



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:14 PM GMT

PDB ID : 4E85
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

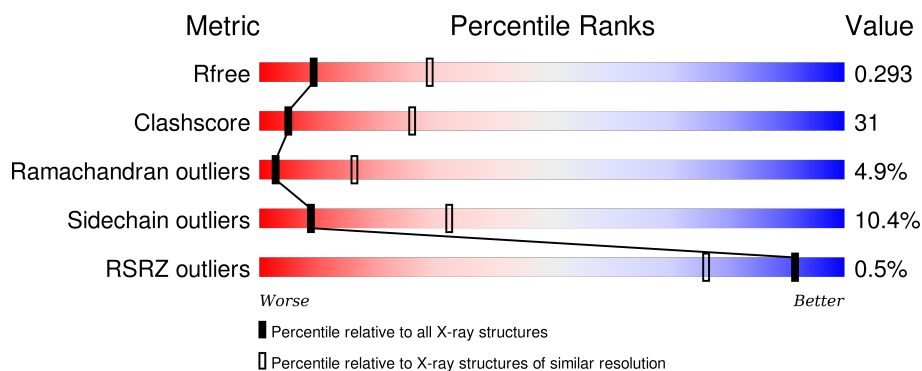
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	678	

2 Entry composition

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
1	A	555	Total	C	N	O	S	0	0	0
			4623	2976	765	856	26			
1	B	552	Total	C	N	O	S	0	0	0
			4598	2962	760	851	25			

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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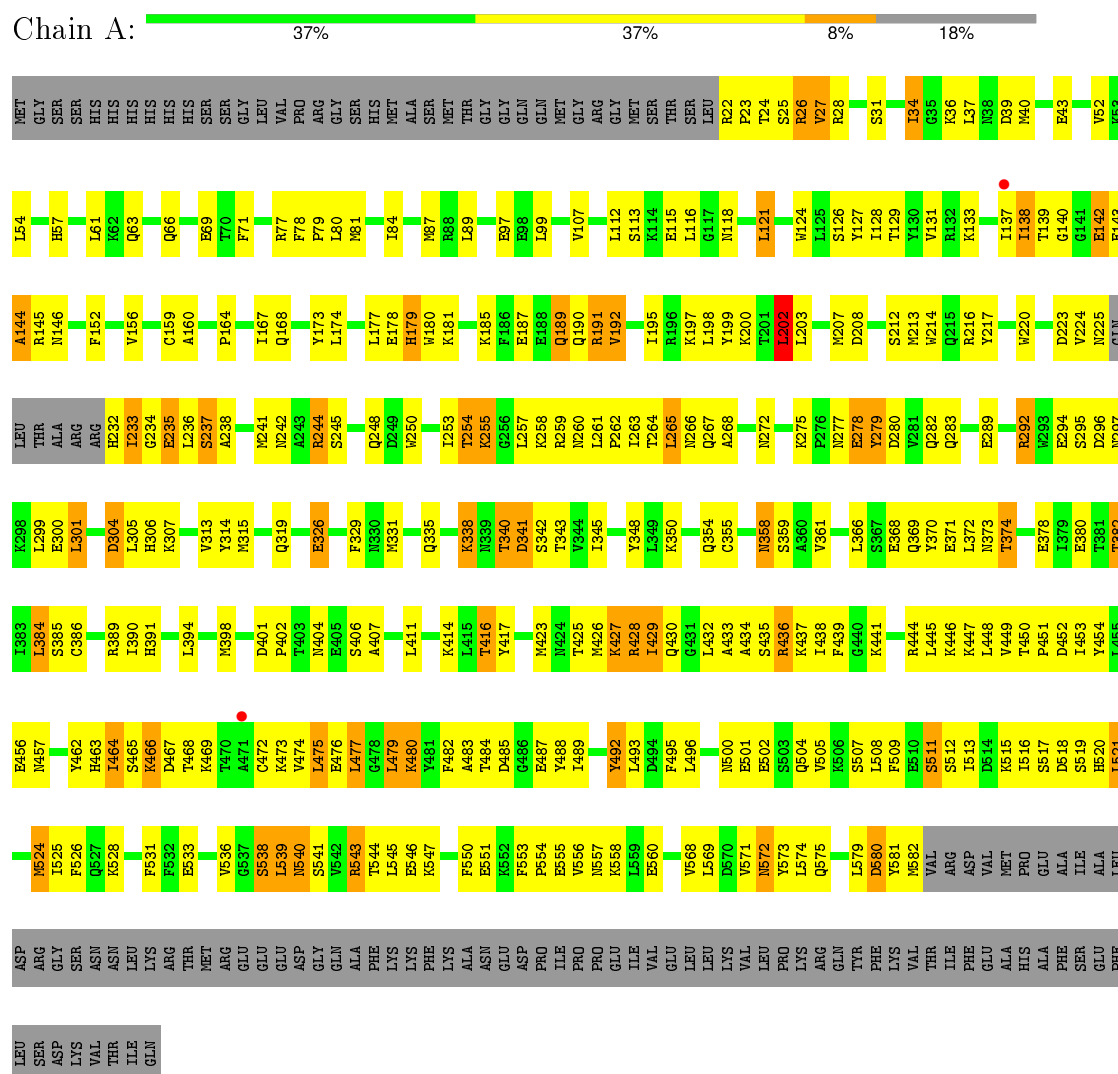
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Chain	Residue	Modelled	Actual	Comment	Reference
B	17	MET	-	EXPRESSION TAG	UNP Q6CII8

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



GLN	LYS	E533	H463	N373	E278	S212	K133	K56	MET
ARG	THR	S538	I464	T374	Y279	S213	I137	L61	GLY
MET	ARG	L539	K466	E378	D280	W214	I138	K62	SER
GLU	GLU	M540	D467	T379	Y281	Q215	T139	Q63	HIS
GLU	GLU	V542	T468	E380	Q282	R216	G140	K65	HIS
ASP	ASP	R543	A471	T382	Q283	Y217	G141	Q66	HIS
GLY	GLY	T544	C472	T383	L284	W220	E142	V67	HIS
GLN	GLN	L545	L384	L384	L288	E221	A143	V68	HIS
ALA	ALA	E546	L476	S385	E289	Q222	E145	E69	SER
PHE	PHE	K547	E476	C386	W290	D223	N146	T70	SER
LYS	LYS	F550	L478	T387	I291	V224	F152	D72	GLY
LYS	LYS	E551	G478	R388	W292	M225	F152	D72	LEU
PHE	PHE	K552	K480	R389	W293	Q226	F155	K73	VAL
ALA	ALA	F553	A483	H391	D286	L227	V155	L74	PRO
ASN	ASN	E554	T484	L394	K297	T228	V156	L74	ARG
GLU	GLU	E555	L489	L394	K298	R230	C159	R77	GLY
ASP	ASP	K558	L489	M398	L299	R231	A160	F78	SER
PRO	PRO	L559	Y492	D401	E300	H232	I161	P79	HIS
ILE	ILE	T563	L493	L401	E304	G234	F162	M81	ALA
PRO	PRO	M564	D494	N404	K307	S237	F166	T84	MET
GLU	GLU	K565	F495	S406	A308	E238	I167	M85	SER
ILE	ILE	Y566	N500	S406	R309	Q239	Q168	R88	GLY
VAL	VAL	K567	E501	L411	V313	W240	F169	L89	GLN
GLU	GLU	V568	E501	K412	Y314	M241	L191	S90	GLN
LEU	LEU	L569	E502	S413	Y314	N242	L191	S90	MET
LYS	LYS	D570	S503	S413	Q319	A243	Y173	L91	MET
VAL	VAL	M572	W505	T416	Q319	R244	L174	E97	GLY
LEU	LEU	Y573	K506	L416	A324	S245	L177	E98	GLY
PRO	PRO	L574	S507	T425	A324	L246	E178	L99	MET
LYS	LYS	L577	L508	T426	A324	L246	H179	V103	SER
ARG	ARG	E578	F509	K427	I327	D249	H179	V103	THR
GLN	GLN	E578	E510	R428	W328	W250	H180	P106	SER
TYR	TYR	L579	S511	L429	W328	L251	K181	P106	LEU
PHE	PHE	D580	S512	Q430	E337	N252	P182	P106	ARG
LYS	LYS	Y581	S513	E431	E337	L253	K185	L108	PRO
VAL	VAL	MET	D514	L432	N339	T254	K185	L108	THR
THR	THR	VAL	K515	L433	T340	K256	E188	C111	SER
ILE	ILE	ARG	I516	A434	D341	G256	Q189	L112	ARG
PHE	PHE	ASP	K516	S435	S342	L257	Q190	S113	VAL
GLU	GLU	VAL	D518	R436	T343	K258	R191	K114	ARG
ALA	ALA	MET	S519	K437	T343	R259	R191	E115	ASP
PRO	PRO	PRO	H520	K437	K347	K259	V192	L116	ASP
ALA	ALA	GLU	L521	K447	K347	N260	V192	L116	E30
GLU	GLU	ALA	E521	K447	K347	N260	V192	L116	E30
PHE	PHE	SER	L522	L448	I356	L261	I195	N118	K36
ILE	ILE	ASP	K523	L449	P357	P262	R196	N119	L37
ALA	ALA	THR	L524	T450	N358	L263	K197	D120	N38
GLU	GLU	PHE	M524	T451	T264	L264	L198	L121	D39
PHE	PHE	LEU	I525	P451	L265	L265	Y199	S122	M40
ASP	ASP	ASP	F526	D452	L366	N266	K200	L123	M40
SER	SER	ARG	Q527	D452	S367	Q267	T201	W124	F49
GLY	GLY	ASP	K528	E456	E368	A268	L201	L125	L50

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 – 2.99	Depositor EDS
% Data completeness (in resolution range)	87.8 (46.77-3.00) 87.2 (46.77-2.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.233 , 0.293 0.233 , 0.293	Depositor DCC
R_{free} test set	1195 reflections (4.80%)	DCC
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 26521 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9221	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage'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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	1/4724 (0.0%)	0.81	2/6385 (0.0%)
1	B	0.64	0/4699	0.80	1/6353 (0.0%)
All	All	0.66	1/9423 (0.0%)	0.80	3/12738 (0.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	CYS	CB-SG	-5.01	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	LEU	CA-CB-CG	6.11	129.35	115.30
1	A	202	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	27	VAL	N-CA-C	-5.15	97.10	111.00

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	296	0
1	B	4598	0	4598	296	0
All	All	9221	0	9218	576	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 31.

All (576) 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:HB3	1:B:244:ARG:HH11	1.27	0.98
1:A:475:LEU:H	1:A:475:LEU:HD12	1.25	0.97
1:A:428:ARG:HG2	1:A:428:ARG:HH11	1.26	0.97
1:A:264:THR:HB	1:A:267:GLN:HG3	1.43	0.96
1:B:475:LEU:H	1:B:475:LEU:HD12	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:A:480:LYS:HE2	1:A:480:LYS:HA	1.59	0.84
1:B:115:GLU:H	1:B:115:GLU:CD	1.82	0.83
1:B:299:LEU:HB3	1:B:301:LEU:HD21	1.61	0.83
1:A:428:ARG:HH11	1:A:428:ARG:CG	1.92	0.82
1:A:115:GLU:HG2	1:A:116:LEU:H	1.45	0.82
1:A:560:GLU:HA	1:A:582:MET:HE1	1.62	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:O	1:B:231:ARG:HD2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:546:GLU:O	1:B:550:PHE:HD1	1.63	0.79
1:A:202:LEU:HD21	1:A:213:MET:HG2	1.62	0.79
1:B:480:LYS:HA	1:B:480:LYS:HE2	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: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:B:230:ARG:NH1	1:B:230:ARG:HB3	2.01	0.75
1:A:427:LYS:HB2	1:A:435:SER:OG	1.87	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
1:A:200:LYS:HD3	1:A:236:LEU:HD21	1.68	0.75
1:A:258:LYS:H	1:A:283:GLN:HE22	1.36	0.74
1:A:536:VAL:O	1:A:536:VAL:HG12	1.87	0.74
1:A:423:MET:HA	1:A:438:ILE:HD12	1.69	0.73
1:A:538:SER:C	1:A:540:ASN:H	1.92	0.73
1:B:231:ARG:HG3	1:B:232:HIS:HD2	1.54	0.73
1:B:224:VAL:O	1:B:225:ASN:HB2	1.87	0.72
1:B:128:ILE:HD11	1:B:152:PHE:HA	1.70	0.72
1:B:238:ALA:HB3	1:B:239:GLN:NE2	2.04	0.72
1:B:230:ARG:HB3	1:B:230:ARG:HH11	1.53	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: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:B:299:LEU:HB3	1:B:301:LEU:CD2	2.22	0.70
1:A:546:GLU:O	1:A:550:PHE:CD1	2.40	0.70
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:A:501:GLU:O	1:A:504:GLN:HB2	1.92	0.69
1:A:292:ARG:HB3	1:A:292:ARG:HH11	1.56	0.69
1:A:167:ILE:HG23	1:A:168:GLN:N	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LEU:HD11	1:A:398:MET:HE3	1.75	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:B:202:LEU:HD21	1:B:213:MET:HG2	1.74	0.68
1:A:214:TRP:CH2	1:A:233:ILE:HG23	2.29	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:A:358:ASN:C	1:A:358:ASN:HD22	1.96	0.68
1:B:538:SER:C	1:B:540:ASN:H	1.98	0.68
1:B:521:LEU:O	1:B:525:ILE:HG13	1.93	0.68
1:B:244:ARG:NH1	1:B:244:ARG:HB3	2.06	0.67
1:A:350:LYS:NZ	1:A:354:GLN:HE21	1.92	0.67
1:B:358:ASN:HD22	1:B:358:ASN:C	1.98	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:290:TRP:HD1	1:B:290:TRP:O	1.79	0.66
1:B:99:LEU:HD11	1:B:133:LYS:HD3	1.77	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:428:ARG:NH1	1:A:428:ARG:CG	2.57	0.65
1:A:282:GLN:HA	1:A:282:GLN:HE21	1.60	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:A:394:LEU:CD1	1:A:398:MET:HE3	2.27	0.64
1:B:78:PHE:HB3	1:B:81:MET:HG2	1.79	0.64
1:B:307:LYS:HZ1	1:B:338:LYS:HG3	1.62	0.63
1:B:138:ILE:HG22	1:B:139:THR:N	2.13	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:546:GLU:O	1:B:550:PHE:CD1	2.50	0.63
1:B:543:ARG:HA	1:B:543:ARG:HH11	1.63	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:480:LYS:HA	1:A:480:LYS:CE	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ARG:O	1:B:145:ARG:HG2	1.98	0.62
1:A:456:GLU:CG	1:B:568:VAL:HG13	2.29	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:115:GLU:H	1:A:115:GLU:CD	2.03	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:B:366:LEU:HD22	1:B:370:TYR:CE1	2.35	0.61
1:B:37:LEU:HD23	1:B:54:LEU:HA	1.82	0.61
1:B:142:GLU:HG3	1:B:143:GLU:N	2.15	0.61
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:B:162:PHE:CD2	1:B:309:ARG:HG3	2.36	0.61
1:A:489:ILE:HD12	1:A:508:LEU:HD11	1.81	0.61
1:A:394:LEU:CG	1:A:398:MET:HE3	2.31	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:264:THR:HG22	1:B:266:ASN:H	1.66	0.60
1:B:61:LEU:CD1	1:B:63:GLN:HE21	2.10	0.60
1:B:290:TRP:CD1	1:B:290:TRP:O	2.54	0.60
1:A:282:GLN:HA	1:A:282:GLN:NE2	2.16	0.60
1:A:167:ILE:HB	1:A:208:ASP:OD1	2.02	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:B:538:SER:O	1:B:540:ASN:N	2.35	0.59
1:A:368:GLU:O	1:A:372:LEU:HD13	2.01	0.59
1:A:254:THR:HG23	1:A:257:LEU:HB2	1.84	0.59
1:A:23:PRO:O	1:A:25:SER:N	2.34	0.59
1:A:178:GLU:C	1:A:180:TRP:H	2.05	0.59
1:A:427:LYS:O	1:A:427:LYS:HE2	2.02	0.59
1:B:254:THR:HG23	1:B:257:LEU:HB2	1.84	0.59
1:A:173:TYR:CE2	1:A:198:LEU:HD13	2.38	0.59
1:B:140:GLY:HA3	1:B:144:ALA:HB2	1.85	0.59
1:B:528:LYS:NZ	1:B:528:LYS:HB2	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:280:ASP:OD1	1:A:282:GLN:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLN:HE21	1:A:190:GLN:N	2.01	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:B:538:SER:HB2	1:B:541:SER:OG	2.04	0.58
1:A:533:GLU:HG3	1:A:545:LEU:HD11	1.86	0.58
1:B:232:HIS:O	1:B:234:GLY:N	2.37	0.57
1:A:429:ILE:HG22	1:A:430:GLN:HG3	1.84	0.57
1:B:264:THR:HB	1:B:267:GLN:CG	2.24	0.57
1:A:236:LEU:O	1:A:238:ALA:N	2.37	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:538:SER:O	1:A:540:ASN:N	2.37	0.57
1:A:429:ILE:CG2	1:A:430:GLN:HG3	2.34	0.57
1:B:55:LEU:HD21	1:B:70:THR:HB	1.87	0.57
1:A:417:TYR:CD1	1:B:573:TYR:HB2	2.38	0.57
1:A:26:ARG:NH1	1:A:26:ARG:HG2	2.16	0.57
1:B:292:ARG:HH11	1:B:292:ARG:HB3	1.70	0.57
1:A:475:LEU:N	1:A:475:LEU:HD12	2.07	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:520:HIS:HE1	1:A:524:MET:CE	2.18	0.57
1:A:394:LEU:HG	1:A:398:MET:HE3	1.85	0.57
1:A:142:GLU:HG3	1:A:143:GLU:N	2.20	0.57
1:B:299:LEU:CB	1:B:301:LEU:HD21	2.34	0.56
1:A:143:GLU:HA	1:A:146:ASN:HB3	1.86	0.56
1:B:559:LEU:HD21	1:B:579:LEU:CD1	2.35	0.56
1:A:521:LEU:O	1:A:525:ILE:HG13	2.05	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:B:220:TRP:O	1:B:224:VAL:HG23	2.06	0.56
1:A:432:LEU:HD23	1:A:436:ARG:HD3	1.88	0.56
1:A:167:ILE:HG23	1:A:168:GLN:H	1.70	0.55
1:B:450:THR:HG23	1:B:452:ASP:H	1.72	0.55
1:B:61:LEU:CD1	1:B:63:GLN:NE2	2.56	0.55
1:A:202:LEU:HD12	1:A:202:LEU:C	2.27	0.55
1:A:224:VAL:HG12	1:A:224:VAL:O	2.07	0.55
1:B:520:HIS:HE1	1:B:524:MET:CE	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:SER:C	1:A:540:ASN:N	2.60	0.55
1:B:178:GLU:C	1:B:180:TRP:H	2.10	0.55
1:B:178:GLU:O	1:B:180:TRP:N	2.39	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:232:HIS:O	1:A:234:GLY:N	2.40	0.54
1:A:66:GLN:HA	1:A:69:GLU:HG3	1.90	0.54
1:A:26:ARG:O	1:A:28:ARG:N	2.40	0.54
1:B:230:ARG:CB	1:B:230:ARG:HH11	2.20	0.54
1:A:456:GLU:HG3	1:B:568:VAL:HG13	1.89	0.54
1:A:181:LYS:H	1:A:181:LYS:NZ	2.06	0.54
1:B:173:TYR:CE2	1:B:198:LEU:HD13	2.43	0.54
1:A:350:LYS:HZ1	1:A:354:GLN:HE21	1.54	0.54
1:A:345:ILE:HB	1:A:369:GLN:OE1	2.08	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:B:291:ILE:HD13	1:B:314:TYR:CE1	2.42	0.54
1:B:428:ARG:HG2	1:B:428:ARG:NH1	2.23	0.53
1:A:489:ILE:HG13	1:A:516:ILE:HD11	1.90	0.53
1:A:99:LEU:HD13	1:A:133:LYS:HD3	1.89	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:426:MET:HA	1:B:426:MET:HE2	1.89	0.53
1:B:342:SER:HB2	1:B:373:ASN:OD1	2.08	0.53
1:A:531:PHE:O	1:A:531:PHE:CD1	2.61	0.53
1:A:518:ASP:CG	1:A:519:SER:H	2.12	0.53
1:B:202:LEU:HD12	1:B:202:LEU:C	2.29	0.53
1:B:551:GLU:O	1:B:554:PRO:HD3	2.09	0.53
1:A:199:TYR:CD1	1:A:217:TYR:HB2	2.43	0.53
1:A:432:LEU:CD2	1:A:436:ARG:HD3	2.39	0.53
1:A:531:PHE:C	1:A:531:PHE:CD1	2.82	0.53
1:A:245:SER:O	1:A:248:GLN:HB2	2.09	0.53
1:B:202:LEU:HD12	1:B:203:LEU:N	2.24	0.53
1:A:511:SER:O	1:A:515:LYS:HE2	2.09	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:340:THR:O	1:A:341:ASP:HB3	2.09	0.52
1:A:299:LEU:O	1:A:300:GLU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:HIS:N	1:A:232:HIS:CD2	2.77	0.52
1:B:238:ALA:HB3	1:B:239:GLN:HE21	1.73	0.52
1:A:307:LYS:HE3	1:A:335:GLN:HE22	1.74	0.52
1:B:509:PHE:O	1:B:513:ILE:HG13	2.09	0.52
1:B:137:ILE:CD1	1:B:138:ILE:HG13	2.37	0.52
1:B:468:THR:O	1:B:468:THR:HG22	2.10	0.52
1:B:531:PHE:CD1	1:B:531:PHE:C	2.83	0.52
1:A:401:ASP:CG	1:A:401:ASP:O	2.47	0.52
1:A:264:THR:HG22	1:A:265:LEU:N	2.24	0.52
1:A:156:VAL:HA	1:A:160:ALA:HB3	1.92	0.52
1:B:432:LEU:HD23	1:B:432:LEU:C	2.30	0.52
1:B:433:ALA:O	1:B:437:LYS:HG3	2.10	0.52
1:B:231:ARG:HG3	1:B:232:HIS:CD2	2.39	0.51
1:B:37:LEU:HD23	1:B:54:LEU:HB2	1.92	0.51
1:A:307:LYS:HE3	1:A:335:GLN:NE2	2.26	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:B:162:PHE:HD2	1:B:309:ARG:HG3	1.75	0.51
1:A:192:VAL:HG12	1:A:220:TRP:HZ2	1.75	0.51
1:A:547:LYS:O	1:A:551:GLU:HG3	2.10	0.51
1:A:579:LEU:C	1:A:581:TYR:H	2.12	0.51
1:B:520:HIS:HE1	1:B:524:MET:HE1	1.75	0.51
1:A:304:ASP:N	1:A:304:ASP:OD2	2.44	0.51
1:B:307:LYS:HZ2	1:B:338:LYS:HG3	1.76	0.50
1:B:68:TYR:CD2	1:B:68:TYR:N	2.78	0.50
1:B:202:LEU:HD21	1:B:213:MET:CG	2.42	0.50
1:A:189:GLN:C	1:A:189:GLN:NE2	2.65	0.50
1:A:292:ARG:O	1:A:295:SER:OG	2.23	0.50
1:B:81:MET:CE	1:B:319:GLN:HA	2.41	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:A:259:ARG:C	1:A:260:ASN:HD22	2.13	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:538:SER:OG	1:A:541:SER:HB2	2.12	0.50
1:B:290:TRP:C	1:B:290:TRP:CD1	2.84	0.50
1:A:89:LEU:HD21	1:A:107:VAL:CG1	2.41	0.50
1:B:189:GLN:HE21	1:B:190:GLN:N	2.08	0.50
1:A:326:GLU:O	1:A:326:GLU:HG3	2.09	0.50
1:B:544:THR:O	1:B:547:LYS:N	2.45	0.50
1:B:509:PHE:CE2	1:B:513:ILE:HD11	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:MET:HG3	1:A:331:MET:HE3	1.94	0.50
1:B:432:LEU:HD23	1:B:436:ARG:HD3	1.94	0.50
1:A:493:LEU:HD23	1:A:496:LEU:HD12	1.93	0.50
1:A:262:PRO:HG3	1:A:272:ASN:ND2	2.27	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: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:81:MET:CE	1:A:319:GLN:HA	2.42	0.49
1:A:426:MET:HG3	1:A:438:ILE:HD11	1.93	0.49
1:B:280:ASP:OD1	1:B:282:GLN:HB3	2.13	0.49
1:B:192:VAL:HG12	1:B:220:TRP:CZ2	2.47	0.49
1:A:167:ILE:CG2	1:A:168:GLN:N	2.75	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:493:LEU:O	1:B:494:ASP:C	2.50	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:A:22:ARG:CZ	1:A:22:ARG:HA	2.43	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:371:GLU:CD	1:B:539:LEU:HD22	2.33	0.49
1:B:299:LEU:O	1:B:300:GLU:HB2	2.13	0.49
1:B:282:GLN:NE2	1:B:282:GLN:HA	2.27	0.49
1:A:294:GLU:HG3	1:A:313:VAL:HG21	1.95	0.49
1:A:366:LEU:O	1:A:369:GLN:N	2.46	0.48
1:B:394:LEU:HG	1:B:398: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:B:542:VAL:HG12	1:B:546:GLU:HG3	1.95	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:B:214:TRP:CH2	1:B:233:ILE:HG23	2.48	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:428:ARG:NH2	1:B:539:LEU:HD13	2.29	0.48
1:B:550:PHE:CE2	1:B:558:LYS:HD3	2.48	0.48
1:A:145:ARG:HG2	1:A:145:ARG:O	2.12	0.48
1:A:474:VAL:O	1:A:477:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:TRP:CE3	1:A:191:ARG:HG3	2.48	0.48
1:B:55:LEU:HD22	1:B:67:VAL:HG13	1.94	0.48
1:B:292:ARG:O	1:B:293:TRP:C	2.50	0.48
1:A:89:LEU:HD21	1:A:107:VAL:HG12	1.95	0.48
1:A:181:LYS:H	1:A:181:LYS:HZ3	1.61	0.48
1:A:553:PHE:HB3	1:A:556:VAL:CG2	2.44	0.48
1:A:359:SER:HA	1:B:578:GLU:OE2	2.13	0.48
1:A:52:VAL:HG11	1:A:268:ALA:HB3	1.95	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:350:LYS:HZ1	1:A:354:GLN:NE2	2.12	0.48
1:B:189:GLN:NE2	1:B:190:GLN:N	2.62	0.48
1:B:539:LEU:HA	1:B:542:VAL:CG2	2.43	0.47
1:B:224:VAL:O	1:B:224:VAL:HG12	2.14	0.47
1:B:358:ASN:ND2	1:B:358:ASN:C	2.66	0.47
1:A:192:VAL:HG12	1:A:220:TRP:CZ2	2.49	0.47
1:B:225:ASN:C	1:B:227:LEU:H	2.18	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:B:55:LEU:CD2	1:B:70:THR:HB	2.44	0.47
1:B:432:LEU:CD2	1:B:436:ARG:HD3	2.44	0.47
1:A:462:TYR:C	1:A:464:ILE:H	2.17	0.47
1:B:518:ASP:CG	1:B:519:SER:H	2.17	0.47
1:B:121:LEU:HD21	1:B:169:PHE:HB2	1.96	0.47
1:B:538:SER:C	1:B:540:ASN:N	2.66	0.47
1:A:372:LEU:C	1:A:374:THR:H	2.17	0.47
1:B:246:LEU:HD22	1:B:293:TRP:CZ2	2.50	0.47
1:B:222:GLN:C	1:B:224:VAL:H	2.18	0.47
1:B:293:TRP:NE1	1:B:298:LYS:HD2	2.29	0.47
1:A:553:PHE:C	1:A:554:PRO:O	2.50	0.47
1:A:212:SER:O	1:A:216:ARG:HG3	2.14	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:B:221:GLU:HA	1:B:221:GLU:OE1	2.15	0.47
1:A:445:LEU:O	1:A:446:LYS:HB2	2.14	0.47
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:297:ASN:HB2	1:A:306:HIS:CD2	2.50	0.46
1:A:329:PHE:CG	1:B:559:LEU:HD13	2.51	0.46
1:A:479:LEU:HD12	1:A:483:ALA:CA	2.44	0.46
1:B:112:LEU:HD22	1:B:124:TRP:CH2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:PHE:HZ	1:A:526:PHE:CE2	2.34	0.46
1:B:307:LYS:CD	1:B:338:LYS:HD2	2.38	0.46
1:A:543:ARG:NH1	1:A:543:ARG:HA	2.30	0.46
1:A:520:HIS:HE1	1:A:524:MET:HE1	1.80	0.46
1:A:350:LYS:HZ2	1:A:354:GLN:HE21	1.63	0.46
1:B:568:VAL:O	1:B:569:LEU:HB2	2.15	0.46
1:A:407:ALA:O	1:A:411:LEU:HD13	2.15	0.46
1:B:284:LEU:O	1:B:288:LEU:HG	2.15	0.46
1:A:439:PHE:CD2	1:A:457:ASN:OD1	2.69	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:B:77:ARG:C	1:B:79:PRO:HD3	2.36	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:HA	1:B:448:LEU:HD12	1.75	0.46
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:B:401:ASP:O	1:B:401:ASP:CG	2.55	0.45
1:A:519:SER:OG	1:A:520:HIS:N	2.49	0.45
1:B:107:VAL:HG12	1:B:108:LEU:N	2.31	0.45
1:A:142:GLU:O	1:A:146:ASN:HB2	2.16	0.45
1:B:452:ASP:O	1:B:456:GLU:HB2	2.17	0.45
1:B:209:CYS:O	1:B:213:MET:HB2	2.16	0.45
1:B:484:THR:HG22	1:B:484:THR:O	2.16	0.45
1:A:550:PHE:CD2	1:A:558:LYS:HD3	2.52	0.45
1:B:125:LEU:HA	1:B:125:LEU:HD23	1.53	0.45
1:A:569:LEU:O	1:A:571:VAL:HG23	2.16	0.45
1:B:416:THR:HG21	1:B:450:THR:HG22	1.99	0.45
1:B:425:THR:HG22	1:B:426:MET:HE3	1.97	0.45
1:B:564:ASN:O	1:B:567:LYS:HG3	2.16	0.45
1:A:264:THR:HG22	1:A:266:ASN:H	1.81	0.45
1:A:37:LEU:HD23	1:A:54:LEU:HA	1.98	0.45
1:A:484:THR:HG22	1:A:484:THR:O	2.16	0.45
1:A:560:GLU:HA	1:A:582:MET:HE3	1.97	0.45
1:B:144:ALA:C	1:B:146:ASN:H	2.19	0.45
1:B:380:GLU:O	1:B:384:LEU:HB2	2.17	0.45
1:A:475:LEU:H	1:A:475:LEU:CD1	2.04	0.45
1:B:115:GLU:N	1:B:115:GLU:CD	2.60	0.45
1:A:115:GLU:HG2	1:A:116:LEU:N	2.23	0.45
1:A:236:LEU:O	1:A:237:SER:C	2.55	0.45
1:B:523:LYS:HB2	1:B:553:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:PHE:HD1	1:B:273:LEU:HD12	1.82	0.45
1:A:128:ILE:HD11	1:A:152:PHE:HA	1.99	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:B:125:LEU:CD1	1:B:168:GLN:NE2	2.80	0.44
1:B:519:SER:O	1:B:521:LEU:N	2.50	0.44
1:B:565:LYS:NZ	1:B:565:LYS:HB3	2.32	0.44
1:B:182:PRO:HG2	1:B:188:GLU:HA	1.98	0.44
1:A:573:TYR:O	1:A:574:LEU:C	2.56	0.44
1:B:200:LYS:HD3	1:B:236:LEU:CD2	2.20	0.44
1:B:115:GLU:HG2	1:B:116:LEU:N	2.27	0.44
1:B:520:HIS:O	1:B:520:HIS:ND1	2.49	0.44
1:B:436:ARG:O	1:B:437:LYS:C	2.55	0.44
1:A:485:ASP:CG	1:A:487:GLU:HB3	2.38	0.44
1:A:428:ARG:HD2	1:A:428:ARG:O	2.17	0.44
1:B:337:GLU:O	1:B:338:LYS:O	2.35	0.44
1:A:244:ARG:HB3	1:A:244:ARG:HH11	1.81	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:B:177:LEU:HA	1:B:177:LEU:HD23	1.77	0.44
1:A:81:MET:HE2	1:A:319:GLN:HA	1.98	0.44
1:A:508:LEU:HD12	1:A:508:LEU:O	2.17	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:560:GLU:HG3	1:A:582:MET:HE3	2.00	0.44
1:B:140:GLY:CA	1:B:144:ALA:HB2	2.46	0.44
1:A:520:HIS:HE1	1:A:524:MET:HE3	1.81	0.44
1:A:572:ASN:HD21	1:A:574:LEU:HB2	1.83	0.44
1:B:79:PRO:HB3	1:B:116:LEU:HD13	1.99	0.44
1:B:493:LEU:HD22	1:B:505:VAL:HG13	1.99	0.44
1:B:174:LEU:HA	1:B:174:LEU:HD23	1.77	0.44
1:A:454:TYR:HE1	1:A:482:PHE:HE1	1.64	0.44
1:A:438:ILE:O	1:A:441:LYS:HG2	2.18	0.44
1:A:468:THR:CG2	1:A:468:THR:O	2.65	0.44
1:A:579:LEU:HD23	1:A:579:LEU:N	2.32	0.44
1:A:25:SER:O	1:A:27:VAL:N	2.46	0.43
1:B:508:LEU:O	1:B:508:LEU:HD12	2.17	0.43
1:A:207:MET:HB3	1:A:207:MET:HE3	1.64	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:B:214:TRP:O	1:B:215:GLN:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LYS:H	1:B:181:LYS:NZ	2.16	0.43
1:A:477:LEU:HD13	1:A:477:LEU:HA	1.87	0.43
1:B:225:ASN:O	1:B:227:LEU:N	2.51	0.43
1:B:426:MET:CE	1:B:426:MET:HA	2.48	0.43
1:A:52:VAL:HG11	1:A:268:ALA:CB	2.48	0.43
1:A:528:LYS:HB2	1:A:528:LYS:NZ	2.33	0.43
1:A:197:LYS:O	1:A:197:LYS:HG2	2.19	0.43
1:A:22:ARG:HB3	1:A:23:PRO:HD3	2.00	0.43
1:A:456:GLU:HG3	1:B:568:VAL:CG1	2.48	0.43
1:A:187:GLU:C	1:A:189:GLN:N	2.70	0.43
1:B:137:ILE:HD12	1:B:138:ILE:N	2.33	0.43
1:A:84:ILE:HA	1:A:87:MET:CE	2.49	0.43
1:B:539:LEU:HA	1:B:542:VAL:HG23	2.00	0.43
1:B:115:GLU:HB2	1:B:347:LYS:NZ	2.33	0.43
1:A:441:LYS:O	1:A:444:ARG:HB3	2.19	0.43
1:A:121:LEU:O	1:A:121:LEU:HD23	2.19	0.43
1:B:372:LEU:C	1:B:374:THR:H	2.22	0.43
1:B:492:TYR:O	1:B:495:PHE:HB3	2.19	0.43
1:B:462:TYR:O	1:B:464:ILE:N	2.52	0.43
1:A:385:SER:O	1:A:386:CYS:C	2.56	0.43
1:B:37:LEU:CD2	1:B:54:LEU:HA	2.48	0.43
1:B:56:LYS:CG	1:B:265:LEU:HD23	2.48	0.43
1:B:232:HIS:C	1:B:234:GLY:N	2.72	0.43
1:B:143:GLU:HA	1:B:146:ASN:HB3	2.01	0.43
1:A:520:HIS:CE1	1:A:524:MET:HE3	2.54	0.43
1:B:259:ARG:C	1:B:260:ASN:HD22	2.21	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:B:366:LEU:O	1:B:367:SER:C	2.57	0.42
1:B:366:LEU:O	1:B:369:GLN:N	2.52	0.42
1:B:37:LEU:HD23	1:B:54:LEU:CB	2.49	0.42
1:A:451:PRO:HG3	1:A:482:PHE:CG	2.54	0.42
1:B:191:ARG:O	1:B:191:ARG:HG2	2.18	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:A:430:GLN:O	1:A:434:ALA:HB2	2.19	0.42
1:A:297:ASN:CG	1:A:297:ASN:O	2.56	0.42
1:A:492:TYR:O	1:A:495:PHE:HB3	2.19	0.42
1:B:90:SER:O	1:B:91:LEU:C	2.58	0.42
1:B:471:ALA:O	1:B:475:LEU:HD11	2.19	0.42
1:A:180:TRP:C	1:A:180:TRP:CD1	2.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LYS:HE3	1:B:208:ASP:HB3	2.02	0.42
1:B:140:GLY:C	1:B:144:ALA:HB2	2.38	0.42
1:B:368:GLU:O	1:B:372:LEU:HD13	2.20	0.42
1:B:137:ILE:HG22	1:B:145:ARG:HB2	2.01	0.42
1:A:436:ARG:HG2	1:A:436:ARG:HH11	1.85	0.42
1:B:460:ILE:C	1:B:462:TYR:N	2.73	0.42
1:A:575:GLN:O	1:A:580:ASP:HA	2.19	0.42
1:A:479:LEU:HD12	1:A:479:LEU:HA	1.78	0.42
1:A:232:HIS:O	1:A:235:GLU:OE1	2.37	0.42
1:B:531:PHE:O	1:B:531:PHE:CD1	2.72	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:279:TYR:CE2	1:B:324:ALA:HA	2.54	0.42
1:B:262:PRO:HG2	1:B:268:ALA:HA	2.02	0.42
1:B:77:ARG:O	1:B:79:PRO:HD3	2.20	0.42
1:B:512:SER:HB2	1:B:516:ILE:HG13	2.01	0.42
1:A:493:LEU:HD23	1:A:493:LEU:HA	1.89	0.42
1:B:263:ILE:HG13	1:B:263:ILE:H	1.80	0.42
1:B:231:ARG:HD2	1:B:231:ARG:C	2.40	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:A:112:LEU:HD22	1:A:124:TRP:CH2	2.54	0.41
1:B:412:LYS:NZ	1:B:447:LYS:O	2.39	0.41
1:B:51:TYR:CD2	1:B:74:LEU:HD21	2.55	0.41
1:A:550:PHE:CE2	1:A:558:LYS:HA	2.55	0.41
1:A:236:LEU:C	1:A:238:ALA:N	2.71	0.41
1:B:202:LEU:HD11	1:B:213:MET:HG2	2.02	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:B:142:GLU:C	1:B:144:ALA:N	2.74	0.41
1:A:37:LEU:HD23	1:A:54:LEU:CA	2.50	0.41
1:B:119:ASN:OD1	1:B:159:CYS:HB2	2.19	0.41
1:B:81:MET:HE2	1:B:319:GLN:HA	2.01	0.41
1:A:539:LEU:HD23	1:B:372:LEU:HD11	2.01	0.41
1:A:446:LYS:HB3	1:A:447:LYS:H	1.45	0.41
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.84	0.41
1:B:164:PRO:HG2	1:B:250:TRP:CZ2	2.55	0.41
1:A:195:ILE:HG22	1:A:195:ILE:O	2.21	0.41
1:B:519:SER:C	1:B:521:LEU:N	2.74	0.41
1:B:144:ALA:C	1:B:146:ASN:N	2.74	0.41
1:B:249:ASP:O	1:B:250:TRP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:HD21	1:B:169:PHE:HD1	1.85	0.41
1:A:138:ILE:HG22	1:A:139:THR:HG23	2.02	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:A:164:PRO:HG3	1:A:250:TRP:CE2	2.55	0.41
1:A:479:LEU:HD11	1:A:483:ALA:HA	2.01	0.41
1:A:187:GLU:O	1:A:189:GLN:N	2.54	0.41
1:B:394:LEU:CG	1:B:398:MET:HE3	2.51	0.41
1:A:253:ILE:HG23	1:A:289:GLU:HG3	2.02	0.41
1:B:526:PHE:O	1:B:530:ILE:HG13	2.21	0.41
1:B:232:HIS:HA	1:B:235:GLU:OE1	2.20	0.41
1:A:464:ILE:HB	1:A:465:SER:H	1.65	0.41
1:B:195:ILE:HG22	1:B:195:ILE:O	2.20	0.41
1:B:243:ALA:O	1:B:246:LEU:N	2.54	0.41
1:A:493:LEU:HD22	1:A:505:VAL:HG13	2.02	0.41
1:B:464:ILE:HB	1:B:465:SER:H	1.71	0.41
1:B:137:ILE:H	1:B:137:ILE:HG13	1.69	0.41
1:B:574:LEU:HA	1:B:574:LEU:HD23	1.81	0.41
1:B:246:LEU:HA	1:B:246:LEU:HD23	1.86	0.41
1:A:579:LEU:O	1:A:581:TYR:N	2.54	0.41
1:A:485:ASP:OD2	1:A:487:GLU:HB3	2.21	0.41
1:B:465:SER:O	1:B:467:ASP:N	2.54	0.41
1:B:74:LEU:HA	1:B:74:LEU:HD23	1.86	0.41
1:A:466:LYS:HZ1	1:B:500:ASN:HB3	1.86	0.41
1:A:416:THR:HG23	1:A:449:VAL:HB	2.03	0.41
1:A:24:THR:CB	1:A:43:GLU:OE2	2.69	0.41
1:A:466:LYS:HA	1:A:466:LYS:HD3	1.94	0.41
1:A:77:ARG:C	1:A:79:PRO:HD3	2.42	0.41
1:B:463:HIS:CD2	1:B:466:LYS:HE2	2.55	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:A:178:GLU:C	1:A:180:TRP:N	2.72	0.40
1:A:394:LEU:HD21	1:A:398:MET:HE1	2.03	0.40
1:A:358:ASN:C	1:A:358:ASN:ND2	2.66	0.40
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:340:THR:O	1:B:341:ASP:HB3	2.21	0.40
1:A:301:LEU:HB3	1:A:305:LEU:HB3	2.03	0.40
1:A:254:THR:HG22	1:A:255:LYS:N	2.36	0.40
1:A:34:ILE:CG1	1:A:57:HIS:CD2	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:538:SER:CB	1:A:541:SER:OG	2.69	0.40
1:A:292:ARG:CB	1:A:292:ARG:HH11	2.27	0.40
1:A:358:ASN:O	1:A:414:LYS:NZ	2.54	0.40
1:A:533:GLU:HG3	1:A:545:LEU:CD1	2.50	0.40
1:A:417:TYR:OH	1:B:574:LEU:HG	2.20	0.40
1:A:520:HIS:ND1	1:A:520:HIS:O	2.54	0.40
1:A:366:LEU:HD22	1:A:370:TYR:CE1	2.56	0.40
1:B:464:ILE:HG13	1:B:464:ILE:H	1.74	0.40
1:B:74:LEU:HD13	1:B:84:ILE:HD13	2.04	0.40
1:A:453:ILE:HA	1:A:453:ILE:HD12	1.93	0.40
1:A:389:ARG:HD2	1:A:389:ARG:HA	1.86	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
1:B:394:LEU:HG	1:B:398:MET:CE	2.51	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

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%)	2	14
1	B	550/678 (81%)	439 (80%)	87 (16%)	24 (4%)	3	18
All	All	1101/1356 (81%)	869 (79%)	178 (16%)	54 (5%)	3	16

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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	468 (90%)	49 (10%)	11	38
1	B	513/623 (82%)	455 (89%)	58 (11%)	7	28
All	All	1030/1246 (83%)	923 (90%)	107 (10%)	9	32

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	39	ASP
1	A	71	PHE
1	A	97	GLU
1	A	121	LEU
1	A	126	SER
1	A	129	THR
1	A	159	CYS
1	A	174	LEU
1	A	179	HIS
1	A	185	LYS
1	A	189	GLN

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Mol	Chain	Res	Type
1	A	191	ARG
1	A	192	VAL
1	A	202	LEU
1	A	242	ASN
1	A	244	ARG
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	314	TYR
1	A	326	GLU
1	A	358	ASN
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	436	ARG
1	A	448	LEU
1	A	450	THR
1	A	475	LEU
1	A	477	LEU
1	A	479	LEU
1	A	480	LYS
1	A	492	TYR
1	A	507	SER
1	A	521	LEU
1	A	540	ASN
1	A	543	ARG
1	A	544	THR
1	A	572	ASN
1	B	39	ASP
1	B	71	PHE
1	B	77	ARG
1	B	97	GLU
1	B	115	GLU

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Mol	Chain	Res	Type
1	B	121	LEU
1	B	128	ILE
1	B	129	THR
1	B	159	CYS
1	B	174	LEU
1	B	179	HIS
1	B	185	LYS
1	B	189	GLN
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	265	LEU
1	B	278	GLU
1	B	292	ARG
1	B	296	ASP
1	B	301	LEU
1	B	304	ASP
1	B	314	TYR
1	B	339	ASN
1	B	356	ILE
1	B	358	ASN
1	B	366	LEU
1	B	388	ASP
1	B	391	HIS
1	B	401	ASP
1	B	406	SER
1	B	413	SER
1	B	416	THR
1	B	427	LYS
1	B	428	ARG
1	B	429	ILE
1	B	435	SER
1	B	436	ARG
1	B	448	LEU
1	B	450	THR
1	B	475	LEU
1	B	477	LEU

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Mol	Chain	Res	Type
1	B	479	LEU
1	B	492	TYR
1	B	507	SER
1	B	510	GLU
1	B	521	LEU
1	B	539	LEU
1	B	540	ASN
1	B	543	ARG
1	B	544	THR
1	B	565	LYS
1	B	572	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	118	ASN
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	330	ASN
1	A	335	GLN
1	A	354	GLN
1	A	504	GLN
1	A	520	HIS
1	A	527	GLN
1	A	572	ASN
1	B	63	GLN
1	B	66	GLN
1	B	118	ASN
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

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Mol	Chain	Res	Type
1	B	391	HIS
1	B	410	GLN
1	B	500	ASN
1	B	504	GLN
1	B	520	HIS
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.13	2 (0%) 93 80	30, 69, 113, 128	0
1	B	552/678 (81%)	-0.14	3 (0%) 91 76	30, 70, 115, 138	0
All	All	1107/1356 (81%)	-0.13	5 (0%) 91 76	30, 70, 114, 138	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	LEU	3.5
1	A	137	ILE	3.1
1	B	30	GLU	2.6
1	B	231	ARG	2.3
1	A	471	ALA	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.