493:LEU:HD22	1:A:505:VAL:HG13	2.02	0.41
1:B:195:ILE:O	1:B:195:ILE:HG22	2.20	0.41
1:B:232:HIS:HA	1:B:235:GLU:OE1	2.20	0.41
1:B:243:ALA:O	1:B:246:LEU:N	2.54	0.41
1:B:464:ILE:HB	1:B:465:SER:H	1.71	0.41
1:A:24:THR:CB	1:A:43:GLU:OE2	2.69	0.41
1:A:416:THR:HG23	1:A:449:VAL:HB	2.03	0.41
1:A:465:SER:C	1:A:467:ASP:N	2.79	0.41
1:A:466:LYS:HA	1:A:466:LYS:HD3	1.94	0.41
1:A:485:ASP:OD2	1:A:487:GLU:HB3	2.21	0.41
1:A:579:LEU:O	1:A:581:TYR:N	2.54	0.41
1:B:74:LEU:HD23	1:B:74:LEU:HA	1.86	0.41
1:B:137:ILE:H	1:B:137:ILE:HG13	1.69	0.41
1:B:246:LEU:HD23	1:B:246:LEU:HA	1.86	0.41
1:B:465:SER:O	1:B:467:ASP:N	2.54	0.41
1:B:574:LEU:HD23	1:B:574:LEU:HA	1.81	0.41
1:A:81:MET:CE	1:A:319:GLN:HA	2.42	0.41
1:A:127:TYR:O	1:A:131:VAL:HG23	2.21	0.41
1:B:85:TRP:CD2	1:B:111:CYS:HB3	2.56	0.41
1:B:397:LEU:C	1:B:399:GLU:N	2.78	0.41
1:B:416:THR:O	1:B:417:TYR:C	2.62	0.41
1:B:463:HIS:CD2	1:B:466:LYS:HE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:PHE:C	1:B:554:PRO:O	2.62	0.41
1:A:299:LEU:O	1:A:300:GLU:CB	2.68	0.40
1:A:411:LEU:N	1:A:411:LEU:CD1	2.84	0.40
1:A:469:LYS:O	1:A:473:LYS:HG3	2.21	0.40
1:B:32:ASP:O	1:B:32:ASP:CG	2.64	0.40
1:A:34:ILE:CG1	1:A:57:HIS:CD2	3.04	0.40
1:A:254:THR:HG22	1:A:255:LYS:N	2.36	0.40
1:A:301:LEU:HB3	1:A:305:LEU:HB3	2.03	0.40
1:B:236:LEU:C	1:B:238:ALA:N	2.78	0.40
1:B:340:THR:O	1:B:341:ASP:HB3	2.21	0.40
1:B:510:GLU:OE1	1:B:510:GLU:HA	2.19	0.40
1:A:202:LEU:HD12	1:A:203:LEU:N	2.36	0.40
1:A:292:ARG:HH11	1:A:292:ARG:CB	2.27	0.40
1:A:358:ASN:O	1:A:414:LYS:NZ	2.54	0.40
1:A:366:LEU:HD22	1:A:370:TYR:CE1	2.56	0.40
1:A:417:TYR:OH	1:B:574:LEU:HG	2.20	0.40
1:A:453:ILE:HD12	1:A:453:ILE:HA	1.93	0.40
1:A:508:LEU:O	1:A:509:PHE:C	2.64	0.40
1:A:520:HIS:O	1:A:520:HIS:ND1	2.54	0.40
1:A:533:GLU:HG3	1:A:545:LEU:CD1	2.50	0.40
1:A:538:SER:CB	1:A:541:SER:OG	2.69	0.40
1:B:74:LEU:HD13	1:B:84:ILE:HD13	2.04	0.40
1:B:464:ILE:H	1:B:464:ILE:HG13	1.74	0.40
1:A:222:GLN:C	1:A:224:VAL:H	2.29	0.40
1:A:389:ARG:HA	1:A:389:ARG:HD2	1.86	0.40
1:A:128:ILE:HD13	1:A:152:PHE:CE1	2.57	0.40
1:B:85:TRP:CD2	1:B:111:CYS:CB	3.05	0.40
1:B:173:TYR:CD2	1:B:198:LEU:CD1	3.04	0.40
1:B:394:LEU:HA	1:B:411:LEU:HD23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/678 (81%)	430 (78%)	91 (16%)	30 (5%)	1	9
1	B	550/678 (81%)	439 (80%)	87 (16%)	24 (4%)	2	12
All	All	1101/1356 (81%)	869 (79%)	178 (16%)	54 (5%)	1	10

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	SER
1	A	142	GLU
1	A	179	HIS
1	A	233	ILE
1	A	338	LYS
1	A	340	THR
1	A	463	HIS
1	A	466	LYS
1	B	113	SER
1	B	142	GLU
1	B	179	HIS
1	B	225	ASN
1	B	255	LYS
1	B	338	LYS
1	A	144	ALA
1	A	237	SER
1	A	464	ILE
1	A	500	ASN
1	A	502	GLU
1	A	517	SER
1	B	144	ALA
1	B	226	GLN
1	B	233	ILE
1	B	237	SER
1	B	279	TYR
1	B	341	ASP
1	B	463	HIS
1	B	466	LYS
1	B	500	ASN
1	B	502	GLU
1	B	539	LEU
1	A	31	SER
1	A	255	LYS
1	A	580	ASP
1	B	405	GLU

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Mol	Chain	Res	Type
1	B	464	ILE
1	B	511	SER
1	A	223	ASP
1	A	235	GLU
1	A	279	TYR
1	A	538	SER
1	A	539	LEU
1	A	557	ASN
1	B	138	ILE
1	B	197	LYS
1	B	517	SER
1	A	34	ILE
1	A	138	ILE
1	A	254	THR
1	A	341	ASP
1	A	374	THR
1	A	511	SER
1	A	524	MET
1	B	223	ASP

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	517/623 (83%)	459 (89%)	58 (11%)	6 24
1	B	513/623 (82%)	458 (89%)	55 (11%)	6 26
All	All	1030/1246 (83%)	917 (89%)	113 (11%)	6 25

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	39	ASP
1	A	97	GLU
1	A	104	ILE

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Mol	Chain	Res	Type
1	A	115	GLU
1	A	121	LEU
1	A	128	ILE
1	A	129	THR
1	A	137	ILE
1	A	147	ILE
1	A	149	ILE
1	A	154	VAL
1	A	156	VAL
1	A	159	CYS
1	A	174	LEU
1	A	179	HIS
1	A	181	LYS
1	A	189	GLN
1	A	192	VAL
1	A	202	LEU
1	A	232	HIS
1	A	242	ASN
1	A	244	ARG
1	A	252	ASN
1	A	263	ILE
1	A	265	LEU
1	A	278	GLU
1	A	292	ARG
1	A	296	ASP
1	A	301	LEU
1	A	304	ASP
1	A	326	GLU
1	A	358	ASN
1	A	366	LEU
1	A	382	THR
1	A	384	LEU
1	A	391	HIS
1	A	406	SER
1	A	416	THR
1	A	427	LYS
1	A	428	ARG
1	A	429	ILE
1	A	448	LEU
1	A	450	THR
1	A	475	LEU
1	A	477	LEU

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Mol	Chain	Res	Type
1	A	479	LEU
1	A	480	LYS
1	A	507	SER
1	A	510	GLU
1	A	521	LEU
1	A	528	LYS
1	A	539	LEU
1	A	540	ASN
1	A	543	ARG
1	A	544	THR
1	A	565	LYS
1	A	579	LEU
1	B	37	LEU
1	B	39	ASP
1	B	97	GLU
1	B	115	GLU
1	B	121	LEU
1	B	128	ILE
1	B	129	THR
1	B	154	VAL
1	B	156	VAL
1	B	159	CYS
1	B	174	LEU
1	B	179	HIS
1	B	192	VAL
1	B	202	LEU
1	B	209	CYS
1	B	226	GLN
1	B	231	ARG
1	B	242	ASN
1	B	244	ARG
1	B	252	ASN
1	B	263	ILE
1	B	265	LEU
1	B	278	GLU
1	B	292	ARG
1	B	296	ASP
1	B	301	LEU
1	B	304	ASP
1	B	326	GLU
1	B	356	ILE
1	B	358	ASN

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Mol	Chain	Res	Type
1	B	366	LEU
1	B	384	LEU
1	B	391	HIS
1	B	401	ASP
1	B	406	SER
1	B	416	THR
1	B	427	LYS
1	B	428	ARG
1	B	429	ILE
1	B	435	SER
1	B	448	LEU
1	B	450	THR
1	B	475	LEU
1	B	477	LEU
1	B	479	LEU
1	B	507	SER
1	B	510	GLU
1	B	521	LEU
1	B	524	MET
1	B	528	LYS
1	B	539	LEU
1	B	540	ASN
1	B	543	ARG
1	B	544	THR
1	B	565	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	118	ASN
1	A	175	HIS
1	A	179	HIS
1	A	189	GLN
1	A	232	HIS
1	A	239	GLN
1	A	260	ASN
1	A	282	GLN
1	A	283	GLN
1	A	306	HIS
1	A	330	ASN
1	A	335	GLN

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Mol	Chain	Res	Type
1	A	354	GLN
1	A	504	GLN
1	A	527	GLN
1	B	63	GLN
1	B	66	GLN
1	B	118	ASN
1	B	150	GLN
1	B	168	GLN
1	B	189	GLN
1	B	232	HIS
1	B	239	GLN
1	B	260	ASN
1	B	282	GLN
1	B	283	GLN
1	B	330	ASN
1	B	335	GLN
1	B	391	HIS
1	B	457	ASN
1	B	463	HIS
1	B	500	ASN
1	B	527	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	555/678 (81%)	-0.00	7 (1%) 75 53	30, 69, 113, 128	0
1	B	552/678 (81%)	-0.05	3 (0%) 87 72	30, 70, 115, 138	0
All	All	1107/1356 (81%)	-0.03	10 (0%) 81 61	30, 70, 114, 138	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	ILE	2.7
1	A	99	LEU	2.6
1	A	33	VAL	2.6
1	A	232	HIS	2.5
1	B	232	HIS	2.3
1	A	97	GLU	2.2
1	A	27	VAL	2.1
1	B	229	ALA	2.1
1	B	260	ASN	2.0
1	A	468	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.