Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 06:44 AM EDT

PDB ID	:	1UK0
Title	:	Crystal structure of catalytic domain of human poly(ADP-ribose) polymerase with a novel inhibitor
Authors	:	Kinoshita, T.
Deposited on	:	2003-08-13
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 (i) 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 (i)) were used in the production of this report:

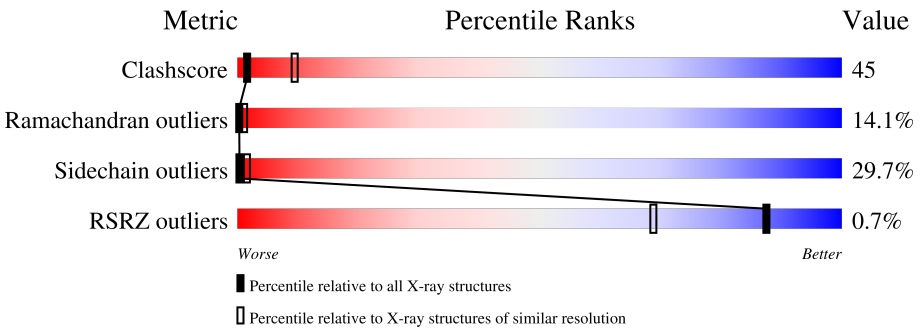
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	350	% 15% 34% 29% 22%
1	B	350	% 8% 30% 37% 25%

2 Entry composition (i)

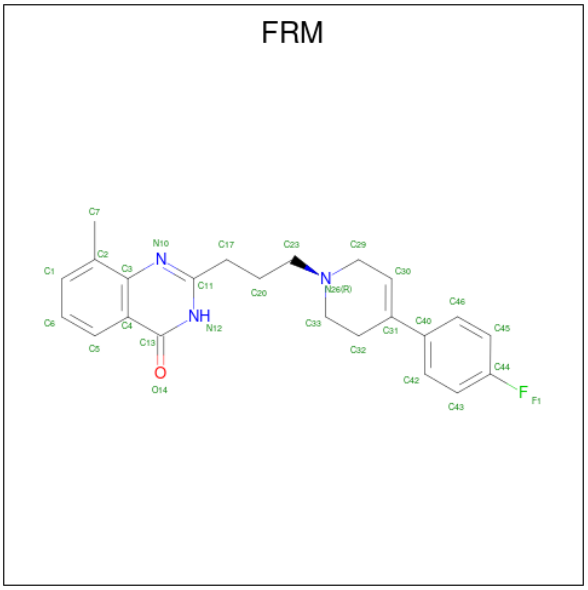
There are 3 unique types of molecules in this entry. The entry contains 5817 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Poly [ADP-ribose] polymerase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	350	2754	1752	465	526	11	0	0	0
			Total	C	N	O	S			
1	B	350	2754	1752	465	526	11	0	0	0

- Molecule 2 is 2-{3-[4-(4-FLUOROPHENYL)-3,6-DIHYDRO-1(2H)-PYRIDINYL]PROPYL}-8-METHYL-4(3H)-QUINAZOLINONE (three-letter code: FRM) (formula: $C_{23}H_{24}FN_3O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	28	23	1	3	1	0	0
			Total	C	F	N	O		
2	B	1	28	23	1	3	1	0	0

- Molecule 3 is water.

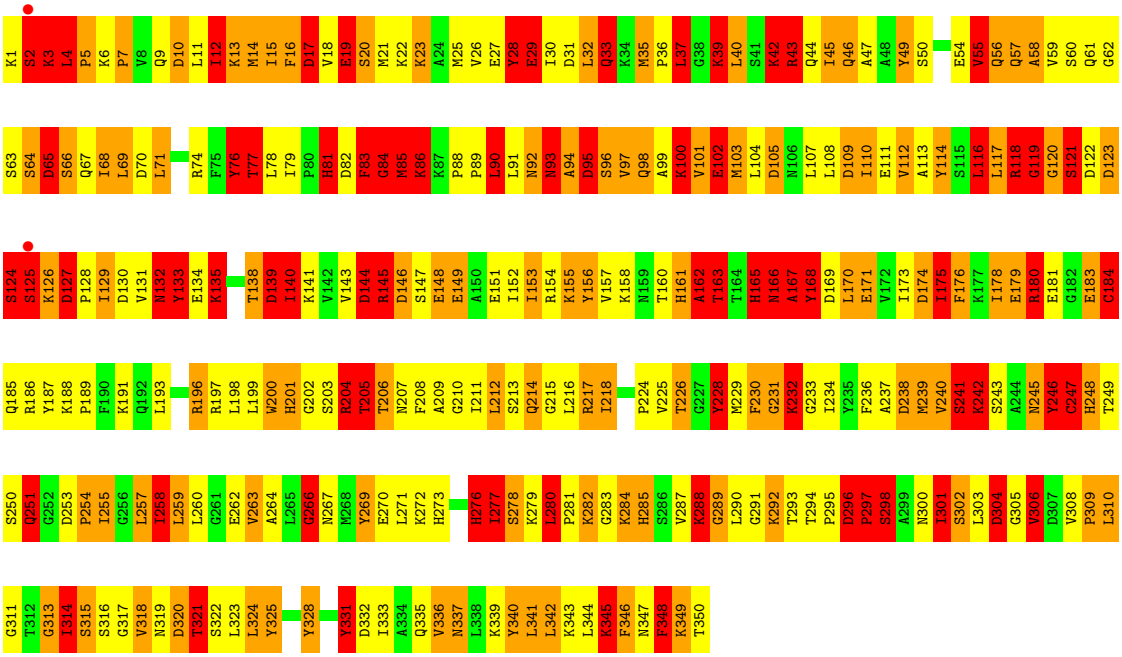
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	124	124	124	0	0
			Total	O		
3	B	129	129	129	0	0

3 Residue-property plots (i)

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.

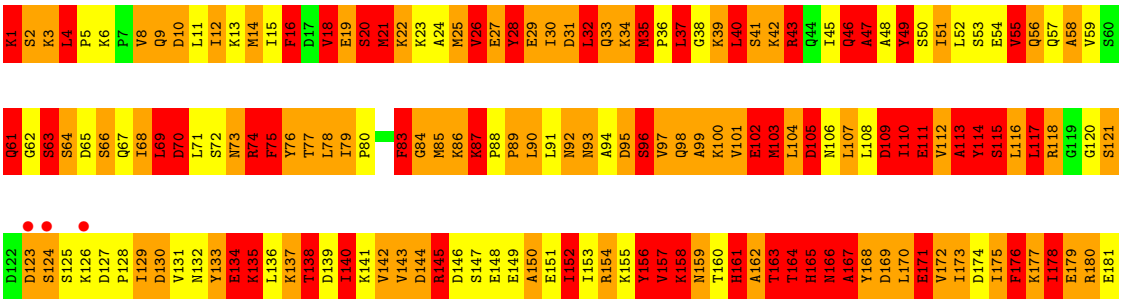
• Molecule 1: Poly [ADP-ribose] polymerase-1

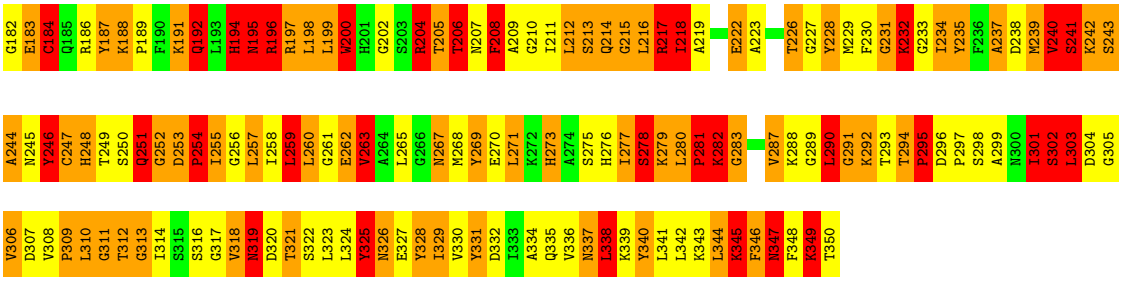
Chain A:



• Molecule 1: Poly [ADP-ribose] polymerase-1

Chain B:




G182 E183 C184 Q185 R186 Y187 K188 P189 F190 K191 Q192 L193 H194 N195 R196 R197 L198 L199 W200 H201 G202 S203 R204 T205 T206 N207 F208 A209 G210 I211 L212 S213 Q214 G215 L216 R217 I218 A219 E222 A223 T226 G227 Y228 M229 F230 G231 K232 G233 I234 Y235 F236 A237 D238 M239 V240 S241 K242 S243
A244 N245 Y246 C247 H248 T249 S250 Q251 G252 D253 P254 I255 G256 L257 I258 L259 L260 G261 E262 V263 A264 L265 G266 N267 M268 Y269 E270 L271 K272 H273 A274 S275 H276 I277 S278 K279 L280 P281 K282 G283 V287 K288 G289 L290 G291 K292 T293 T294 P295 D296 P297 S298 A299 N300 I301 S302 L303 D304 G305
V306 D307 V308 P309 L310 G311 T312 G313 I314 S315 S316 G317 V318 N319 D320 T321 S322 L323 L324 Y325 N326 E327 Y328 I329 V330 Y331 D332 I333 A334 Q335 V336 N337 L338 K339 Y340 L341 L342 K343 L344 K345 F346 N347 F348 K349 T350

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	179.82Å 53.55Å 92.01Å 90.00° 114.40° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 95.8 (50.90-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.01Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.219 , 0.246 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 113.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5817	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.69	32/2806 (1.1%)	2.79	273/3786 (7.2%)
1	B	1.76	28/2806 (1.0%)	2.89	311/3786 (8.2%)
All	All	1.73	60/5612 (1.1%)	2.84	584/7572 (7.7%)

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	47
1	B	0	39
All	All	0	86

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	LYS	C-N	11.68	1.54	1.33
1	B	262	GLU	CD-OE2	11.28	1.38	1.25
1	B	304	ASP	CB-CG	10.02	1.72	1.51
1	B	282	LYS	C-O	-9.09	1.06	1.23
1	B	282	LYS	CA-C	8.97	1.76	1.52
1	B	322	SER	CB-OG	8.92	1.53	1.42
1	B	184	CYS	CB-SG	7.96	1.95	1.82
1	B	242	LYS	CD-CE	7.95	1.71	1.51
1	B	305	GLY	CA-C	7.82	1.64	1.51
1	B	2	SER	CA-CB	7.31	1.64	1.52
1	A	315	SER	CA-CB	-7.19	1.42	1.52
1	B	304	ASP	CA-CB	6.95	1.69	1.53
1	A	200	TRP	NE1-CE2	6.80	1.46	1.37
1	A	28	TYR	CE1-CZ	6.79	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ARG	NE-CZ	6.67	1.41	1.33
1	B	154	ARG	NE-CZ	6.57	1.41	1.33
1	A	350	THR	CA-C	6.31	1.69	1.52
1	B	121	SER	CA-CB	6.23	1.62	1.52
1	A	241	SER	C-N	6.22	1.48	1.34
1	B	125	SER	CB-OG	6.05	1.50	1.42
1	A	161	HIS	CB-CG	6.04	1.60	1.50
1	A	242	LYS	CG-CD	6.02	1.73	1.52
1	B	282	LYS	CD-CE	5.98	1.66	1.51
1	B	213	SER	CB-OG	5.91	1.50	1.42
1	A	81	HIS	CA-C	5.89	1.68	1.52
1	A	206	THR	CB-OG1	5.88	1.55	1.43
1	B	21	MET	CA-C	5.85	1.68	1.52
1	B	346	PHE	CB-CG	-5.83	1.41	1.51
1	B	322	SER	CA-CB	5.83	1.61	1.52
1	A	28	TYR	CG-CD1	5.82	1.46	1.39
1	A	110	ILE	CA-CB	-5.82	1.41	1.54
1	B	282	LYS	N-CA	5.79	1.57	1.46
1	A	197	ARG	NE-CZ	5.77	1.40	1.33
1	A	242	LYS	CD-CE	5.76	1.65	1.51
1	A	251	GLN	C-N	5.70	1.43	1.33
1	B	183	GLU	CD-OE1	-5.67	1.19	1.25
1	A	288	LYS	CA-C	5.66	1.67	1.52
1	A	57	GLN	CG-CD	5.62	1.64	1.51
1	A	109	ASP	CA-C	5.60	1.67	1.52
1	A	317	GLY	N-CA	5.59	1.54	1.46
1	A	204	ARG	CZ-NH2	5.47	1.40	1.33
1	A	119	GLY	CA-C	5.46	1.60	1.51
1	A	122	ASP	CA-C	5.46	1.67	1.52
1	B	308	VAL	C-N	5.45	1.44	1.34
1	A	296	ASP	C-N	5.33	1.44	1.34
1	B	161	HIS	CG-CD2	5.32	1.44	1.35
1	A	313	GLY	C-N	5.29	1.46	1.34
1	B	306	VAL	C-O	-5.27	1.13	1.23
1	A	60	SER	CB-OG	5.25	1.49	1.42
1	A	217	ARG	NE-CZ	5.23	1.39	1.33
1	A	183	GLU	CD-OE1	-5.15	1.20	1.25
1	B	192	GLN	CG-CD	5.15	1.62	1.51
1	A	322	SER	CB-OG	5.14	1.49	1.42
1	A	144	ASP	CB-CG	5.09	1.62	1.51
1	B	151	GLU	CG-CD	5.04	1.59	1.51
1	B	283	GLY	CA-C	-5.04	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	GLU	CG-CD	5.04	1.59	1.51
1	A	33	GLN	CG-CD	5.04	1.62	1.51
1	B	121	SER	CB-OG	5.03	1.48	1.42
1	A	217	ARG	CZ-NH1	5.01	1.39	1.33

All (584) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	ARG	NE-CZ-NH1	17.58	129.09	120.30
1	B	43	ARG	NE-CZ-NH1	-16.29	112.15	120.30
1	A	43	ARG	NE-CZ-NH1	15.72	128.16	120.30
1	A	118	ARG	NE-CZ-NH2	-14.63	112.98	120.30
1	A	204	ARG	NE-CZ-NH1	-14.05	113.27	120.30
1	B	235	TYR	CB-CG-CD2	-13.77	112.74	121.00
1	A	49	TYR	CB-CG-CD2	-13.58	112.85	121.00
1	B	156	TYR	CB-CG-CD1	13.39	129.03	121.00
1	B	328	TYR	CB-CG-CD2	-13.25	113.05	121.00
1	B	306	VAL	CA-CB-CG2	13.12	130.59	110.90
1	B	61	GLN	N-CA-CB	-13.08	87.06	110.60
1	B	93	ASN	N-CA-CB	-12.80	87.56	110.60
1	A	331	TYR	CB-CG-CD2	-12.35	113.59	121.00
1	A	10	ASP	CB-CG-OD2	-12.17	107.35	118.30
1	B	54	GLU	CA-CB-CG	-11.81	87.41	113.40
1	B	262	GLU	OE1-CD-OE2	-11.75	109.20	123.30
1	A	196	ARG	NE-CZ-NH1	11.69	126.15	120.30
1	A	180	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	B	325	TYR	CB-CG-CD2	-11.52	114.09	121.00
1	A	200	TRP	CG-CD2-CE3	-11.46	123.58	133.90
1	A	168	TYR	CB-CG-CD1	-11.35	114.19	121.00
1	B	217	ARG	NE-CZ-NH2	-11.30	114.65	120.30
1	B	235	TYR	CB-CG-CD1	11.27	127.76	121.00
1	B	347	ASN	N-CA-CB	-10.91	90.97	110.60
1	A	186	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	A	47	ALA	CB-CA-C	-10.82	93.87	110.10
1	B	346	PHE	CB-CG-CD1	-10.80	113.24	120.80
1	B	169	ASP	CB-CG-OD2	10.65	127.89	118.30
1	B	21	MET	CG-SD-CE	-10.64	83.18	100.20
1	A	149	GLU	CA-CB-CG	10.64	136.80	113.40
1	B	25	MET	CA-CB-CG	-10.57	95.34	113.30
1	B	282	LYS	CA-C-N	-10.52	95.15	116.20
1	B	74	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	B	281	PRO	N-CA-CB	-10.46	90.74	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	8	VAL	CA-CB-CG2	-10.36	95.36	110.90
1	A	178	ILE	CB-CA-C	-10.33	90.93	111.60
1	B	282	LYS	O-C-N	10.23	140.60	123.20
1	A	74	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	B	346	PHE	CD1-CG-CD2	10.16	131.50	118.30
1	B	9	GLN	CA-CB-CG	10.10	135.63	113.40
1	B	306	VAL	CG1-CB-CG2	-10.04	94.84	110.90
1	B	49	TYR	CB-CG-CD2	-9.89	115.06	121.00
1	B	35	MET	CA-CB-CG	9.83	130.01	113.30
1	A	118	ARG	CB-CG-CD	9.77	137.00	111.60
1	B	268	MET	CG-SD-CE	9.69	115.70	100.20
1	B	156	TYR	CB-CG-CD2	-9.69	115.19	121.00
1	A	145	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	B	282	LYS	C-N-CA	-9.48	102.38	122.30
1	B	49	TYR	CB-CG-CD1	9.30	126.58	121.00
1	B	4	LEU	CB-CA-C	-9.22	92.69	110.20
1	B	318	VAL	C-N-CA	-9.20	98.70	121.70
1	A	258	ILE	CB-CG1-CD1	-9.19	88.17	113.90
1	B	209	ALA	CB-CA-C	-9.10	96.44	110.10
1	B	74	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	B	226	THR	CA-CB-CG2	9.06	125.09	112.40
1	A	337	ASN	N-CA-CB	-8.96	94.47	110.60
1	B	112	VAL	CG1-CB-CG2	-8.95	96.57	110.90
1	A	175	ILE	CA-CB-CG1	8.94	127.99	111.00
1	B	303	LEU	CB-CG-CD1	-8.94	95.80	111.00
1	A	156	TYR	CB-CG-CD2	-8.66	115.80	121.00
1	B	107	LEU	CB-CA-C	-8.64	93.79	110.20
1	B	145	ARG	CD-NE-CZ	-8.60	111.56	123.60
1	A	277	ILE	CA-CB-CG1	8.58	127.31	111.00
1	B	177	LYS	CA-CB-CG	8.53	132.17	113.40
1	A	56	GLN	N-CA-CB	8.52	125.94	110.60
1	A	340	TYR	CB-CG-CD1	-8.52	115.89	121.00
1	A	118	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	103	MET	CA-CB-CG	8.49	127.73	113.30
1	A	197	ARG	CB-CA-C	-8.46	93.48	110.40
1	B	197	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	A	217	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	A	28	TYR	CB-CG-CD2	-8.41	115.95	121.00
1	A	301	ILE	CA-CB-CG1	-8.39	95.05	111.00
1	A	197	ARG	CD-NE-CZ	-8.39	111.86	123.60
1	B	79	ILE	CA-CB-CG2	8.38	127.67	110.90
1	A	40	LEU	C-N-CA	-8.36	100.80	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	169	ASP	C-N-CA	-8.35	100.83	121.70
1	B	345	LYS	CA-C-N	-8.32	98.90	117.20
1	B	242	LYS	CA-CB-CG	8.31	131.69	113.40
1	B	304	ASP	CA-CB-CG	8.30	131.67	113.40
1	A	203	SER	N-CA-CB	-8.29	98.07	110.50
1	A	168	TYR	CG-CD2-CE2	-8.27	114.69	121.30
1	A	315	SER	N-CA-CB	-8.26	98.11	110.50
1	A	316	SER	C-N-CA	-8.21	105.06	122.30
1	A	320	ASP	CB-CG-OD1	8.20	125.68	118.30
1	B	61	GLN	CB-CG-CD	-8.18	90.32	111.60
1	A	178	ILE	CA-CB-CG1	8.16	126.50	111.00
1	B	209	ALA	N-CA-CB	8.13	121.49	110.10
1	A	246	TYR	CB-CG-CD2	-8.12	116.12	121.00
1	B	75	PHE	CB-CG-CD1	-8.08	115.14	120.80
1	A	288	LYS	N-CA-CB	-8.06	96.10	110.60
1	A	200	TRP	CD1-NE1-CE2	-8.04	101.77	109.00
1	A	201	HIS	CA-CB-CG	-8.01	99.98	113.60
1	B	200	TRP	CB-CG-CD2	8.01	137.01	126.60
1	A	263	VAL	CG1-CB-CG2	-8.00	98.10	110.90
1	B	273	HIS	CB-CA-C	-8.00	94.40	110.40
1	B	55	VAL	C-N-CA	-7.99	101.74	121.70
1	A	243	SER	CB-CA-C	-7.98	94.94	110.10
1	A	228	TYR	CB-CG-CD2	-7.98	116.21	121.00
1	B	68	ILE	CG1-CB-CG2	-7.95	93.90	111.40
1	B	349	LYS	CA-CB-CG	7.95	130.90	113.40
1	B	346	PHE	CB-CG-CD2	-7.95	115.24	120.80
1	B	77	THR	OG1-CB-CG2	7.93	128.25	110.00
1	B	14	MET	CB-CG-SD	-7.92	88.65	112.40
1	A	255	ILE	CA-CB-CG1	-7.90	96.00	111.00
1	B	99	ALA	CB-CA-C	-7.89	98.26	110.10
1	B	346	PHE	CG-CD2-CE2	-7.82	112.20	120.80
1	B	242	LYS	CD-CE-NZ	7.81	129.65	111.70
1	A	124	SER	N-CA-CB	7.78	122.17	110.50
1	B	170	LEU	CB-CA-C	7.76	124.95	110.20
1	B	301	ILE	CA-CB-CG1	-7.76	96.25	111.00
1	B	140	ILE	CA-CB-CG1	7.76	125.74	111.00
1	B	26	VAL	CA-CB-CG2	7.75	122.53	110.90
1	B	346	PHE	CA-CB-CG	-7.75	95.29	113.90
1	A	257	LEU	CB-CG-CD1	-7.71	97.89	111.00
1	B	93	ASN	CB-CA-C	7.69	125.78	110.40
1	B	145	ARG	N-CA-CB	7.67	124.41	110.60
1	B	218	ILE	CA-CB-CG1	7.66	125.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	17	ASP	CB-CG-OD1	-7.66	111.41	118.30
1	B	344	LEU	N-CA-CB	-7.65	95.10	110.40
1	B	34	LYS	C-N-CA	-7.64	102.59	121.70
1	B	183	GLU	CB-CA-C	-7.64	95.11	110.40
1	A	200	TRP	NE1-CE2-CZ2	-7.63	122.00	130.40
1	B	99	ALA	N-CA-CB	7.59	120.73	110.10
1	A	76	TYR	CA-CB-CG	-7.58	99.00	113.40
1	A	335	GLN	N-CA-CB	-7.58	96.96	110.60
1	B	1	LYS	CB-CA-C	7.54	125.48	110.40
1	A	240	VAL	CA-CB-CG2	7.53	122.20	110.90
1	B	240	VAL	CG1-CB-CG2	7.44	122.80	110.90
1	B	168	TYR	N-CA-C	7.43	131.07	111.00
1	B	70	ASP	N-CA-CB	7.41	123.93	110.60
1	A	323	LEU	CB-CG-CD2	7.38	123.55	111.00
1	A	69	LEU	C-N-CA	-7.36	103.31	121.70
1	B	212	LEU	CB-CG-CD2	-7.33	98.54	111.00
1	B	74	ARG	CB-CG-CD	-7.32	92.57	111.60
1	A	199	LEU	CB-CG-CD2	7.29	123.40	111.00
1	A	340	TYR	N-CA-CB	-7.29	97.47	110.60
1	A	200	TRP	CD1-CG-CD2	-7.29	100.47	106.30
1	A	99	ALA	CB-CA-C	-7.29	99.17	110.10
1	A	199	LEU	CB-CG-CD1	-7.28	98.63	111.00
1	A	197	ARG	NE-CZ-NH2	7.27	123.94	120.30
1	B	327	GLU	N-CA-CB	-7.27	97.52	110.60
1	A	68	ILE	CA-CB-CG1	-7.22	97.28	111.00
1	B	145	ARG	CB-CA-C	-7.21	95.97	110.40
1	B	61	GLN	CA-CB-CG	7.21	129.26	113.40
1	A	282	LYS	N-CA-CB	-7.20	97.65	110.60
1	A	311	GLY	C-N-CA	-7.19	103.72	121.70
1	B	97	VAL	CA-CB-CG2	-7.19	100.12	110.90
1	A	93	ASN	N-CA-CB	-7.18	97.68	110.60
1	A	302	SER	CB-CA-C	-7.18	96.46	110.10
1	B	229	MET	CG-SD-CE	-7.17	88.73	100.20
1	B	316	SER	C-N-CA	-7.17	107.25	122.30
1	B	248	HIS	C-N-CA	-7.16	103.79	121.70
1	B	134	GLU	CA-CB-CG	7.16	129.15	113.40
1	A	121	SER	C-N-CA	-7.16	103.81	121.70
1	B	200	TRP	N-CA-CB	7.15	123.47	110.60
1	B	138	THR	CA-CB-CG2	7.13	122.38	112.40
1	A	7	PRO	C-N-CA	-7.13	103.88	121.70
1	A	103	MET	CG-SD-CE	-7.12	88.80	100.20
1	A	123	ASP	O-C-N	-7.12	111.31	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	144	ASP	CB-CG-OD1	7.09	124.69	118.30
1	A	322	SER	N-CA-CB	7.08	121.13	110.50
1	A	331	TYR	CB-CG-CD1	7.08	125.25	121.00
1	B	106	ASN	CB-CA-C	-7.07	96.25	110.40
1	B	247	CYS	CA-CB-SG	7.06	126.72	114.00
1	A	168	TYR	CD1-CE1-CZ	-7.05	113.45	119.80
1	A	184	CYS	CA-CB-SG	-7.03	101.34	114.00
1	B	336	VAL	CA-CB-CG2	7.03	121.44	110.90
1	A	197	ARG	N-CA-CB	7.03	123.25	110.60
1	A	181	GLU	C-N-CA	-7.02	107.55	122.30
1	A	350	THR	N-CA-CB	-6.96	97.07	110.30
1	B	302	SER	N-CA-CB	6.95	120.93	110.50
1	A	168	TYR	N-CA-C	6.94	129.75	111.00
1	A	196	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	B	43	ARG	CA-CB-CG	6.93	128.66	113.40
1	B	304	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	336	VAL	CA-CB-CG2	6.92	121.27	110.90
1	B	263	VAL	CA-CB-CG2	6.92	121.27	110.90
1	A	83	PHE	N-CA-C	6.90	129.62	111.00
1	A	238	ASP	N-CA-CB	6.90	123.01	110.60
1	A	313	GLY	CA-C-O	-6.89	108.20	120.60
1	A	126	LYS	CB-CA-C	6.89	124.17	110.40
1	B	179	GLU	N-CA-C	6.84	129.47	111.00
1	B	217	ARG	NH1-CZ-NH2	6.84	126.92	119.40
1	B	329	ILE	CB-CG1-CD1	-6.81	94.84	113.90
1	A	39	LYS	CB-CA-C	-6.78	96.83	110.40
1	A	206	THR	C-N-CA	6.78	138.64	121.70
1	A	229	MET	CA-CB-CG	6.77	124.81	113.30
1	B	329	ILE	CG1-CB-CG2	-6.77	96.51	111.40
1	B	176	PHE	N-CA-C	6.77	129.27	111.00
1	B	28	TYR	CB-CG-CD2	-6.76	116.94	121.00
1	A	47	ALA	N-CA-CB	6.76	119.56	110.10
1	B	227	GLY	O-C-N	6.74	133.49	122.70
1	A	332	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	A	43	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	B	260	LEU	CB-CA-C	-6.71	97.44	110.20
1	A	318	VAL	CG1-CB-CG2	-6.71	100.16	110.90
1	B	118	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	146	ASP	C-N-CA	-6.68	105.00	121.70
1	B	138	THR	CA-CB-OG1	-6.68	94.98	109.00
1	A	269	TYR	CG-CD2-CE2	-6.66	115.98	121.30
1	A	167	ALA	C-N-CA	6.65	138.33	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	278	SER	N-CA-CB	6.65	120.48	110.50
1	B	340	TYR	N-CA-CB	-6.64	98.64	110.60
1	B	232	LYS	C-N-CA	-6.63	108.37	122.30
1	B	208	PHE	CB-CG-CD1	-6.63	116.16	120.80
1	B	242	LYS	N-CA-CB	6.63	122.53	110.60
1	A	289	GLY	CA-C-O	6.61	132.50	120.60
1	B	340	TYR	CB-CG-CD1	-6.58	117.05	121.00
1	B	197	ARG	CD-NE-CZ	6.58	132.81	123.60
1	A	58	ALA	C-N-CA	-6.57	105.29	121.70
1	B	104	LEU	C-N-CA	6.57	138.11	121.70
1	B	143	VAL	CA-CB-CG1	6.56	120.74	110.90
1	B	178	ILE	C-N-CA	-6.56	105.31	121.70
1	A	111	GLU	CA-CB-CG	6.55	127.82	113.40
1	B	234	ILE	CA-CB-CG2	-6.55	97.80	110.90
1	A	188	LYS	CA-CB-CG	-6.54	99.01	113.40
1	B	242	LYS	C-N-CA	-6.54	105.34	121.70
1	A	76	TYR	CB-CA-C	6.53	123.46	110.40
1	B	150	ALA	CB-CA-C	-6.52	100.32	110.10
1	B	157	VAL	CG1-CB-CG2	-6.52	100.47	110.90
1	A	314	ILE	CA-CB-CG2	6.50	123.91	110.90
1	B	322	SER	O-C-N	-6.50	112.30	122.70
1	A	14	MET	CG-SD-CE	6.50	110.60	100.20
1	A	74	ARG	CA-CB-CG	-6.50	99.11	113.40
1	B	51	ILE	CB-CG1-CD1	-6.50	95.71	113.90
1	B	278	SER	O-C-N	6.50	133.09	122.70
1	B	302	SER	CB-CA-C	-6.49	97.77	110.10
1	A	273	HIS	CA-CB-CG	-6.49	102.57	113.60
1	B	277	ILE	C-N-CA	-6.49	105.48	121.70
1	A	304	ASP	C-N-CA	-6.48	108.69	122.30
1	A	57	GLN	CA-CB-CG	6.48	127.65	113.40
1	B	69	LEU	N-CA-CB	-6.47	97.46	110.40
1	B	269	TYR	CG-CD1-CE1	-6.46	116.13	121.30
1	A	280	LEU	CA-CB-CG	6.46	130.15	115.30
1	B	325	TYR	CD1-CG-CD2	6.45	125.00	117.90
1	A	320	ASP	N-CA-C	6.45	128.40	111.00
1	A	3	LYS	CA-CB-CG	6.44	127.57	113.40
1	A	74	ARG	CD-NE-CZ	6.44	132.62	123.60
1	A	165	HIS	CA-CB-CG	6.43	124.53	113.60
1	A	294	THR	CA-CB-CG2	6.43	121.40	112.40
1	A	306	VAL	CG1-CB-CG2	-6.42	100.62	110.90
1	A	77	THR	CA-CB-CG2	6.42	121.39	112.40
1	A	90	LEU	CA-C-O	6.41	133.56	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	31	ASP	O-C-N	6.41	132.96	122.70
1	B	222	GLU	N-CA-C	6.41	128.30	111.00
1	B	338	LEU	CB-CA-C	6.40	122.36	110.20
1	B	349	LYS	CD-CE-NZ	-6.40	96.99	111.70
1	B	110	ILE	C-N-CA	-6.39	105.73	121.70
1	B	184	CYS	N-CA-CB	6.38	122.08	110.60
1	B	229	MET	CA-C-O	6.37	133.48	120.10
1	B	337	ASN	C-N-CA	-6.36	105.80	121.70
1	B	105	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	269	TYR	C-N-CA	-6.35	105.82	121.70
1	B	324	LEU	CB-CA-C	-6.35	98.14	110.20
1	B	100	LYS	CB-CG-CD	6.34	128.09	111.60
1	B	12	ILE	CA-CB-CG2	6.34	123.58	110.90
1	B	34	LYS	N-CA-CB	6.33	121.99	110.60
1	A	135	LYS	CB-CG-CD	6.32	128.04	111.60
1	A	238	ASP	CB-CA-C	-6.32	97.76	110.40
1	A	129	ILE	C-N-CA	-6.31	105.92	121.70
1	B	41	SER	N-CA-CB	-6.30	101.05	110.50
1	A	91	LEU	CB-CA-C	6.29	122.15	110.20
1	B	295	PRO	CA-N-CD	-6.29	102.69	111.50
1	A	348	PHE	CG-CD2-CE2	-6.29	113.88	120.80
1	A	105	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	70	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	B	58	ALA	CB-CA-C	-6.27	100.69	110.10
1	A	109	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	230	PHE	C-N-CA	-6.25	109.17	122.30
1	A	127	ASP	N-CA-CB	-6.24	99.36	110.60
1	B	214	GLN	N-CA-CB	6.24	121.83	110.60
1	A	225	VAL	CG1-CB-CG2	-6.22	100.94	110.90
1	A	64	SER	N-CA-CB	-6.21	101.18	110.50
1	B	228	TYR	CB-CG-CD1	-6.21	117.27	121.00
1	B	144	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	B	139	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	180	ARG	CD-NE-CZ	-6.20	114.92	123.60
1	A	90	LEU	CB-CA-C	6.19	121.96	110.20
1	A	110	ILE	CA-CB-CG1	-6.19	99.24	111.00
1	B	347	ASN	C-N-CA	-6.19	106.23	121.70
1	B	237	ALA	O-C-N	6.19	132.60	122.70
1	A	147	SER	CB-CA-C	-6.18	98.36	110.10
1	A	292	LYS	N-CA-C	6.17	127.67	111.00
1	B	277	ILE	CA-C-N	-6.17	103.62	117.20
1	A	297	PRO	N-CA-CB	-6.17	95.81	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	348	PHE	CB-CG-CD2	-6.17	116.48	120.80
1	A	205	THR	C-N-CA	6.16	137.11	121.70
1	B	292	LYS	CA-CB-CG	6.16	126.96	113.40
1	B	69	LEU	CB-CG-CD2	-6.16	100.53	111.00
1	A	242	LYS	CG-CD-CE	6.16	130.37	111.90
1	A	86	LYS	N-CA-C	6.15	127.61	111.00
1	A	84	GLY	C-N-CA	-6.15	106.33	121.70
1	B	317	GLY	N-CA-C	6.14	128.46	113.10
1	A	282	LYS	CB-CA-C	6.14	122.69	110.40
1	A	314	ILE	CG1-CB-CG2	-6.13	97.91	111.40
1	A	282	LYS	C-N-CA	-6.12	109.46	122.30
1	A	259	LEU	CB-CG-CD1	6.11	121.38	111.00
1	B	269	TYR	CD1-CG-CD2	6.11	124.62	117.90
1	B	158	LYS	N-CA-C	6.10	127.47	111.00
1	B	322	SER	CA-CB-OG	6.10	127.67	111.20
1	B	107	LEU	N-CA-CB	6.09	122.59	110.40
1	B	248	HIS	CA-CB-CG	-6.09	103.25	113.60
1	A	205	THR	N-CA-C	6.08	127.42	111.00
1	A	171	GLU	N-CA-C	6.08	127.41	111.00
1	A	248	HIS	CA-C-O	6.07	132.85	120.10
1	B	208	PHE	C-N-CA	-6.07	106.53	121.70
1	A	10	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	151	GLU	CA-CB-CG	6.06	126.74	113.40
1	A	277	ILE	CA-CB-CG2	-6.06	98.78	110.90
1	A	126	LYS	N-CA-CB	-6.03	99.74	110.60
1	B	304	ASP	OD1-CG-OD2	-6.03	111.84	123.30
1	A	49	TYR	CA-C-N	-6.02	103.95	117.20
1	B	239	MET	O-C-N	-6.02	113.06	122.70
1	A	109	ASP	N-CA-CB	-6.02	99.77	110.60
1	B	139	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	179	GLU	C-N-CA	-6.02	106.66	121.70
1	A	126	LYS	O-C-N	-6.01	113.08	122.70
1	B	344	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	B	56	GLN	CB-CA-C	6.01	122.41	110.40
1	B	172	VAL	C-N-CA	-6.01	106.68	121.70
1	B	322	SER	N-CA-CB	6.00	119.50	110.50
1	B	338	LEU	N-CA-CB	-6.00	98.41	110.40
1	B	200	TRP	CG-CD2-CE3	-5.99	128.51	133.90
1	A	246	TYR	C-N-CA	-5.99	106.72	121.70
1	B	140	ILE	CB-CA-C	-5.98	99.64	111.60
1	A	17	ASP	N-CA-C	5.97	127.13	111.00
1	B	251	GLN	N-CA-C	5.97	127.12	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	VAL	CA-CB-CG1	5.96	119.85	110.90
1	B	206	THR	CA-CB-CG2	-5.95	104.06	112.40
1	B	306	VAL	CA-C-N	-5.95	104.11	117.20
1	B	46	GLN	N-CA-CB	-5.94	99.90	110.60
1	A	313	GLY	O-C-N	5.93	132.20	122.70
1	B	175	ILE	CG1-CB-CG2	-5.93	98.36	111.40
1	A	214	GLN	CA-CB-CG	5.92	126.43	113.40
1	B	306	VAL	CA-C-O	5.92	132.54	120.10
1	A	345	LYS	N-CA-C	-5.92	95.03	111.00
1	B	304	ASP	CB-CG-OD1	5.92	123.62	118.30
1	A	126	LYS	CA-C-O	5.91	132.52	120.10
1	A	70	ASP	C-N-CA	-5.91	106.92	121.70
1	B	287	VAL	CA-CB-CG2	5.91	119.77	110.90
1	B	197	ARG	CG-CD-NE	5.91	124.21	111.80
1	A	320	ASP	O-C-N	-5.90	113.26	122.70
1	B	167	ALA	N-CA-CB	5.90	118.36	110.10
1	A	344	LEU	CA-CB-CG	-5.90	101.73	115.30
1	B	214	GLN	O-C-N	5.89	133.22	123.20
1	B	241	SER	N-CA-CB	-5.89	101.66	110.50
1	B	269	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	B	290	LEU	CB-CG-CD2	5.86	120.96	111.00
1	B	90	LEU	CB-CG-CD1	5.86	120.96	111.00
1	B	192	GLN	CB-CG-CD	5.85	126.81	111.60
1	A	118	ARG	CA-CB-CG	-5.84	100.56	113.40
1	B	325	TYR	CG-CD2-CE2	-5.83	116.63	121.30
1	B	116	LEU	CB-CG-CD2	5.83	120.91	111.00
1	B	163	THR	CB-CA-C	-5.81	95.91	111.60
1	B	89	PRO	N-CA-C	5.81	127.20	112.10
1	A	200	TRP	CG-CD1-NE1	5.81	115.91	110.10
1	B	111	GLU	N-CA-CB	5.81	121.05	110.60
1	A	231	GLY	C-N-CA	-5.80	107.21	121.70
1	B	196	ARG	CD-NE-CZ	-5.80	115.48	123.60
1	A	93	ASN	C-N-CA	-5.79	107.22	121.70
1	B	228	TYR	CZ-CE2-CD2	-5.79	114.59	119.80
1	A	318	VAL	CA-CB-CG2	-5.76	102.26	110.90
1	B	83	PHE	C-N-CA	5.76	134.40	122.30
1	B	64	SER	N-CA-CB	5.76	119.14	110.50
1	B	115	SER	CB-CA-C	-5.76	99.16	110.10
1	A	269	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	B	345	LYS	CA-C-O	5.75	132.18	120.10
1	B	4	LEU	CB-CG-CD2	-5.75	101.22	111.00
1	B	118	ARG	C-N-CA	-5.75	110.22	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	250	SER	CA-C-N	-5.75	104.56	117.20
1	A	304	ASP	CB-CA-C	-5.74	98.92	110.40
1	A	263	VAL	N-CA-CB	5.73	124.11	111.50
1	B	1	LYS	CB-CG-CD	5.73	126.51	111.60
1	A	100	LYS	CA-CB-CG	5.73	126.00	113.40
1	B	290	LEU	N-CA-C	5.72	126.45	111.00
1	A	276	HIS	N-CA-C	5.71	126.42	111.00
1	B	336	VAL	CA-CB-CG1	5.71	119.47	110.90
1	A	187	TYR	CD1-CE1-CZ	-5.71	114.66	119.80
1	A	66	SER	CB-CA-C	-5.71	99.25	110.10
1	B	183	GLU	C-N-CA	-5.71	107.43	121.70
1	B	204	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	57	GLN	CB-CG-CD	5.70	126.43	111.60
1	B	188	LYS	CA-CB-CG	5.70	125.95	113.40
1	A	170	LEU	CA-CB-CG	5.70	128.41	115.30
1	B	217	ARG	CB-CA-C	-5.70	99.01	110.40
1	A	39	LYS	N-CA-C	5.69	126.36	111.00
1	B	271	LEU	C-N-CA	-5.69	107.48	121.70
1	A	94	ALA	N-CA-CB	5.68	118.05	110.10
1	B	74	ARG	CD-NE-CZ	-5.67	115.66	123.60
1	A	325	TYR	CZ-CE2-CD2	-5.67	114.70	119.80
1	B	118	ARG	CG-CD-NE	5.67	123.71	111.80
1	A	112	VAL	CA-CB-CG2	5.65	119.38	110.90
1	B	255	ILE	CA-CB-CG1	5.65	121.74	111.00
1	B	278	SER	CA-C-N	-5.65	104.78	117.20
1	A	293	THR	C-N-CA	-5.64	107.61	121.70
1	B	309	PRO	N-CA-CB	-5.64	96.40	102.60
1	A	189	PRO	CA-C-N	-5.63	104.81	117.20
1	B	303	LEU	CB-CG-CD2	5.63	120.57	111.00
1	A	123	ASP	C-N-CA	5.63	135.77	121.70
1	B	168	TYR	CB-CA-C	-5.62	99.16	110.40
1	B	328	TYR	C-N-CA	-5.62	107.65	121.70
1	B	148	GLU	N-CA-CB	5.61	120.70	110.60
1	A	186	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	168	TYR	N-CA-CB	-5.60	100.53	110.60
1	B	46	GLN	N-CA-C	5.60	126.11	111.00
1	B	133	TYR	CB-CG-CD1	-5.59	117.65	121.00
1	A	282	LYS	CB-CG-CD	5.58	126.12	111.60
1	B	269	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	A	162	ALA	N-CA-CB	-5.57	102.30	110.10
1	B	303	LEU	N-CA-C	5.56	126.02	111.00
1	B	114	TYR	CD1-CE1-CZ	-5.56	114.80	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	167	ALA	CB-CA-C	-5.54	101.78	110.10
1	B	105	ASP	N-CA-CB	-5.54	100.64	110.60
1	B	307	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	A	85	MET	CA-CB-CG	5.53	122.70	113.30
1	B	101	VAL	CG1-CB-CG2	-5.52	102.06	110.90
1	A	237	ALA	C-N-CA	-5.51	107.92	121.70
1	B	308	VAL	CG1-CB-CG2	5.51	119.72	110.90
1	B	92	ASN	CA-C-N	-5.51	105.08	117.20
1	A	163	THR	N-CA-CB	-5.50	99.84	110.30
1	B	281	PRO	CB-CA-C	5.50	125.75	112.00
1	A	155	LYS	CB-CG-CD	5.50	125.89	111.60
1	B	291	GLY	CA-C-O	5.50	130.49	120.60
1	A	204	ARG	CD-NE-CZ	-5.49	115.91	123.60
1	B	299	ALA	CB-CA-C	-5.49	101.86	110.10
1	A	122	ASP	CB-CA-C	5.49	121.38	110.40
1	A	341	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	B	232	LYS	CA-C-O	5.48	131.62	120.10
1	A	340	TYR	CD1-CG-CD2	5.48	123.93	117.90
1	A	152	ILE	CA-CB-CG1	5.47	121.40	111.00
1	B	262	GLU	CG-CD-OE2	5.47	129.25	118.30
1	B	142	VAL	CA-CB-CG1	-5.47	102.70	110.90
1	A	200	TRP	CH2-CZ2-CE2	-5.45	111.95	117.40
1	A	321	THR	CA-CB-CG2	-5.45	104.77	112.40
1	A	302	SER	N-CA-C	5.45	125.70	111.00
1	B	135	LYS	C-N-CA	-5.45	108.09	121.70
1	B	344	LEU	CB-CA-C	5.44	120.54	110.20
1	B	208	PHE	N-CA-C	5.44	125.69	111.00
1	B	151	GLU	CB-CA-C	5.43	121.27	110.40
1	B	246	TYR	CA-C-O	5.43	131.51	120.10
1	B	328	TYR	CB-CA-C	-5.43	99.53	110.40
1	A	145	ARG	N-CA-C	5.43	125.66	111.00
1	A	90	LEU	CB-CG-CD2	5.42	120.21	111.00
1	A	109	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	B	187	TYR	C-N-CA	-5.41	108.18	121.70
1	A	23	LYS	N-CA-CB	-5.41	100.87	110.60
1	B	117	LEU	CB-CA-C	5.40	120.46	110.20
1	A	306	VAL	C-N-CA	-5.39	108.21	121.70
1	B	241	SER	N-CA-C	5.39	125.56	111.00
1	A	98	GLN	CA-CB-CG	5.39	125.26	113.40
1	B	165	HIS	N-CA-C	5.39	125.55	111.00
1	B	191	LYS	C-N-CA	-5.38	108.25	121.70
1	B	151	GLU	N-CA-CB	-5.38	100.92	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	146	ASP	CA-CB-CG	-5.38	101.57	113.40
1	B	32	LEU	C-N-CA	-5.38	108.26	121.70
1	B	343	LYS	C-N-CA	-5.38	108.26	121.70
1	A	40	LEU	CB-CA-C	-5.37	99.99	110.20
1	A	120	GLY	C-N-CA	-5.37	108.27	121.70
1	B	228	TYR	CG-CD1-CE1	-5.37	117.00	121.30
1	B	171	GLU	CA-CB-CG	5.36	125.20	113.40
1	B	130	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	92	ASN	CA-C-O	5.35	131.34	120.10
1	A	135	LYS	CB-CA-C	-5.34	99.73	110.40
1	B	346	PHE	C-N-CA	-5.33	108.37	121.70
1	B	263	VAL	CA-C-O	5.33	131.29	120.10
1	A	49	TYR	CB-CG-CD1	5.33	124.20	121.00
1	A	204	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	A	60	SER	CB-CA-C	5.32	120.21	110.10
1	B	257	LEU	CB-CA-C	-5.31	100.11	110.20
1	A	266	GLY	N-CA-C	5.31	126.38	113.10
1	A	306	VAL	CA-CB-CG1	-5.30	102.94	110.90
1	B	166	ASN	CA-C-N	-5.30	105.54	117.20
1	A	45	ILE	CA-CB-CG1	5.30	121.07	111.00
1	B	21	MET	CA-CB-CG	-5.30	104.29	113.30
1	A	133	TYR	CB-CA-C	-5.29	99.82	110.40
1	A	114	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	B	106	ASN	CA-C-O	-5.28	109.02	120.10
1	B	254	PRO	N-CA-CB	-5.27	96.80	102.60
1	B	289	GLY	CA-C-N	-5.27	105.60	117.20
1	B	267	ASN	N-CA-CB	-5.27	101.11	110.60
1	A	186	ARG	CA-CB-CG	5.27	124.99	113.40
1	B	110	ILE	N-CA-C	5.27	125.22	111.00
1	B	200	TRP	CG-CD1-NE1	5.27	115.37	110.10
1	A	4	LEU	CB-CG-CD1	5.26	119.94	111.00
1	B	69	LEU	C-N-CA	-5.26	108.55	121.70
1	A	144	ASP	O-C-N	-5.26	114.28	122.70
1	A	247	CYS	CA-CB-SG	5.26	123.47	114.00
1	B	63	SER	N-CA-CB	-5.26	102.61	110.50
1	A	29	GLU	N-CA-CB	5.26	120.06	110.60
1	A	183	GLU	CB-CA-C	5.26	120.92	110.40
1	B	28	TYR	N-CA-C	5.26	125.19	111.00
1	B	21	MET	N-CA-C	5.25	125.18	111.00
1	B	102	GLU	CA-C-N	-5.25	105.64	117.20
1	A	239	MET	CA-CB-CG	5.25	122.23	113.30
1	B	145	ARG	O-C-N	5.25	131.09	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	271	LEU	CA-CB-CG	-5.25	103.23	115.30
1	B	40	LEU	C-N-CA	-5.24	108.59	121.70
1	A	239	MET	C-N-CA	-5.24	108.60	121.70
1	A	146	ASP	CB-CA-C	5.24	120.88	110.40
1	B	116	LEU	C-N-CA	-5.24	108.61	121.70
1	A	99	ALA	N-CA-CB	5.24	117.43	110.10
1	B	31	ASP	CA-C-N	-5.24	105.68	117.20
1	B	263	VAL	CB-CA-C	5.24	121.35	111.40
1	B	16	PHE	CB-CA-C	-5.23	99.93	110.40
1	B	258	ILE	C-N-CA	-5.23	108.62	121.70
1	A	232	LYS	CA-C-N	-5.23	105.75	116.20
1	A	346	PHE	CB-CA-C	5.23	120.85	110.40
1	B	304	ASP	N-CA-CB	5.23	120.01	110.60
1	A	209	ALA	N-CA-CB	-5.22	102.79	110.10
1	B	54	GLU	N-CA-C	5.22	125.08	111.00
1	A	336	VAL	N-CA-CB	5.21	122.97	111.50
1	A	54	GLU	OE1-CD-OE2	-5.21	117.05	123.30
1	A	240	VAL	O-C-N	5.21	131.03	122.70
1	A	133	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	120	GLY	N-CA-C	5.20	126.11	113.10
1	B	109	ASP	O-C-N	-5.20	114.38	122.70
1	B	43	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	B	199	LEU	C-N-CA	-5.20	108.71	121.70
1	A	246	TYR	CB-CG-CD1	5.20	124.12	121.00
1	B	39	LYS	N-CA-CB	5.19	119.95	110.60
1	A	292	LYS	O-C-N	-5.19	114.40	122.70
1	A	178	ILE	CA-CB-CG2	-5.18	100.53	110.90
1	B	18	VAL	N-CA-C	5.18	125.00	111.00
1	A	26	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	A	332	ASP	C-N-CA	-5.18	108.75	121.70
1	B	74	ARG	O-C-N	5.18	130.99	122.70
1	B	244	ALA	CB-CA-C	5.18	117.87	110.10
1	A	85	MET	CB-CA-C	5.17	120.75	110.40
1	B	29	GLU	CA-CB-CG	-5.17	102.03	113.40
1	B	318	VAL	CA-CB-CG1	5.17	118.65	110.90
1	A	95	ASP	CA-CB-CG	-5.16	102.05	113.40
1	B	232	LYS	CD-CE-NZ	-5.16	99.84	111.70
1	B	187	TYR	CD1-CE1-CZ	-5.16	115.16	119.80
1	A	318	VAL	N-CA-CB	-5.15	100.16	111.50
1	A	345	LYS	O-C-N	5.15	130.94	122.70
1	B	63	SER	O-C-N	-5.15	114.45	122.70
1	B	329	ILE	CA-CB-CG2	5.15	121.20	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	125	SER	N-CA-C	5.15	124.90	111.00
1	A	46	GLN	CB-CA-C	5.15	120.70	110.40
1	A	28	TYR	C-N-CA	5.13	134.53	121.70
1	A	35	MET	CA-C-O	5.12	130.86	120.10
1	B	29	GLU	CB-CA-C	5.12	120.65	110.40
1	B	302	SER	N-CA-C	5.12	124.83	111.00
1	B	164	THR	CA-CB-CG2	5.12	119.56	112.40
1	B	259	LEU	N-CA-C	5.10	124.78	111.00
1	A	148	GLU	CA-CB-CG	5.10	124.62	113.40
1	A	85	MET	N-CA-C	5.10	124.76	111.00
1	B	96	SER	C-N-CA	-5.10	108.95	121.70
1	B	335	GLN	CA-CB-CG	5.10	124.61	113.40
1	B	295	PRO	N-CD-CG	5.09	110.84	103.20
1	A	116	LEU	CB-CG-CD2	5.08	119.64	111.00
1	A	242	LYS	CB-CG-CD	5.08	124.80	111.60
1	B	319	ASN	CB-CA-C	5.08	120.55	110.40
1	A	139	ASP	CB-CG-OD1	5.07	122.87	118.30
1	A	269	TYR	CD1-CG-CD2	5.07	123.48	117.90
1	A	314	ILE	CB-CG1-CD1	-5.07	99.70	113.90
1	A	102	GLU	C-N-CA	-5.07	109.03	121.70
1	A	110	ILE	CB-CG1-CD1	-5.07	99.71	113.90
1	B	47	ALA	C-N-CA	-5.07	109.03	121.70
1	B	123	ASP	CA-CB-CG	-5.07	102.25	113.40
1	B	37	LEU	C-N-CA	-5.06	111.67	122.30
1	B	152	ILE	CB-CG1-CD1	-5.06	99.74	113.90
1	A	292	LYS	CA-CB-CG	5.05	124.52	113.40
1	B	73	ASN	CA-CB-CG	-5.05	102.29	113.40
1	B	74	ARG	CA-CB-CG	5.05	124.51	113.40
1	B	180	ARG	CA-CB-CG	5.04	124.50	113.40
1	B	158	LYS	O-C-N	-5.04	114.64	122.70
1	B	35	MET	N-CA-CB	5.04	119.66	110.60
1	A	175	ILE	CB-CG1-CD1	-5.03	99.81	113.90
1	A	43	ARG	CA-CB-CG	5.03	124.47	113.40
1	B	77	THR	CA-C-N	-5.03	106.13	117.20
1	A	140	ILE	CA-C-O	5.02	130.64	120.10
1	A	174	ASP	CB-CA-C	-5.02	100.37	110.40
1	A	49	TYR	CA-C-O	5.01	130.63	120.10
1	A	84	GLY	N-CA-C	5.01	125.63	113.10
1	B	200	TRP	CB-CG-CD1	-5.01	120.49	127.00
1	B	346	PHE	CG-CD1-CE1	-5.01	115.29	120.80
1	A	124	SER	C-N-CA	-5.01	109.18	121.70
1	A	288	LYS	CB-CA-C	5.01	120.41	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	THR	N-CA-CB	-5.00	100.79	110.30
1	A	28	TYR	CD1-CE1-CZ	-5.00	115.30	119.80
1	A	349	LYS	C-N-CA	5.00	134.20	121.70
1	B	347	ASN	CB-CA-C	5.00	120.40	110.40

There are no chirality outliers.

All (86) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLY	Peptide
1	A	120	GLY	Peptide
1	A	121	SER	Peptide
1	A	125	SER	Peptide
1	A	131	VAL	Mainchain
1	A	132	ASN	Peptide
1	A	133	TYR	Sidechain
1	A	144	ASP	Peptide
1	A	145	ARG	Sidechain
1	A	154	ARG	Sidechain
1	A	16	PHE	Sidechain
1	A	160	THR	Peptide
1	A	162	ALA	Peptide
1	A	165	HIS	Peptide
1	A	166	ASN	Peptide
1	A	167	ALA	Peptide
1	A	168	TYR	Sidechain
1	A	169	ASP	Peptide
1	A	184	CYS	Peptide
1	A	2	SER	Peptide
1	A	205	THR	Peptide
1	A	217	ARG	Sidechain
1	A	228	TYR	Sidechain
1	A	230	PHE	Sidechain
1	A	246	TYR	Sidechain
1	A	251	GLN	Peptide
1	A	269	TYR	Sidechain
1	A	276	HIS	Sidechain
1	A	28	TYR	Sidechain
1	A	319	ASN	Peptide
1	A	328	TYR	Sidechain
1	A	331	TYR	Peptide
1	A	340	TYR	Peptide,Sidechain

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Mol	Chain	Res	Type	Group
1	A	348	PHE	Sidechain
1	A	37	LEU	Peptide
1	A	39	LYS	Mainchain,Peptide
1	A	42	LYS	Peptide
1	A	43	ARG	Sidechain
1	A	49	TYR	Sidechain
1	A	65	ASP	Peptide
1	A	71	LEU	Peptide
1	A	76	TYR	Sidechain
1	A	83	PHE	Peptide,Sidechain
1	A	84	GLY	Peptide
1	B	102	GLU	Peptide
1	B	109	ASP	Peptide
1	B	113	ALA	Peptide
1	B	114	TYR	Sidechain
1	B	146	ASP	Peptide
1	B	156	TYR	Sidechain
1	B	160	THR	Peptide
1	B	162	ALA	Peptide
1	B	169	ASP	Peptide
1	B	175	ILE	Peptide
1	B	176	PHE	Sidechain
1	B	18	VAL	Peptide
1	B	194	HIS	Peptide
1	B	196	ARG	Sidechain
1	B	20	SER	Peptide
1	B	217	ARG	Sidechain
1	B	240	VAL	Peptide
1	B	246	TYR	Sidechain
1	B	252	GLY	Peptide
1	B	259	LEU	Peptide
1	B	28	TYR	Peptide,Sidechain
1	B	294	THR	Peptide
1	B	311	GLY	Peptide
1	B	319	ASN	Peptide
1	B	325	TYR	Peptide
1	B	328	TYR	Sidechain
1	B	331	TYR	Sidechain
1	B	347	ASN	Peptide
1	B	349	LYS	Peptide
1	B	35	MET	Peptide
1	B	46	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	B	49	TYR	Sidechain
1	B	50	SER	Peptide
1	B	76	TYR	Sidechain
1	B	83	PHE	Peptide
1	B	84	GLY	Peptide
1	B	87	LYS	Peptide
1	B	93	ASN	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2754	0	2798	212	0
1	B	2754	0	2798	294	0
2	A	28	0	24	2	0
2	B	28	0	24	0	0
3	A	124	0	0	11	0
3	B	129	0	0	23	0
All	All	5817	0	5644	506	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 45.

All (506) 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:282:LYS:C	1:B:282:LYS:CA	1.76	1.51
1:A:138:THR:HG23	1:A:180:ARG:HB3	1.49	0.95
1:A:138:THR:HG21	1:A:212:LEU:HD23	1.52	0.90
1:B:202:GLY:HA3	1:B:243:SER:O	1.74	0.88
1:A:133:TYR:HE1	1:A:140:ILE:HG13	1.38	0.88
1:A:59:VAL:HG21	1:A:92:ASN:HA	1.56	0.87
1:A:296:ASP:HB2	1:A:314:ILE:HD13	1.57	0.86
1:A:301:ILE:HD12	1:A:310:LEU:HD11	1.56	0.85
1:A:123:ASP:HA	1:A:124:SER:HB3	1.59	0.84
1:B:67:GLN:NE2	1:B:71:LEU:HG	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:HIS:CD2	1:A:241:SER:HB3	2.14	0.82
1:A:112:VAL:O	1:A:116:LEU:HB2	1.78	0.82
1:B:230:PHE:HA	1:B:275:SER:O	1.79	0.82
1:B:109:ASP:HB2	1:B:207:ASN:OD1	1.78	0.81
1:B:170:LEU:HD21	1:B:344:LEU:HD21	1.60	0.81
1:B:282:LYS:CA	1:B:283:GLY:N	2.44	0.81
1:A:318:VAL:HG12	1:A:321:THR:CG2	2.12	0.80
1:B:37:LEU:HD22	1:B:114:TYR:HD1	1.47	0.80
1:A:90:LEU:HB3	1:A:92:ASN:OD1	1.82	0.79
1:A:149:GLU:O	1:A:153:ILE:HG13	1.83	0.78
1:A:318:VAL:HG12	1:A:321:THR:HG21	1.66	0.77
1:A:280:LEU:HD12	1:A:281:PRO:HD2	1.67	0.77
1:A:19:GLU:HG2	3:A:530:HOH:O	1.85	0.76
1:B:171:GLU:HG2	1:B:345:LYS:HZ2	1.51	0.75
1:B:84:GLY:H	1:B:85:MET:HA	1.52	0.75
1:B:138:THR:HG22	1:B:140:ILE:HD13	1.69	0.75
1:A:184:CYS:SG	1:A:191:LYS:NZ	2.60	0.75
1:A:118:ARG:HD3	3:A:504:HOH:O	1.86	0.74
1:B:43:ARG:H	1:B:43:ARG:HE	1.33	0.74
1:B:156:TYR:OH	1:B:309:PRO:HD2	1.87	0.74
1:B:198:LEU:HG	1:B:260:LEU:HD22	1.70	0.74
1:A:315:SER:HB2	3:A:523:HOH:O	1.88	0.74
1:A:109:ASP:HB3	1:A:207:ASN:HA	1.69	0.73
1:A:173:ILE:HB	1:A:343:LYS:HG2	1.68	0.73
1:B:45:ILE:HG23	1:B:104:LEU:HD22	1.70	0.73
1:B:37:LEU:HA	3:B:524:HOH:O	1.87	0.73
1:B:269:TYR:HE2	3:B:613:HOH:O	1.72	0.73
1:A:31:ASP:HB2	1:A:82:ASP:N	2.05	0.72
1:A:133:TYR:CE1	1:A:140:ILE:HG13	2.25	0.71
1:B:161:HIS:NE2	1:B:168:TYR:HE1	1.89	0.71
1:A:45:ILE:HG23	1:A:104:LEU:HD22	1.71	0.71
1:B:61:GLN:HB3	3:B:548:HOH:O	1.89	0.71
1:B:154:ARG:HG2	1:B:172:VAL:HG21	1.72	0.71
1:A:21:MET:O	1:A:25:MET:HG3	1.91	0.71
1:A:144:ASP:HA	1:A:145:ARG:HD2	1.73	0.70
1:A:93:ASN:HD21	1:A:96:SER:H	1.38	0.70
1:B:208:PHE:O	1:B:212:LEU:HG	1.93	0.69
1:A:11:LEU:HG	1:A:15:ILE:HD13	1.73	0.69
1:A:28:TYR:CG	1:A:103:MET:HB2	2.27	0.69
1:A:64:SER:HB3	1:A:67:GLN:HB2	1.73	0.69
1:B:242:LYS:HD3	1:B:325:TYR:HD2	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:VAL:O	1:B:101:VAL:HG23	1.93	0.69
1:B:15:ILE:HG13	1:B:16:PHE:HD2	1.57	0.68
1:B:96:SER:O	1:B:100:LYS:HG2	1.92	0.68
1:B:210:GLY:HA2	1:B:213:SER:OG	1.94	0.68
1:B:84:GLY:N	1:B:85:MET:HA	2.08	0.68
1:B:86:LYS:HD3	1:B:87:LYS:N	2.07	0.68
1:B:67:GLN:HE21	1:B:71:LEU:HG	1.58	0.67
1:B:186:ARG:HB3	3:B:577:HOH:O	1.95	0.67
1:B:238:ASP:HA	3:B:612:HOH:O	1.95	0.67
1:B:195:ASN:O	1:B:265:LEU:HB2	1.94	0.67
1:B:349:LYS:HD3	1:B:350:THR:H	1.59	0.67
1:B:165:HIS:CD2	1:B:245:ASN:HD21	2.13	0.66
1:B:292:LYS:HE3	1:B:319:ASN:HB2	1.76	0.66
1:A:93:ASN:HD21	1:A:96:SER:N	1.93	0.66
1:B:301:ILE:HG22	1:B:303:LEU:HB3	1.77	0.65
1:B:204:ARG:O	1:B:207:ASN:HB2	1.97	0.65
1:A:168:TYR:HB3	1:A:348:PHE:CD2	2.32	0.65
1:A:246:TYR:HD1	3:A:518:HOH:O	1.79	0.65
1:A:68:ILE:HG21	1:A:92:ASN:HB3	1.78	0.64
1:B:167:ALA:HA	1:B:349:LYS:HB3	1.77	0.64
1:B:260:LEU:HD11	3:B:590:HOH:O	1.96	0.64
1:B:144:ASP:O	1:B:147:SER:HB3	1.98	0.64
1:A:183:GLU:OE1	1:A:337:ASN:HA	1.96	0.64
1:A:287:VAL:HG23	1:A:331:TYR:HE1	1.64	0.63
1:A:15:ILE:CG2	1:A:257:LEU:HD11	2.27	0.63
1:A:234:ILE:HG22	1:A:236:PHE:CE1	2.34	0.63
1:A:234:ILE:HD11	1:A:333:ILE:HG22	1.81	0.63
1:B:32:LEU:HB2	3:B:572:HOH:O	1.98	0.63
1:B:75:PHE:CD2	1:B:91:LEU:HD11	2.34	0.62
1:B:295:PRO:HA	1:B:311:GLY:O	1.99	0.62
1:B:28:TYR:C	1:B:29:GLU:HG3	2.19	0.62
1:B:282:LYS:C	1:B:282:LYS:CB	2.65	0.62
1:B:292:LYS:HE3	1:B:319:ASN:ND2	2.14	0.62
1:A:324:LEU:HD22	1:A:325:TYR:CE2	2.35	0.62
1:B:161:HIS:CE1	1:B:168:TYR:CE1	2.88	0.62
1:B:153:ILE:HD13	3:B:563:HOH:O	1.99	0.62
1:A:292:LYS:HB3	1:A:318:VAL:O	2.00	0.61
1:A:35:MET:HG2	1:A:39:LYS:HG2	1.82	0.61
1:B:246:TYR:N	1:B:246:TYR:CD2	2.68	0.61
1:B:279:LYS:HA	3:B:536:HOH:O	2.00	0.61
1:A:84:GLY:HA3	3:A:587:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ILE:HG12	1:B:206:THR:HB	1.82	0.61
1:B:78:LEU:O	1:B:79:ILE:HD13	2.01	0.61
1:A:138:THR:HG21	1:A:212:LEU:CD2	2.28	0.61
1:B:339:LYS:HB3	1:B:340:TYR:CD2	2.36	0.61
1:A:23:LYS:O	1:A:27:GLU:HG3	2.00	0.61
1:B:194:HIS:HB2	3:B:625:HOH:O	2.01	0.60
1:A:110:ILE:O	1:A:113:ALA:HB3	2.00	0.60
1:B:161:HIS:NE2	1:B:168:TYR:CE1	2.68	0.60
1:B:186:ARG:HE	1:B:334:ALA:HA	1.66	0.60
1:A:43:ARG:HD3	1:A:43:ARG:N	2.17	0.60
1:A:144:ASP:CG	1:A:145:ARG:HD2	2.21	0.60
1:B:13:LYS:CG	1:B:129:ILE:HD11	2.32	0.60
1:A:37:LEU:H	1:A:37:LEU:HD12	1.65	0.60
1:B:62:GLY:HA3	3:B:603:HOH:O	2.02	0.60
1:B:246:TYR:H	1:B:246:TYR:HD2	1.50	0.59
1:B:247:CYS:SG	3:B:573:HOH:O	2.52	0.59
1:A:155:LYS:O	1:A:158:LYS:HB3	2.03	0.59
1:B:86:LYS:HD3	1:B:87:LYS:H	1.66	0.59
1:A:144:ASP:HA	1:A:145:ARG:CD	2.33	0.59
1:B:187:TYR:CD2	1:B:337:ASN:HB2	2.38	0.59
1:A:18:VAL:HG12	1:A:22:LYS:HE2	1.85	0.58
1:B:20:SER:HA	1:B:23:LYS:HB3	1.85	0.58
1:B:161:HIS:HD2	1:B:240:VAL:HG13	1.69	0.58
1:A:55:VAL:HG22	1:A:68:ILE:HD12	1.85	0.58
1:A:196:ARG:HG3	1:A:264:ALA:HA	1.85	0.58
1:B:214:GLN:HG2	1:B:217:ARG:CZ	2.34	0.58
1:A:68:ILE:HD13	1:A:71:LEU:HD12	1.84	0.58
1:B:55:VAL:HG12	1:B:56:GLN:HG3	1.86	0.58
1:B:180:ARG:HB2	1:B:183:GLU:HG3	1.85	0.58
1:B:25:MET:HE3	1:B:107:LEU:HD22	1.85	0.58
1:A:193:LEU:HD11	1:A:266:GLY:HA3	1.85	0.58
1:B:141:LYS:O	1:B:176:PHE:HA	2.04	0.58
1:B:152:ILE:HA	1:B:155:LYS:HE3	1.85	0.58
1:B:293:THR:HB	1:B:325:TYR:HD1	1.68	0.58
1:A:20:SER:O	1:A:23:LYS:HB2	2.03	0.57
1:B:234:ILE:O	1:B:329:ILE:HA	2.04	0.57
1:A:280:LEU:HD22	1:A:331:TYR:CD1	2.39	0.57
1:B:161:HIS:NE2	1:B:170:LEU:HB2	2.20	0.57
1:B:242:LYS:HD3	1:B:325:TYR:CD2	2.40	0.57
1:A:86:LYS:O	1:A:88:PRO:HD3	2.04	0.57
1:A:104:LEU:HD23	1:A:107:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LYS:HD2	1:B:43:ARG:CZ	2.34	0.57
1:B:111:GLU:O	1:B:115:SER:HB2	2.05	0.57
1:A:42:LYS:HG3	1:A:43:ARG:CD	2.35	0.57
1:A:45:ILE:HD13	1:A:108:LEU:HD23	1.86	0.57
1:B:157:VAL:HG13	1:B:240:VAL:HG11	1.86	0.57
1:B:214:GLN:HG2	1:B:217:ARG:NE	2.20	0.57
1:B:94:ALA:O	1:B:98:GLN:HG2	2.05	0.57
1:A:15:ILE:HG22	1:A:257:LEU:HD11	1.86	0.56
1:B:180:ARG:NH1	1:B:214:GLN:HA	2.20	0.56
1:A:144:ASP:CA	1:A:145:ARG:HD2	2.35	0.56
1:B:255:ILE:HD13	1:B:345:LYS:HG2	1.87	0.56
1:A:94:ALA:O	1:A:97:VAL:HG12	2.05	0.56
1:B:12:ILE:HD12	1:B:133:TYR:HB2	1.86	0.56
1:A:262:GLU:HG3	1:A:306:VAL:HG11	1.88	0.56
1:B:296:ASP:HB2	1:B:314:ILE:HD12	1.87	0.56
1:A:218:ILE:HG22	1:A:234:ILE:HD11	1.87	0.55
1:B:13:LYS:HG3	1:B:129:ILE:HD11	1.87	0.55
1:B:321:THR:OG1	1:B:323:LEU:N	2.40	0.55
1:A:224:PRO:O	1:A:228:TYR:CE1	2.60	0.55
1:A:42:LYS:HG3	1:A:43:ARG:HD3	1.88	0.55
1:B:271:LEU:HD13	1:B:275:SER:OG	2.06	0.55
1:A:11:LEU:HG	1:A:15:ILE:CD1	2.37	0.55
1:A:242:LYS:O	1:A:246:TYR:CE2	2.60	0.55
1:B:12:ILE:HD11	1:B:133:TYR:HD1	1.71	0.55
1:B:161:HIS:NE2	1:B:170:LEU:HD22	2.20	0.55
1:B:109:ASP:O	1:B:112:VAL:N	2.40	0.55
1:B:292:LYS:HE3	1:B:319:ASN:HD22	1.71	0.55
1:A:116:LEU:HD12	1:A:135:LYS:NZ	2.23	0.54
1:B:234:ILE:HG22	1:B:235:TYR:H	1.72	0.54
1:B:267:ASN:OD1	1:B:283:GLY:O	2.25	0.54
1:B:43:ARG:H	1:B:43:ARG:NE	2.04	0.54
1:B:187:TYR:OH	1:B:262:GLU:HG2	2.08	0.54
1:A:22:LYS:HB3	1:A:32:LEU:HD11	1.90	0.54
1:A:200:TRP:CE3	1:A:258:ILE:HD11	2.43	0.54
1:A:58:ALA:HB1	1:A:63:SER:HB2	1.90	0.54
1:A:205:THR:HA	1:A:208:PHE:CD1	2.43	0.54
1:B:24:ALA:O	1:B:27:GLU:HG2	2.08	0.54
1:B:12:ILE:CD1	1:B:133:TYR:HB2	2.37	0.54
1:B:51:ILE:CD1	1:B:74:ARG:HG3	2.38	0.54
1:B:85:MET:SD	1:B:85:MET:N	2.81	0.54
1:B:165:HIS:HE1	1:B:325:TYR:HE2	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:O	1:A:114:TYR:CE2	2.61	0.54
1:B:55:VAL:O	1:B:59:VAL:HG23	2.08	0.54
1:A:133:TYR:OH	1:A:139:ASP:HA	2.08	0.53
1:B:35:MET:SD	1:B:80:PRO:HD2	2.48	0.53
1:A:198:LEU:HG	1:A:260:LEU:HD22	1.90	0.53
1:A:218:ILE:HD12	1:A:233:GLY:HA2	1.90	0.53
1:A:12:ILE:HG13	1:A:129:ILE:HG23	1.90	0.53
1:B:24:ALA:HA	1:B:27:GLU:OE2	2.08	0.53
1:B:36:PRO:O	1:B:39:LYS:N	2.42	0.53
1:B:170:LEU:CD2	1:B:344:LEU:HD21	2.33	0.53
1:A:134:GLU:HB3	3:A:531:HOH:O	2.08	0.53
1:A:210:GLY:HA2	1:A:213:SER:OG	2.09	0.53
1:A:224:PRO:O	1:A:228:TYR:HE1	1.91	0.53
1:B:215:GLY:O	1:B:216:LEU:C	2.47	0.53
1:A:10:ASP:HA	1:A:13:LYS:HE3	1.90	0.53
1:B:211:ILE:O	1:B:215:GLY:HA2	2.08	0.53
1:A:124:SER:H	1:A:127:ASP:HA	1.74	0.53
1:A:132:ASN:N	1:A:132:ASN:OD1	2.38	0.52
1:B:231:GLY:H	1:B:276:HIS:HA	1.74	0.52
1:A:242:LYS:O	1:A:246:TYR:CD2	2.62	0.52
1:B:28:TYR:CD1	1:B:103:MET:HG3	2.45	0.52
1:B:259:LEU:HD22	1:B:338:LEU:HD22	1.92	0.52
1:B:117:LEU:C	1:B:117:LEU:HD12	2.30	0.52
1:A:205:THR:HA	1:A:208:PHE:HD1	1.74	0.52
1:B:5:PRO:O	1:B:6:LYS:C	2.48	0.52
1:B:349:LYS:HB2	3:B:619:HOH:O	2.09	0.52
1:A:42:LYS:N	1:A:43:ARG:HD3	2.24	0.52
1:A:36:PRO:O	1:A:39:LYS:N	2.43	0.52
1:B:77:THR:C	3:B:631:HOH:O	2.48	0.52
1:B:158:LYS:HG3	1:B:159:ASN:OD1	2.10	0.52
1:A:153:ILE:HD12	1:A:175:ILE:HD11	1.92	0.52
1:A:207:ASN:O	1:A:211:ILE:HG13	2.10	0.52
1:B:19:GLU:HA	1:B:22:LYS:HE2	1.91	0.52
1:B:75:PHE:O	1:B:78:LEU:HB2	2.10	0.52
1:B:123:ASP:HA	1:B:124:SER:OG	2.10	0.52
1:B:161:HIS:CE1	1:B:168:TYR:CD1	2.97	0.52
1:A:37:LEU:HD12	1:A:37:LEU:N	2.24	0.51
1:B:346:PHE:N	1:B:346:PHE:CD1	2.73	0.51
1:A:83:PHE:CE2	1:A:89:PRO:HD2	2.45	0.51
1:B:233:GLY:HA3	1:B:330:VAL:O	2.10	0.51
1:B:1:LYS:HG3	1:B:2:SER:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:THR:HB	1:B:325:TYR:CD1	2.44	0.51
1:B:72:SER:HB2	1:B:91:LEU:HB2	1.91	0.51
1:B:262:GLU:OE1	1:B:306:VAL:CG2	2.58	0.51
1:B:279:LYS:HD2	1:B:280:LEU:O	2.10	0.51
1:B:301:ILE:CG2	1:B:303:LEU:HB3	2.40	0.51
1:B:138:THR:HG23	1:B:178:ILE:HG22	1.93	0.51
1:B:4:LEU:CD2	1:B:8:VAL:HG12	2.40	0.51
1:B:346:PHE:HB3	1:B:348:PHE:CZ	2.46	0.51
1:A:165:HIS:NE2	1:A:241:SER:HB3	2.26	0.51
1:B:249:THR:HG22	1:B:253:ASP:OD2	2.10	0.51
1:B:121:SER:HB2	1:B:131:VAL:HG11	1.92	0.50
1:A:104:LEU:HA	1:A:107:LEU:HB2	1.93	0.50
1:A:123:ASP:HA	1:A:124:SER:CB	2.38	0.50
1:B:112:VAL:O	1:B:113:ALA:O	2.29	0.50
1:B:259:LEU:HD22	1:B:338:LEU:CD2	2.41	0.50
1:B:259:LEU:HD13	1:B:338:LEU:HD21	1.94	0.50
1:A:218:ILE:HG22	1:A:234:ILE:CD1	2.40	0.50
1:B:133:TYR:HA	1:B:136:LEU:HD12	1.93	0.50
1:B:87:LYS:N	1:B:87:LYS:HD2	2.26	0.50
1:B:174:ASP:HB2	1:B:176:PHE:CE2	2.46	0.50
1:A:139:ASP:C	1:A:140:ILE:HG12	2.32	0.50
1:B:135:LYS:O	1:B:136:LEU:C	2.49	0.50
1:B:230:PHE:O	1:B:231:GLY:C	2.50	0.50
1:B:199:LEU:HD12	1:B:263:VAL:HG13	1.93	0.50
1:B:273:HIS:HD2	3:B:558:HOH:O	1.94	0.50
1:A:55:VAL:HG23	1:A:71:LEU:HD13	1.93	0.50
1:A:200:TRP:CE2	1:A:240:VAL:HB	2.47	0.50
1:B:28:TYR:N	1:B:29:GLU:HA	2.26	0.50
1:B:88:PRO:O	1:B:90:LEU:HD22	2.11	0.50
1:B:207:ASN:O	1:B:210:GLY:N	2.45	0.50
1:A:4:LEU:HD21	1:A:133:TYR:CD2	2.46	0.50
1:A:270:GLU:O	1:A:271:LEU:HD23	2.12	0.50
1:A:21:MET:SD	1:A:114:TYR:HB2	2.52	0.49
1:A:210:GLY:O	1:A:214:GLN:N	2.42	0.49
1:B:41:SER:O	1:B:45:ILE:HG13	2.12	0.49
1:B:250:SER:O	1:B:252:GLY:N	2.45	0.49
1:A:157:VAL:HG22	1:A:200:TRP:CH2	2.47	0.49
1:B:10:ASP:O	1:B:11:LEU:C	2.51	0.49
1:B:98:GLN:HB3	3:B:600:HOH:O	2.13	0.49
1:B:46:GLN:HB3	1:B:222:GLU:OE1	2.12	0.49
1:B:345:LYS:HZ3	1:B:347:ASN:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ILE:HG22	1:B:235:TYR:N	2.27	0.49
1:B:311:GLY:O	1:B:312:THR:C	2.51	0.49
1:A:232:LYS:HB2	3:A:507:HOH:O	2.12	0.49
1:A:28:TYR:CD1	1:A:103:MET:HB2	2.47	0.49
1:B:15:ILE:HG13	1:B:16:PHE:CD2	2.44	0.49
1:A:55:VAL:O	1:A:59:VAL:HG23	2.12	0.49
1:B:98:GLN:O	1:B:99:ALA:C	2.50	0.49
1:B:173:ILE:O	1:B:174:ASP:CG	2.52	0.49
1:B:349:LYS:HD3	1:B:350:THR:N	2.26	0.49
1:A:254:PRO:O	1:A:346:PHE:HB2	2.12	0.48
1:A:296:ASP:CB	1:A:314:ILE:HD13	2.38	0.48
1:A:1:LYS:HD2	1:A:127:ASP:OD1	2.14	0.48
1:A:31:ASP:CG	1:A:82:ASP:HB2	2.34	0.48
1:B:150:ALA:HB1	1:B:154:ARG:NH1	2.28	0.48
1:A:102:GLU:O	1:A:103:MET:C	2.48	0.48
1:A:287:VAL:HG23	1:A:331:TYR:CE1	2.47	0.48
1:B:168:TYR:CE1	1:B:170:LEU:HD22	2.49	0.48
1:B:37:LEU:HD22	1:B:114:TYR:CD1	2.36	0.48
1:B:112:VAL:O	1:B:113:ALA:C	2.52	0.48
1:B:218:ILE:HG21	1:B:232:LYS:O	2.13	0.48
1:A:251:GLN:HA	1:A:251:GLN:HE21	1.78	0.48
1:A:341:LEU:O	1:A:342:LEU:HD12	2.14	0.48
1:B:64:SER:O	1:B:67:GLN:N	2.46	0.48
1:B:345:LYS:NZ	1:B:345:LYS:HB3	2.29	0.48
1:B:145:ARG:H	1:B:145:ARG:NE	2.12	0.47
1:A:43:ARG:HD3	1:A:43:ARG:H	1.79	0.47
1:B:30:ILE:HD11	1:B:107:LEU:HD11	1.95	0.47
1:B:260:LEU:HD21	3:B:590:HOH:O	2.14	0.47
1:A:95:ASP:O	1:A:96:SER:C	2.50	0.47
1:A:204:ARG:NH2	1:A:248:HIS:ND1	2.62	0.47
1:A:140:ILE:HG22	1:A:176:PHE:HD1	1.80	0.47
1:B:153:ILE:O	1:B:156:TYR:N	2.47	0.47
1:B:171:GLU:HG2	1:B:345:LYS:HB3	1.96	0.47
1:A:267:ASN:ND2	1:A:285:HIS:CE1	2.82	0.47
1:B:58:ALA:O	1:B:59:VAL:C	2.50	0.47
1:B:198:LEU:HA	1:B:261:GLY:O	2.13	0.47
1:B:23:LYS:O	1:B:26:VAL:HG23	2.15	0.47
1:B:99:ALA:O	1:B:103:MET:HB2	2.15	0.47
1:B:211:ILE:HD13	1:B:211:ILE:HG21	1.70	0.47
1:B:295:PRO:O	1:B:297:PRO:HD3	2.14	0.47
1:A:31:ASP:O	1:A:33:GLN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:MET:HG3	1:A:325:TYR:CD1	2.50	0.47
1:A:43:ARG:CD	1:A:43:ARG:H	2.27	0.47
1:B:15:ILE:HG13	1:B:16:PHE:H	1.80	0.47
1:A:291:GLY:HA3	1:A:325:TYR:C	2.35	0.47
1:B:156:TYR:HH	1:B:309:PRO:HD2	1.79	0.47
1:B:170:LEU:HG	1:B:344:LEU:HD11	1.97	0.47
1:B:345:LYS:HZ2	1:B:345:LYS:HB3	1.79	0.47
1:A:76:TYR:O	1:A:77:THR:C	2.54	0.46
1:B:83:PHE:HB3	1:B:88:PRO:HB3	1.97	0.46
1:B:150:ALA:HB1	1:B:154:ARG:HH12	1.80	0.46
1:B:170:LEU:HD11	1:B:346:PHE:CZ	2.50	0.46
1:B:230:PHE:CD2	1:B:329:ILE:HD11	2.50	0.46
1:A:208:PHE:HA	1:A:211:ILE:HB	1.98	0.46
1:A:211:ILE:HG21	1:A:259:LEU:HD11	1.97	0.46
1:A:236:PHE:CE1	1:A:263:VAL:HG11	2.50	0.46
1:A:280:LEU:HG	1:A:284:LYS:O	2.16	0.46
1:B:102:GLU:O	1:B:105:ASP:HB2	2.16	0.46
1:B:165:HIS:CD2	1:B:241:SER:HB2	2.50	0.46
1:A:205:THR:OG1	1:A:206:THR:N	2.49	0.46
1:B:211:ILE:HG23	1:B:216:LEU:HD23	1.97	0.46
1:A:42:LYS:HG3	1:A:43:ARG:NE	2.30	0.46
1:A:201:HIS:HB3	1:A:259:LEU:HB2	1.97	0.46
1:A:258:ILE:HG21	1:A:258:ILE:HD13	1.35	0.46
1:B:47:ALA:O	1:B:48:ALA:C	2.53	0.46
1:A:262:GLU:HB2	1:A:339:LYS:HD3	1.98	0.46
1:A:345:LYS:HZ1	1:A:347:ASN:CG	2.19	0.46
1:B:16:PHE:CD2	1:B:16:PHE:N	2.84	0.45
1:B:159:ASN:HB3	1:B:312:THR:H	1.81	0.45
1:A:56:GLN:OE1	1:A:226:THR:HB	2.16	0.45
1:B:25:MET:HE3	1:B:107:LEU:CD2	2.45	0.45
1:B:183:GLU:O	1:B:184:CYS:C	2.52	0.45
1:B:199:LEU:HB3	1:B:237:ALA:O	2.16	0.45
1:A:128:PRO:O	1:A:129:ILE:HD13	2.15	0.45
1:B:4:LEU:O	1:B:5:PRO:C	2.53	0.45
1:B:270:GLU:HA	1:B:288:LYS:O	2.15	0.45
1:A:65:ASP:N	1:A:65:ASP:OD1	2.49	0.45
1:A:143:VAL:HG23	1:A:175:ILE:O	2.16	0.45
1:B:19:GLU:OE2	1:B:20:SER:HA	2.16	0.45
1:B:104:LEU:HD23	1:B:107:LEU:HD12	1.98	0.45
1:A:201:HIS:NE2	2:A:501:FRM:H202	2.31	0.45
1:B:15:ILE:HG13	1:B:16:PHE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:PHE:HD2	1:B:16:PHE:N	2.14	0.45
1:B:21:MET:HG3	1:B:206:THR:CG2	2.47	0.45
1:B:129:ILE:O	1:B:132:ASN:N	2.49	0.45
1:B:109:ASP:HB2	1:B:207:ASN:HA	1.98	0.45
1:B:142:VAL:O	1:B:143:VAL:C	2.48	0.45
1:A:296:ASP:OD1	1:A:298:SER:OG	2.34	0.45
1:B:42:LYS:HE3	1:B:43:ARG:NH1	2.31	0.45
1:B:51:ILE:HD13	1:B:74:ARG:HG3	1.99	0.45
1:B:123:ASP:HA	1:B:124:SER:CB	2.46	0.45
1:B:204:ARG:HD3	1:B:248:HIS:ND1	2.31	0.45
1:B:51:ILE:HD13	1:B:51:ILE:HG21	1.73	0.45
1:B:288:LYS:HE2	1:B:326:ASN:HD21	1.82	0.45
1:B:96:SER:N	3:B:581:HOH:O	2.50	0.44
1:B:152:ILE:HG21	1:B:152:ILE:HD13	1.45	0.44
1:B:168:TYR:HE1	1:B:170:LEU:HD22	1.82	0.44
1:A:208:PHE:HB3	1:A:212:LEU:HD12	1.99	0.44
1:B:42:LYS:H	1:B:42:LYS:HG3	1.56	0.44
1:B:281:PRO:O	1:B:282:LYS:C	2.55	0.44
1:A:249:THR:OG1	1:A:346:PHE:CG	2.64	0.44
1:B:188:LYS:O	1:B:189:PRO:C	2.53	0.44
1:B:349:LYS:CD	1:B:350:THR:H	2.27	0.44
1:B:218:ILE:O	1:B:219:ALA:C	2.55	0.44
1:A:145:ARG:H	1:A:145:ARG:HG3	1.69	0.44
1:A:296:ASP:HA	1:A:297:PRO:HD2	1.76	0.44
1:A:304:ASP:O	1:A:305:GLY:C	2.55	0.44
1:B:292:LYS:HG2	1:B:319:ASN:HB2	1.99	0.44
1:B:301:ILE:CG2	1:B:303:LEU:HD13	2.48	0.44
1:A:2:SER:HA	1:A:3:LYS:HD2	1.99	0.44
1:B:37:LEU:HB3	1:B:114:TYR:CE1	2.53	0.44
1:A:267:ASN:ND2	1:A:285:HIS:NE2	2.66	0.44
1:A:310:LEU:H	1:A:310:LEU:HG	1.58	0.44
1:B:4:LEU:HG	1:B:8:VAL:CG1	2.48	0.44
1:A:205:THR:HG22	1:A:257:LEU:H	1.82	0.44
1:A:281:PRO:HG2	1:A:284:LYS:HG3	1.99	0.44
1:A:289:GLY:N	3:A:529:HOH:O	2.51	0.44
1:B:70:ASP:O	1:B:73:ASN:N	2.50	0.44
1:B:241:SER:C	1:B:243:SER:N	2.70	0.44
1:A:202:GLY:N	2:A:501:FRM:O14	2.50	0.43
1:B:49:TYR:HB3	1:B:223:ALA:HA	2.00	0.43
1:B:112:VAL:O	1:B:116:LEU:HB2	2.18	0.43
1:B:200:TRP:NE1	3:B:612:HOH:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:PHE:CE1	1:B:257:LEU:HB2	2.53	0.43
1:B:52:LEU:HA	1:B:52:LEU:HD23	1.77	0.43
1:A:13:LYS:O	1:A:17:ASP:HB3	2.19	0.43
1:A:206:THR:HG22	3:A:615:HOH:O	2.18	0.43
1:B:3:LYS:HE2	1:B:130:ASP:OD2	2.18	0.43
1:B:22:LYS:H	1:B:22:LYS:HG2	1.47	0.43
1:B:33:GLN:HE21	1:B:33:GLN:HB3	1.52	0.43
1:B:84:GLY:O	1:B:85:MET:SD	2.76	0.43
1:B:112:VAL:CG1	1:B:116:LEU:HG	2.48	0.43
1:B:112:VAL:HG12	1:B:116:LEU:HG	1.99	0.43
1:B:9:GLN:O	1:B:10:ASP:C	2.55	0.43
1:B:230:PHE:O	1:B:231:GLY:O	2.36	0.43
1:A:93:ASN:ND2	1:A:96:SER:N	2.64	0.43
1:B:40:LEU:HD23	1:B:40:LEU:HA	1.64	0.43
1:A:126:LYS:HE2	1:A:134:GLU:OE1	2.18	0.43
1:B:71:LEU:HD23	1:B:74:ARG:NH1	2.34	0.43
1:A:43:ARG:N	1:A:43:ARG:CD	2.82	0.43
1:A:270:GLU:HG2	1:A:288:LYS:HB3	2.01	0.43
1:A:39:LYS:O	1:A:40:LEU:C	2.56	0.43
1:A:93:ASN:ND2	1:A:96:SER:H	2.11	0.43
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.85	0.43
1:A:116:LEU:HD12	1:A:135:LYS:HZ2	1.83	0.43
1:A:140:ILE:HG22	1:A:176:PHE:CD1	2.54	0.43
1:B:241:SER:O	1:B:244:ALA:N	2.40	0.43
1:B:135:LYS:HE2	1:B:135:LYS:HB2	1.79	0.43
1:B:153:ILE:HG21	1:B:342:LEU:HD11	2.00	0.43
1:B:159:ASN:HB2	1:B:310:LEU:O	2.18	0.43
1:B:191:LYS:O	1:B:192:GLN:C	2.55	0.43
1:B:288:LYS:HD3	1:B:290:LEU:CD2	2.48	0.43
1:A:161:HIS:NE2	1:A:170:LEU:HB2	2.34	0.42
1:A:166:ASN:HA	1:A:167:ALA:HA	1.27	0.42
1:A:283:GLY:C	3:A:580:HOH:O	2.57	0.42
1:A:296:ASP:CG	1:A:298:SER:HG	2.21	0.42
1:B:21:MET:HG3	1:B:206:THR:HG21	2.00	0.42
1:B:205:THR:HG23	3:B:512:HOH:O	2.18	0.42
1:B:287:VAL:HG23	1:B:331:TYR:HE1	1.83	0.42
1:B:312:THR:O	1:B:313:GLY:C	2.58	0.42
1:A:15:ILE:HG21	1:A:257:LEU:HD11	2.01	0.42
1:A:37:LEU:O	1:A:114:TYR:CD2	2.72	0.42
1:A:95:ASP:O	1:A:97:VAL:N	2.51	0.42
1:A:105:ASP:O	1:A:108:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ILE:HD13	1:A:218:ILE:HG21	1.54	0.42
1:B:78:LEU:O	1:B:80:PRO:HD3	2.19	0.42
1:B:216:LEU:HB3	1:B:234:ILE:HG21	2.00	0.42
1:B:239:MET:CE	1:B:295:PRO:HD3	2.50	0.42
1:B:277:ILE:HB	1:B:278:SER:H	1.58	0.42
1:A:324:LEU:CD2	1:A:325:TYR:CE2	3.01	0.42
1:B:108:LEU:HD23	1:B:108:LEU:HA	1.60	0.42
1:B:157:VAL:HG22	1:B:200:TRP:CH2	2.54	0.42
1:B:153:ILE:HG21	3:B:563:HOH:O	2.18	0.42
1:A:204:ARG:HH22	1:A:248:HIS:CG	2.38	0.42
1:A:218:ILE:HD12	1:A:232:LYS:O	2.19	0.42
1:A:100:LYS:NZ	1:A:103:MET:SD	2.92	0.42
1:A:267:ASN:ND2	1:A:283:GLY:O	2.53	0.42
1:B:26:VAL:HA	1:B:32:LEU:HD12	2.01	0.42
1:B:161:HIS:NE2	1:B:170:LEU:CD2	2.83	0.42
1:A:272:LYS:HG2	1:A:321:THR:HB	2.02	0.42
1:B:167:ALA:CA	1:B:349:LYS:HB3	2.47	0.42
1:B:170:LEU:O	1:B:171:GLU:C	2.58	0.42
1:B:269:TYR:O	1:B:288:LYS:N	2.53	0.42
1:B:149:GLU:O	1:B:152:ILE:N	2.52	0.42
1:A:162:ALA:O	1:A:163:THR:C	2.59	0.41
1:B:256:GLY:HA3	1:B:346:PHE:HE1	1.84	0.41
1:B:349:LYS:HG2	1:B:350:THR:HG23	2.01	0.41
1:A:270:GLU:HB3	1:A:290:LEU:HD11	2.02	0.41
1:B:110:ILE:CG1	1:B:206:THR:HB	2.49	0.41
1:B:249:THR:HB	1:B:254:PRO:HA	2.02	0.41
1:B:291:GLY:O	1:B:318:VAL:HB	2.19	0.41
1:A:76:TYR:O	1:A:78:LEU:N	2.53	0.41
1:A:257:LEU:O	1:A:258:ILE:HG22	2.20	0.41
1:A:284:LYS:HG2	3:A:580:HOH:O	2.20	0.41
1:B:186:ARG:NE	1:B:334:ALA:HA	2.34	0.41
1:A:108:LEU:O	1:A:112:VAL:HG23	2.21	0.41
1:B:38:GLY:HA3	3:B:556:HOH:O	2.21	0.41
1:B:129:ILE:O	1:B:130:ASP:C	2.58	0.41
1:B:332:ASP:OD1	1:B:332:ASP:C	2.58	0.41
1:A:88:PRO:HA	1:A:89:PRO:HD3	1.61	0.41
1:A:285:HIS:CD2	1:A:285:HIS:N	2.88	0.41
1:A:5:PRO:O	1:A:9:GLN:HG3	2.20	0.41
1:A:84:GLY:HA2	1:A:85:MET:HA	1.38	0.41
1:B:292:LYS:HE3	1:B:319:ASN:CB	2.48	0.41
1:A:83:PHE:CE2	1:A:89:PRO:CD	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.76	0.41
1:B:116:LEU:HD22	1:B:135:LYS:HB3	2.02	0.41
1:B:196:ARG:HA	1:B:263:VAL:O	2.20	0.41
1:A:175:ILE:HG21	1:A:175:ILE:HD13	1.16	0.41
1:A:193:LEU:O	1:A:196:ARG:HD3	2.20	0.41
1:A:304:ASP:OD2	1:A:304:ASP:N	2.53	0.41
1:B:256:GLY:O	1:B:257:LEU:HD23	2.20	0.41
1:A:204:ARG:HH21	1:A:204:ARG:HD2	1.70	0.41
1:A:231:GLY:HA3	1:A:277:ILE:O	2.20	0.41
1:B:12:ILE:HA	1:B:12:ILE:HD13	1.90	0.41
1:B:18:VAL:HA	1:B:21:MET:HB2	2.03	0.41
1:B:21:MET:HB3	1:B:37:LEU:HD11	2.03	0.41
1:B:36:PRO:O	1:B:37:LEU:C	2.60	0.41
1:B:138:THR:CG2	1:B:178:ILE:HG22	2.50	0.41
1:B:149:GLU:O	1:B:150:ALA:C	2.59	0.41
1:B:187:TYR:CE2	1:B:191:LYS:HG2	2.56	0.41
1:B:251:GLN:HA	1:B:254:PRO:HB3	2.02	0.41
1:B:287:VAL:HG21	1:B:331:TYR:OH	2.21	0.41
1:B:341:LEU:O	1:B:341:LEU:CD2	2.69	0.41
1:A:31:ASP:HB2	1:A:81:HIS:C	2.40	0.40
1:B:36:PRO:HD2	1:B:39:LYS:HB2	2.03	0.40
1:B:130:ASP:O	1:B:134:GLU:HB2	2.21	0.40
1:B:161:HIS:HE1	1:B:168:TYR:CD1	2.36	0.40
1:B:228:TYR:HD1	1:B:232:LYS:HG2	1.86	0.40
1:A:7:PRO:HB3	1:A:174:ASP:OD1	2.20	0.40
1:A:98:GLN:O	1:A:101:VAL:N	2.54	0.40
1:A:102:GLU:H	1:A:102:GLU:HG2	1.53	0.40
1:A:251:GLN:HA	1:A:251:GLN:NE2	2.36	0.40
1:A:288:LYS:HE3	1:A:328:TYR:CE2	2.57	0.40
1:A:346:PHE:HB3	1:A:348:PHE:CE1	2.56	0.40
1:B:83:PHE:CB	1:B:88:PRO:HB3	2.51	0.40
1:B:104:LEU:HD23	1:B:104:LEU:HA	1.92	0.40
1:B:164:THR:O	1:B:166:ASN:N	2.55	0.40
1:B:212:LEU:HA	1:B:212:LEU:HD23	1.79	0.40
1:A:180:ARG:HH11	1:A:180:ARG:HD2	1.68	0.40
1:A:204:ARG:O	1:A:206:THR:N	2.55	0.40
1:A:245:ASN:O	1:A:247:CYS:N	2.54	0.40
1:A:254:PRO:HG2	1:A:255:ILE:HG13	2.03	0.40
1:B:63:SER:CB	3:B:548:HOH:O	2.70	0.40
1:B:69:LEU:C	1:B:69:LEU:HD22	2.42	0.40
1:A:308:VAL:HA	1:A:309:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LYS:HB3	1:B:196:ARG:NH2	2.36	0.40
1:A:30:ILE:HD11	1:A:103:MET:CG	2.52	0.40
1:A:31:ASP:O	1:A:32:LEU:C	2.60	0.40
1:B:162:ALA:C	1:B:163:THR:O	2.60	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	348/350 (99%)	241 (69%)	61 (18%)	46 (13%)	0 1
1	B	348/350 (99%)	235 (68%)	61 (18%)	52 (15%)	0 1
All	All	696/700 (99%)	476 (68%)	122 (18%)	98 (14%)	0 1

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	12	ILE
1	A	39	LYS
1	A	43	ARG
1	A	66	SER
1	A	95	ASP
1	A	117	LEU
1	A	118	ARG
1	A	124	SER
1	A	133	TYR
1	A	144	ASP
1	A	145	ARG
1	A	168	TYR
1	A	185	GLN

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Mol	Chain	Res	Type
1	A	205	THR
1	A	278	SER
1	A	297	PRO
1	A	313	GLY
1	A	320	ASP
1	A	349	LYS
1	B	10	ASP
1	B	21	MET
1	B	40	LEU
1	B	76	TYR
1	B	95	ASP
1	B	96	SER
1	B	114	TYR
1	B	137	LYS
1	B	161	HIS
1	B	163	THR
1	B	165	HIS
1	B	167	ALA
1	B	176	PHE
1	B	231	GLY
1	B	241	SER
1	B	251	GLN
1	B	312	THR
1	B	320	ASP
1	B	326	ASN
1	A	3	LYS
1	A	13	LYS
1	A	29	GLU
1	A	62	GLY
1	A	163	THR
1	A	166	ASN
1	A	215	GLY
1	A	301	ILE
1	B	26	VAL
1	B	30	ILE
1	B	68	ILE
1	B	75	PHE
1	B	103	MET
1	B	113	ALA
1	B	182	GLY
1	B	208	PHE
1	B	215	GLY

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Mol	Chain	Res	Type
1	B	302	SER
1	B	349	LYS
1	A	32	LEU
1	A	116	LEU
1	A	119	GLY
1	A	132	ASN
1	A	241	SER
1	B	66	SER
1	B	128	PRO
1	B	254	PRO
1	B	282	LYS
1	B	290	LEU
1	B	313	GLY
1	A	77	THR
1	A	86	LYS
1	A	96	SER
1	A	242	LYS
1	B	105	ASP
1	B	110	ILE
1	B	124	SER
1	B	216	LEU
1	B	295	PRO
1	A	295	PRO
1	A	298	SER
1	A	304	ASP
1	B	32	LEU
1	B	120	GLY
1	B	157	VAL
1	B	195	ASN
1	A	276	HIS
1	B	37	LEU
1	B	47	ALA
1	B	65	ASP
1	A	153	ILE
1	B	89	PRO
1	A	127	ASP
1	A	266	GLY
1	B	301	ILE
1	A	5	PRO
1	B	55	VAL
1	B	253	ASP
1	A	296	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	308/308 (100%)	215 (70%)	93 (30%)	0 1
1	B	308/308 (100%)	218 (71%)	90 (29%)	0 2
All	All	616/616 (100%)	433 (70%)	183 (30%)	0 1

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	LEU
1	A	6	LYS
1	A	12	ILE
1	A	14	MET
1	A	15	ILE
1	A	16	PHE
1	A	17	ASP
1	A	19	GLU
1	A	20	SER
1	A	29	GLU
1	A	33	GLN
1	A	37	LEU
1	A	42	LYS
1	A	43	ARG
1	A	44	GLN
1	A	46	GLN
1	A	50	SER
1	A	55	VAL
1	A	57	GLN
1	A	61	GLN
1	A	65	ASP
1	A	69	LEU
1	A	79	ILE
1	A	81	HIS
1	A	83	PHE
1	A	85	MET

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Mol	Chain	Res	Type
1	A	86	LYS
1	A	90	LEU
1	A	92	ASN
1	A	93	ASN
1	A	97	VAL
1	A	100	LYS
1	A	101	VAL
1	A	102	GLU
1	A	116	LEU
1	A	117	LEU
1	A	121	SER
1	A	125	SER
1	A	130	ASP
1	A	135	LYS
1	A	138	THR
1	A	139	ASP
1	A	140	ILE
1	A	141	LYS
1	A	145	ARG
1	A	146	ASP
1	A	148	GLU
1	A	151	GLU
1	A	156	TYR
1	A	165	HIS
1	A	171	GLU
1	A	175	ILE
1	A	176	PHE
1	A	178	ILE
1	A	179	GLU
1	A	180	ARG
1	A	184	CYS
1	A	204	ARG
1	A	212	LEU
1	A	218	ILE
1	A	226	THR
1	A	232	LYS
1	A	238	ASP
1	A	242	LYS
1	A	245	ASN
1	A	247	CYS
1	A	251	GLN
1	A	253	ASP

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Mol	Chain	Res	Type
1	A	254	PRO
1	A	258	ILE
1	A	277	ILE
1	A	279	LYS
1	A	280	LEU
1	A	282	LYS
1	A	284	LYS
1	A	285	HIS
1	A	288	LYS
1	A	298	SER
1	A	300	ASN
1	A	302	SER
1	A	303	LEU
1	A	304	ASP
1	A	306	VAL
1	A	309	PRO
1	A	310	LEU
1	A	314	ILE
1	A	321	THR
1	A	324	LEU
1	A	331	TYR
1	A	336	VAL
1	A	342	LEU
1	A	345	LYS
1	B	1	LYS
1	B	3	LYS
1	B	4	LEU
1	B	14	MET
1	B	16	PHE
1	B	19	GLU
1	B	20	SER
1	B	22	LYS
1	B	26	VAL
1	B	27	GLU
1	B	31	ASP
1	B	33	GLN
1	B	34	LYS
1	B	35	MET
1	B	42	LYS
1	B	43	ARG
1	B	53	SER
1	B	57	GLN

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Mol	Chain	Res	Type
1	B	61	GLN
1	B	63	SER
1	B	66	SER
1	B	69	LEU
1	B	70	ASP
1	B	74	ARG
1	B	78	LEU
1	B	83	PHE
1	B	85	MET
1	B	86	LYS
1	B	87	LYS
1	B	92	ASN
1	B	95	ASP
1	B	96	SER
1	B	98	GLN
1	B	103	MET
1	B	111	GLU
1	B	115	SER
1	B	117	LEU
1	B	118	ARG
1	B	126	LYS
1	B	127	ASP
1	B	129	ILE
1	B	134	GLU
1	B	135	LYS
1	B	137	LYS
1	B	138	THR
1	B	140	ILE
1	B	145	ARG
1	B	152	ILE
1	B	158	LYS
1	B	159	ASN
1	B	161	HIS
1	B	164	THR
1	B	166	ASN
1	B	171	GLU
1	B	173	ILE
1	B	177	LYS
1	B	178	ILE
1	B	179	GLU
1	B	181	GLU
1	B	184	CYS

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Mol	Chain	Res	Type
1	B	192	GLN
1	B	194	HIS
1	B	195	ASN
1	B	197	ARG
1	B	198	LEU
1	B	200	TRP
1	B	204	ARG
1	B	205	THR
1	B	206	THR
1	B	217	ARG
1	B	218	ILE
1	B	226	THR
1	B	232	LYS
1	B	243	SER
1	B	251	GLN
1	B	263	VAL
1	B	278	SER
1	B	279	LYS
1	B	280	LEU
1	B	281	PRO
1	B	294	THR
1	B	295	PRO
1	B	298	SER
1	B	302	SER
1	B	303	LEU
1	B	310	LEU
1	B	319	ASN
1	B	321	THR
1	B	338	LEU
1	B	345	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	93	ASN
1	A	245	ASN
1	A	251	GLN
1	A	267	ASN
1	A	326	ASN
1	A	337	ASN
1	A	347	ASN

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Mol	Chain	Res	Type
1	B	33	GLN
1	B	46	GLN
1	B	67	GLN
1	B	165	HIS
1	B	267	ASN
1	B	273	HIS
1	B	300	ASN
1	B	319	ASN
1	B	326	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FRM	B	502	-	30,31,31	1.70	8 (26%)	37,43,43	3.49	17 (45%)
2	FRM	A	501	-	30,31,31	1.33	4 (13%)	37,43,43	3.64	20 (54%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRM	B	502	-	-	2/10/20/20	0/4/4/4
2	FRM	A	501	-	-	4/10/20/20	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	FRM	C2-C3	-4.27	1.35	1.42
2	B	502	FRM	C29-N26	-4.16	1.42	1.46
2	B	502	FRM	C40-C31	-3.39	1.43	1.48
2	A	501	FRM	C2-C3	-3.34	1.37	1.42
2	B	502	FRM	C7-C2	-2.71	1.45	1.51
2	B	502	FRM	C46-C40	-2.59	1.35	1.39
2	B	502	FRM	C1-C2	2.34	1.42	1.37
2	A	501	FRM	C4-C3	-2.26	1.37	1.41
2	A	501	FRM	C46-C45	-2.08	1.35	1.38
2	B	502	FRM	C33-N26	-2.06	1.41	1.46
2	A	501	FRM	C11-N12	-2.05	1.31	1.33
2	B	502	FRM	C6-C5	2.04	1.41	1.36

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FRM	C11-N10-C3	11.05	124.06	115.42
2	B	502	FRM	C32-C33-N26	10.52	120.58	111.19
2	B	502	FRM	C4-C13-N12	-9.06	115.41	124.68
2	A	501	FRM	C3-C4-C13	-7.22	114.65	119.98
2	B	502	FRM	C3-C4-C13	-7.13	114.72	119.98
2	A	501	FRM	N10-C11-N12	-6.31	117.57	126.09
2	B	502	FRM	N10-C11-N12	-5.96	118.05	126.09
2	A	501	FRM	C46-C40-C31	-5.88	114.18	121.22
2	A	501	FRM	C30-C29-N26	-5.70	108.39	112.89
2	A	501	FRM	C5-C4-C3	5.52	123.23	118.09
2	B	502	FRM	C17-C11-N10	5.50	125.13	116.77
2	B	502	FRM	C29-N26-C33	5.01	114.75	109.78
2	B	502	FRM	C32-C31-C30	-4.52	116.87	120.63
2	A	501	FRM	C43-C42-C40	-4.33	116.18	120.80
2	B	502	FRM	C11-N10-C3	4.25	118.75	115.42
2	A	501	FRM	C4-C13-N12	-4.24	120.34	124.68
2	A	501	FRM	C6-C5-C4	-4.23	114.01	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FRM	C46-C45-C44	-4.05	114.21	118.38
2	A	501	FRM	C17-C11-N12	3.71	122.31	116.73
2	B	502	FRM	C23-N26-C33	3.22	119.82	111.24
2	A	501	FRM	C45-C46-C40	3.22	124.23	120.80
2	B	502	FRM	C20-C23-N26	3.20	122.92	113.93
2	A	501	FRM	C32-C31-C30	-3.17	118.00	120.63
2	A	501	FRM	C20-C23-N26	-3.16	105.05	113.93
2	A	501	FRM	C42-C40-C31	3.14	124.97	121.22
2	A	501	FRM	C32-C33-N26	-3.13	108.39	111.19
2	A	501	FRM	C2-C3-C4	3.03	122.53	120.03
2	A	501	FRM	C7-C2-C3	2.88	122.76	120.05
2	B	502	FRM	C1-C2-C3	2.73	121.37	117.99
2	B	502	FRM	C5-C4-C3	2.72	120.62	118.09
2	B	502	FRM	C30-C29-N26	2.61	114.95	112.89
2	A	501	FRM	F1-C44-C45	-2.57	114.43	118.55
2	A	501	FRM	C42-C43-C44	2.51	120.96	118.38
2	B	502	FRM	C2-C3-N10	2.42	121.02	118.16
2	B	502	FRM	C2-C3-C4	-2.26	118.17	120.03
2	B	502	FRM	F1-C44-C43	2.05	121.84	118.55
2	B	502	FRM	C5-C6-C1	-2.05	117.84	121.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FRM	N12-C11-C17-C20
2	A	501	FRM	C11-C17-C20-C23
2	A	501	FRM	C20-C23-N26-C29
2	A	501	FRM	C20-C23-N26-C33
2	B	502	FRM	C20-C23-N26-C29
2	B	502	FRM	C11-C17-C20-C23

There are no ring outliers.

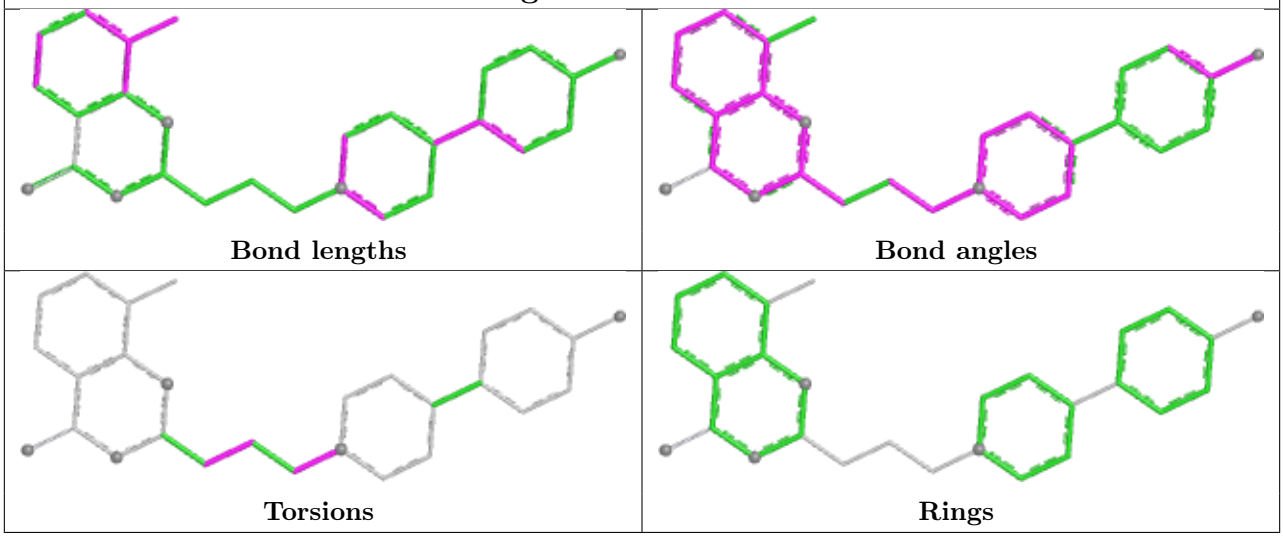
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FRM	2	0

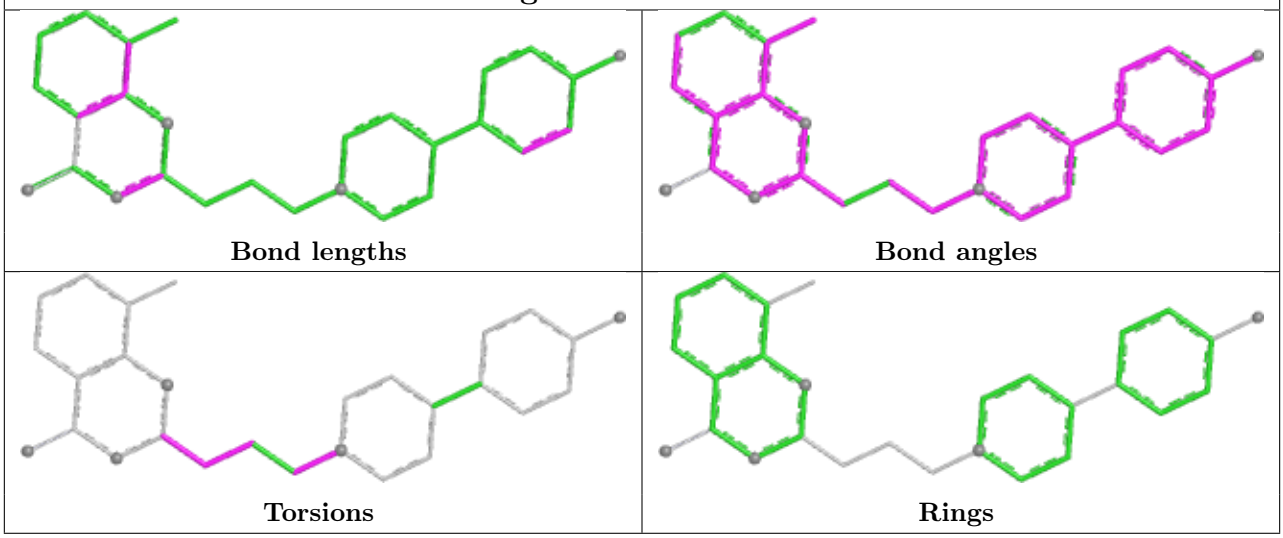
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FRM B 502



Ligand FRM A 501



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	350/350 (100%)	-0.44	2 (0%)	89	72	2, 10, 26, 38	0
1	B	350/350 (100%)	-0.31	3 (0%)	84	63	2, 12, 28, 43	0
All	All	700/700 (100%)	-0.37	5 (0%)	87	69	2, 11, 27, 43	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	SER	3.3
1	A	125	SER	2.3
1	A	2	SER	2.2
1	B	123	ASP	2.1
1	B	126	LYS	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

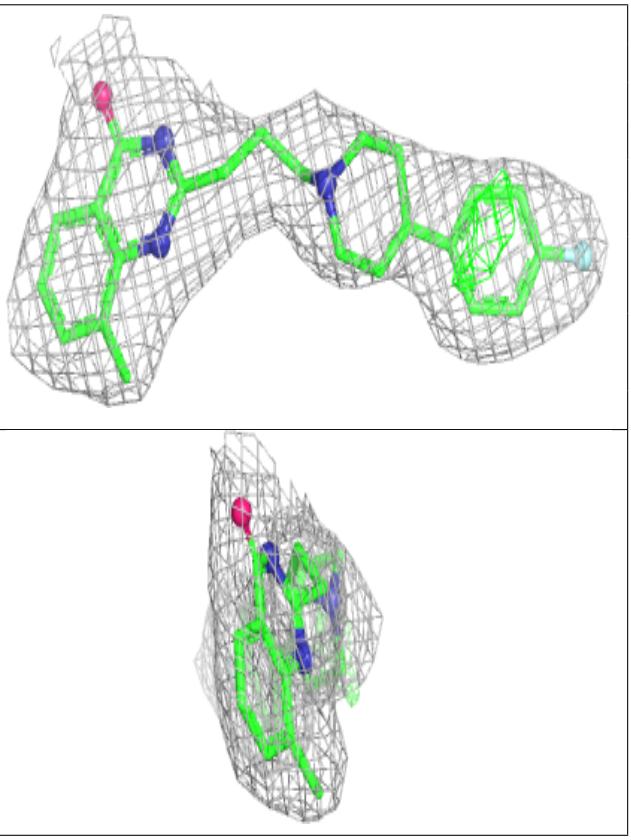
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FRM	A	501	28/28	0.96	0.16	2,7,16,17	0
2	FRM	B	502	28/28	0.97	0.15	2,2,6,9	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

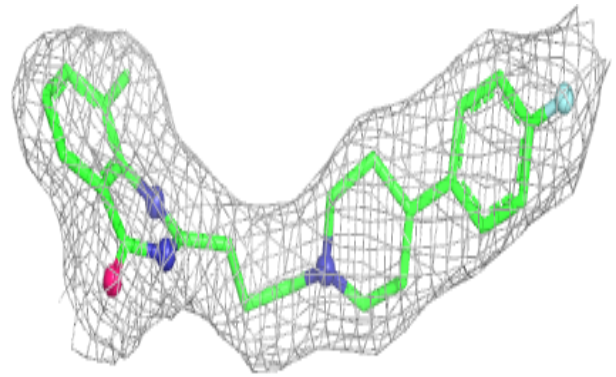
Electron density around FRM A 501:

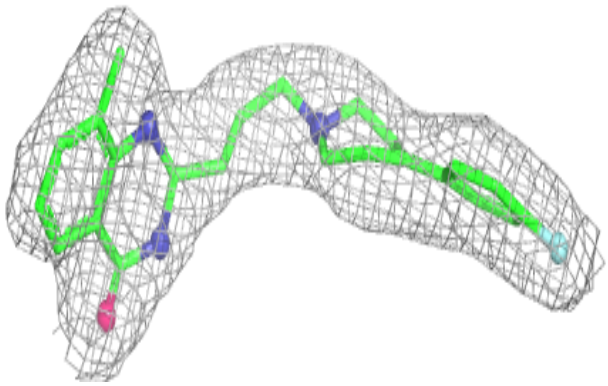
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

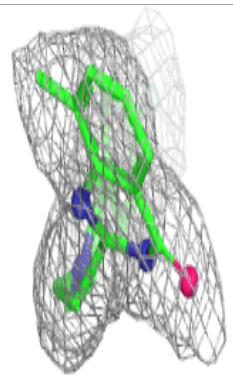


Electron density around FRM B 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.