



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:47 AM UTC

PDB ID : 1LW2 / pdb_00001lw2
Title : CRYSTAL STRUCTURE OF T215Y MUTANT HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH 1051U91
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Deposited on : 2002-05-30
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

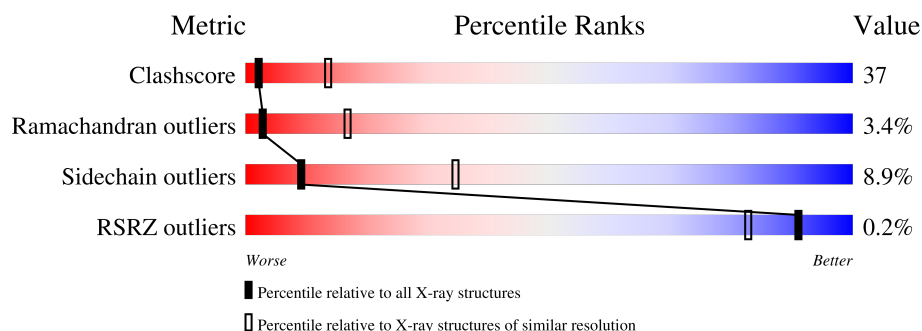
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	440	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7662 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 HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4257	2759	703	787	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	TYR	THR	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

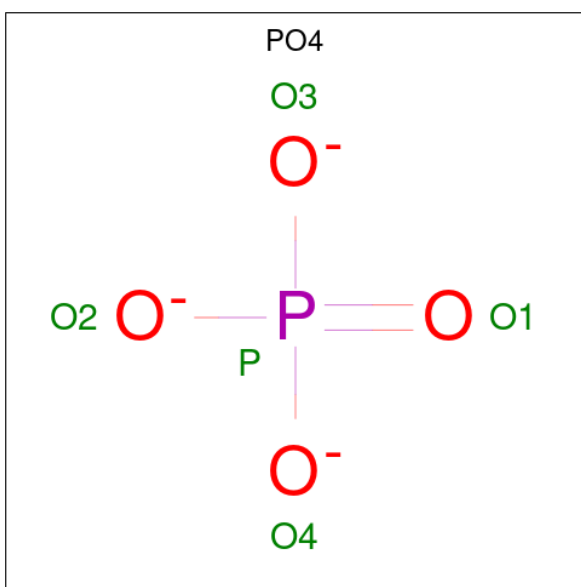
- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	406	Total	C	N	O	S	0	0	0
			3373	2203	555	608	7			

There is a discrepancy between the modelled and reference sequences:

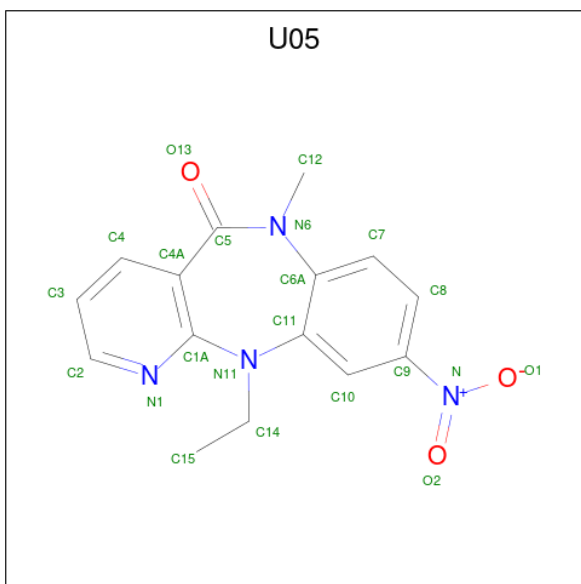
Chain	Residue	Modelled	Actual	Comment	Reference
B	215	TYR	THR	engineered mutation	UNP P04585

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 6,11-DIHYDRO-11-ETHYL-6-METHYL-9-NITRO-5H-PYRIDO[2,3-B][1,5]BENZODIAZEPIN-5-ONE (CCD ID: U05) (formula: C₁₅H₁₄N₄O₃).

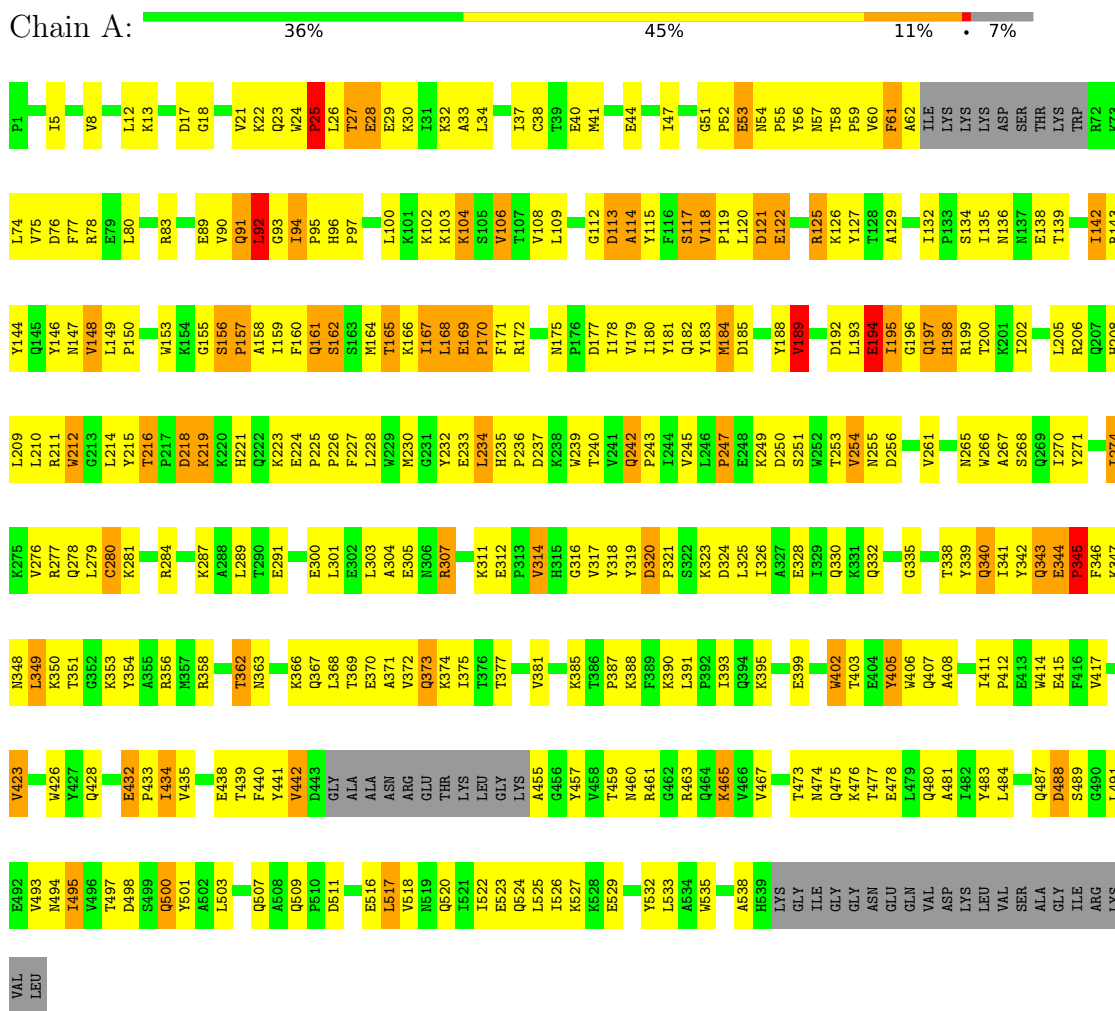


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			22	15	4	3		

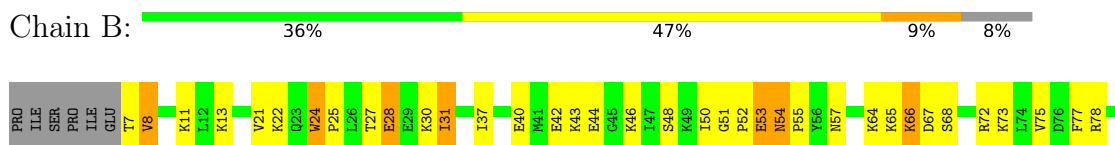
3 Residue-property plots

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

• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE



ILE VAL GLY ALA GLU THR PHE	ALA HIS T362 N363 D364 V365 K366 Q367 L368 T369	L289 T290 E291 V292 P294 L295 T296 E297 E298 A299 E300 L301 E302	HIS GLN K223 E224 P225 F226 F227 L228 W229 M230 G231 Y232 E233 L234 P236 W239	P157 A158 I159 F160 Q161 S162 S163 M164	K82 R83 T84 Q85 D86 F87 W88 GLU VAL GLN LEU GLY I94 P95
P377 E378 S379 I380 V381 I382 W383 G384	V372 Q373 K374	E305 N306 I309 V314 H315 G316 V317 Y318 K323 I326 A327 E328 I329 Q330 K331 Q332 G333 Q334 G335 Q336 W337 T338 Y339 Q340 I341 Y342 E344	Q242 P243 I244 P247 E248 K249 D250 W252 T253 V254 I257 Q258 K259 L260 V261 G262 K263 L264 N265 W266 Q269 I270 P272 G273 I274	Y189 G190 S191 D192 L193 E194 I195 G196 Q197 H198 R199 T200 K201 I202 E203 E204 L205 R206 H208 L209 L210	Y115 F116 S117 V118 P119 L120 D121 R125 A129 F130 T131 I132 P133 S134 I135 N136 W137 E138 T139 P140 G141 I142 R143 Y144
Q418 T419 P420 P421 L422 V423 K424 L425	Q428 LEU GLU LYS GLU PRO	K356 MET ARG GLY	R277 Q278 L279 C280 K281 L282 L283 R284 G285 T286	R211 W212 G213 L214 Y215 T216 PRO ASP LYS LYS	Q145 Y146 N147 V148 L149 P150 Q151 G152 W153 K154

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.30Å 115.20Å 64.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 3.00 29.78 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.78-3.00) 98.5 (29.78-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.267 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 76.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7662	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: U05, PO4, CSD

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	0.70	1/4363 (0.0%)	1.13	33/5934 (0.6%)
2	B	0.70	0/3471	1.12	23/4716 (0.5%)
All	All	0.70	1/7834 (0.0%)	1.13	56/10650 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	ILE	CA-CB	-5.60	1.47	1.54

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	214	LEU	N-CA-C	-12.39	97.62	113.72
1	A	349	LEU	N-CA-C	-11.08	99.27	113.12
2	B	215	TYR	N-CA-C	-10.88	99.66	113.16
1	A	234	LEU	N-CA-C	9.56	124.00	108.41
1	A	343	GLN	N-CA-C	-7.75	103.66	113.43
1	A	189	VAL	N-CA-C	7.13	118.41	107.78
2	B	53	GLU	N-CA-C	-7.11	104.73	113.19
2	B	225	PRO	N-CA-C	7.09	119.35	110.70
1	A	500	GLN	N-CA-C	-7.01	103.64	111.28
1	A	113	ASP	N-CA-C	-6.86	104.03	113.56
1	A	242	GLN	N-CA-C	-6.67	101.93	109.60
1	A	29	GLU	N-CA-C	-6.64	103.97	111.14
2	B	147	ASN	N-CA-C	-6.63	105.82	114.04
1	A	197	GLN	N-CA-C	-6.55	103.25	111.11
1	A	61	PHE	N-CA-C	6.52	117.18	108.38
2	B	401	TRP	N-CA-C	6.37	122.12	113.97
1	A	388	LYS	N-CA-C	-6.36	100.86	110.28
1	A	223	LYS	N-CA-C	-6.33	102.01	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	GLU	N-CA-C	-6.20	101.67	110.35
1	A	242	GLN	CA-C-N	6.17	127.56	119.84
1	A	242	GLN	C-N-CA	6.17	127.56	119.84
1	A	96	HIS	CA-C-N	6.13	127.50	119.84
1	A	96	HIS	C-N-CA	6.13	127.50	119.84
1	A	167	ILE	N-CA-C	-5.89	104.76	110.42
2	B	37	ILE	N-CA-C	5.57	116.21	110.36
1	A	147	ASN	N-CA-C	-5.55	106.41	114.12
1	A	278	GLN	N-CA-C	5.51	117.29	111.28
1	A	125	ARG	N-CA-C	5.49	117.27	111.28
2	B	192	ASP	N-CA-C	-5.46	106.47	114.39
2	B	108	VAL	N-CA-C	5.46	115.81	108.17
2	B	118	VAL	CA-C-N	5.42	125.89	120.14
2	B	118	VAL	C-N-CA	5.42	125.89	120.14
2	B	250	ASP	N-CA-C	-5.40	102.67	111.04
2	B	24	TRP	CA-C-N	5.40	125.40	119.89
2	B	24	TRP	C-N-CA	5.40	125.40	119.89
1	A	267	ALA	N-CA-C	5.38	116.83	111.07
1	A	274	ILE	N-CA-C	-5.34	102.70	109.80
1	A	493	VAL	N-CA-C	5.33	114.89	108.06
2	B	349	LEU	N-CA-C	-5.32	106.80	113.72
1	A	40	GLU	N-CA-C	-5.26	104.80	111.11
1	A	212	TRP	N-CA-C	-5.23	104.08	110.61
1	A	53	GLU	N-CA-C	-5.18	106.96	113.28
2	B	175	ASN	CA-C-N	5.17	126.31	119.84
2	B	175	ASN	C-N-CA	5.17	126.31	119.84
1	A	5	ILE	N-CA-C	5.14	116.10	108.23
1	A	118	VAL	N-CA-C	5.12	113.70	107.61
1	A	405	TYR	N-CA-C	5.11	117.72	110.10
2	B	139	THR	CA-C-N	5.09	126.20	119.84
2	B	139	THR	C-N-CA	5.09	126.20	119.84
1	A	320	ASP	CA-C-N	5.05	126.15	119.84
1	A	320	ASP	C-N-CA	5.05	126.15	119.84
2	B	54	ASN	CA-C-N	5.04	126.98	120.89
2	B	54	ASN	C-N-CA	5.04	126.98	120.89
1	A	442	VAL	N-CA-C	5.03	115.55	108.36
2	B	194	GLU	N-CA-C	-5.02	103.43	110.50
2	B	13	LYS	N-CA-C	-5.01	102.87	109.84

There are no chirality outliers.

There are no planarity outliers.

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	4257	0	4280	339	0
2	B	3373	0	3399	237	0
3	A	10	0	0	2	0
4	A	22	0	14	1	0
All	All	7662	0	7693	568	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 37.

All (568) 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)
2:B:167:ILE:HG21	2:B:214:LEU:HD11	1.30	1.11
1:A:362:THR:HG22	1:A:366:LYS:HD3	1.43	1.00
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.43	0.99
2:B:94:ILE:HD12	2:B:95:PRO:HD2	1.46	0.96
1:A:356:ARG:HE	1:A:358:ARG:HH11	1.14	0.96
1:A:136:ASN:HD22	1:A:139:THR:HG22	1.31	0.95
1:A:206:ARG:HH12	1:A:218:ASP:HB3	1.31	0.95
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.49	0.95
1:A:194:GLU:HG2	1:A:197:GLN:HE21	1.30	0.94
1:A:142:ILE:HD12	1:A:142:ILE:H	1.34	0.91
1:A:476:LYS:HG2	1:A:480:GLN:HE21	1.37	0.89
1:A:442:VAL:HG13	1:A:481:ALA:HB1	1.53	0.89
2:B:282:LEU:HG	2:B:293:ILE:HG21	1.55	0.89
1:A:480:GLN:HG3	1:A:517:LEU:HD11	1.57	0.87
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.11	0.85
1:A:113:ASP:HB3	1:A:117:SER:OG	1.76	0.85
2:B:270:ILE:O	2:B:272:PRO:HD3	1.76	0.85
1:A:92:LEU:HD12	1:A:92:LEU:N	1.92	0.85
2:B:142:ILE:H	2:B:142:ILE:HD12	1.41	0.84
1:A:92:LEU:HD12	1:A:92:LEU:H	1.42	0.83
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.61	0.82
1:A:136:ASN:ND2	1:A:139:THR:HG22	1.93	0.82
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASN:HD21	1:A:138:GLU:HB2	1.46	0.81
1:A:132:ILE:HG13	1:A:142:ILE:HD13	1.63	0.81
2:B:422:LEU:HA	2:B:425:LEU:HD23	1.62	0.80
1:A:372:VAL:HG11	1:A:411:ILE:HD12	1.63	0.79
1:A:253:THR:HG22	1:A:256:ASP:CG	2.07	0.79
2:B:164:MET:SD	2:B:167:ILE:HD11	2.21	0.79
2:B:277:ARG:HH11	2:B:277:ARG:HB2	1.48	0.79
2:B:72:ARG:HH12	2:B:110:ASP:CG	1.90	0.79
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.65	0.78
1:A:307:ARG:HH11	1:A:307:ARG:HG2	1.50	0.77
2:B:173:LYS:HA	2:B:176:PRO:HG3	1.66	0.76
1:A:33:ALA:O	1:A:37:ILE:HG13	1.85	0.76
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.67	0.76
1:A:161:GLN:HA	1:A:182:GLN:HE22	1.51	0.76
1:A:473:THR:O	1:A:477:THR:HG23	1.85	0.76
1:A:142:ILE:HD12	1:A:142:ILE:N	2.01	0.75
1:A:432:GLU:HG3	1:A:433:PRO:HD2	1.69	0.75
1:A:399:GLU:HG2	1:A:402:TRP:CE3	2.22	0.74
2:B:88:TRP:CD1	2:B:88:TRP:C	2.65	0.74
2:B:195:ILE:O	2:B:199:ARG:HG3	1.87	0.74
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.23	0.73
1:A:518:VAL:O	1:A:522:ILE:HG13	1.89	0.72
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.23	0.72
1:A:23:GLN:O	1:A:25:PRO:HD3	1.89	0.72
1:A:22:LYS:HE2	1:A:24:TRP:HD1	1.55	0.72
2:B:282:LEU:HG	2:B:293:ILE:CG2	2.20	0.72
2:B:227:PHE:HB3	2:B:231:GLY:HA2	1.71	0.72
1:A:455:ALA:HB3	1:A:467:VAL:O	1.90	0.71
1:A:92:LEU:HD13	1:A:93:GLY:H	1.55	0.71
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.70	0.71
1:A:524:GLN:HA	1:A:524:GLN:OE1	1.90	0.71
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.72	0.71
1:A:136:ASN:HD22	1:A:139:THR:CG2	2.02	0.71
1:A:277:ARG:HG3	1:A:277:ARG:HH11	1.55	0.71
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.20	0.71
1:A:22:LYS:HE2	1:A:24:TRP:CD1	2.26	0.70
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.21	0.70
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.74	0.70
2:B:175:ASN:ND2	2:B:201:LYS:HD3	2.07	0.70
2:B:230:MET:C	2:B:232:TYR:H	2.00	0.69
1:A:134:SER:OG	1:A:139:THR:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:GLN:HB3	2:B:211:ARG:HD2	1.73	0.69
2:B:170:PRO:HG3	2:B:212:TRP:CZ3	2.28	0.69
1:A:304:ALA:O	1:A:307:ARG:HB2	1.93	0.69
2:B:64:LYS:HZ1	2:B:66:LYS:HA	1.57	0.69
1:A:95:PRO:HB3	2:B:136:ASN:O	1.92	0.69
1:A:162:SER:O	1:A:165:THR:HG23	1.92	0.69
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.74	0.69
2:B:72:ARG:NH1	2:B:110:ASP:OD1	2.26	0.69
2:B:154:LYS:O	2:B:157:PRO:HD2	1.93	0.69
1:A:194:GLU:CG	1:A:197:GLN:HE21	2.03	0.68
2:B:393:ILE:HG12	2:B:394:GLN:H	1.58	0.68
2:B:393:ILE:HG12	2:B:394:GLN:N	2.06	0.68
2:B:167:ILE:CG2	2:B:214:LEU:HD11	2.16	0.68
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.18	0.68
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.75	0.68
1:A:172:ARG:NH1	1:A:180:ILE:HB	2.08	0.67
2:B:110:ASP:HB3	2:B:226:PRO:HG2	1.76	0.67
2:B:31:ILE:HD11	2:B:133:PRO:HG2	1.77	0.67
1:A:354:TYR:CZ	1:A:356:ARG:HB3	2.30	0.67
1:A:28:GLU:HG3	1:A:135:ILE:HG12	1.74	0.67
1:A:170:PRO:HG2	1:A:171:PHE:H	1.61	0.66
1:A:399:GLU:O	1:A:402:TRP:HB3	1.95	0.66
2:B:64:LYS:NZ	2:B:66:LYS:HA	2.10	0.66
2:B:139:THR:HB	2:B:140:PRO:HD2	1.77	0.66
1:A:195:ILE:O	1:A:198:HIS:HB3	1.96	0.66
1:A:350:LYS:HG2	1:A:351:THR:N	2.10	0.65
2:B:362:THR:HG22	2:B:363:ASN:N	2.10	0.65
2:B:148:VAL:HG23	2:B:149:LEU:O	1.95	0.65
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.32	0.65
1:A:183:TYR:CE1	1:A:184:MET:HG3	2.31	0.65
1:A:356:ARG:HE	1:A:358:ARG:NH1	1.90	0.65
2:B:27:THR:OG1	2:B:30:LYS:HG2	1.97	0.65
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.62	0.65
2:B:277:ARG:O	2:B:281:LYS:HG3	1.97	0.65
1:A:319:TYR:OH	1:A:385:LYS:HE2	1.97	0.65
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.32	0.64
2:B:167:ILE:CD1	2:B:168:LEU:HG	2.27	0.64
2:B:88:TRP:C	2:B:88:TRP:HD1	2.06	0.64
1:A:108:VAL:C	1:A:109:LEU:HD12	2.22	0.64
1:A:148:VAL:O	1:A:150:PRO:HD3	1.97	0.64
1:A:206:ARG:HH12	1:A:218:ASP:CB	2.07	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:THR:CG2	2:B:367:GLN:HE21	2.09	0.64
1:A:112:GLY:O	1:A:113:ASP:HB2	1.97	0.64
2:B:78:ARG:HD3	2:B:411:ILE:O	1.98	0.64
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.33	0.64
1:A:89:GLU:OE2	1:A:92:LEU:HA	1.98	0.63
1:A:136:ASN:ND2	1:A:139:THR:H	1.96	0.63
1:A:197:GLN:O	1:A:200:THR:HB	1.98	0.63
2:B:326:ILE:HG22	2:B:327:ALA:N	2.12	0.63
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.29	0.63
2:B:53:GLU:OE1	2:B:53:GLU:N	2.28	0.63
1:A:114:ALA:HB2	1:A:185:ASP:OD2	1.98	0.63
1:A:476:LYS:HG2	1:A:480:GLN:NE2	2.13	0.63
2:B:131:THR:OG1	2:B:143:ARG:HG2	1.99	0.63
1:A:344:GLU:HB3	1:A:347:LYS:HE3	1.81	0.62
2:B:167:ILE:HD12	2:B:168:LEU:N	2.13	0.62
2:B:362:THR:HG21	2:B:367:GLN:HE21	1.64	0.62
1:A:178:ILE:HG22	1:A:179:VAL:N	2.15	0.62
1:A:438:GLU:OE1	1:A:463:ARG:HD3	1.99	0.62
2:B:167:ILE:HD12	2:B:168:LEU:HG	1.81	0.62
2:B:203:GLU:O	2:B:207:GLN:HG3	1.99	0.62
1:A:104:LYS:CB	1:A:192:ASP:HA	2.29	0.61
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.48	0.61
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.34	0.61
1:A:210:LEU:HD23	1:A:210:LEU:O	2.00	0.61
1:A:171:PHE:HE1	1:A:205:LEU:HA	1.65	0.61
2:B:31:ILE:CD1	2:B:133:PRO:HG2	2.30	0.61
1:A:27:THR:HG23	1:A:30:LYS:CG	2.31	0.61
1:A:487:GLN:HA	1:A:524:GLN:NE2	2.16	0.61
1:A:277:ARG:HG3	1:A:277:ARG:NH1	2.15	0.60
2:B:202:ILE:HG22	2:B:203:GLU:N	2.15	0.60
1:A:28:GLU:O	1:A:32:LYS:HG3	2.01	0.60
2:B:340:GLN:HB3	2:B:348:ASN:HD22	1.66	0.60
2:B:210:LEU:HG	2:B:223:LYS:O	2.01	0.60
1:A:34:LEU:HD13	1:A:132:ILE:HG22	1.83	0.60
1:A:399:GLU:HG2	1:A:402:TRP:HE3	1.63	0.60
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.15	0.60
1:A:90:VAL:HG22	1:A:91:GLN:HG2	1.83	0.60
1:A:391:LEU:HD12	1:A:414:TRP:CE3	2.36	0.60
1:A:61:PHE:CE1	1:A:74:LEU:HD23	2.37	0.60
1:A:149:LEU:HD21	1:A:159:ILE:HG21	1.83	0.59
1:A:161:GLN:HG2	1:A:182:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.16	0.59
1:A:228:LEU:HA	1:A:232:TYR:O	2.02	0.59
1:A:60:VAL:HG22	1:A:75:VAL:HG13	1.82	0.59
1:A:303:LEU:C	1:A:303:LEU:HD23	2.27	0.59
1:A:30:LYS:CD	1:A:62:ALA:HB3	2.32	0.59
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.38	0.59
1:A:94:ILE:CD1	1:A:230:MET:HE3	2.32	0.58
1:A:120:LEU:HD23	1:A:125:ARG:HG2	1.86	0.58
1:A:102:LYS:O	1:A:103:LYS:HD3	2.04	0.58
1:A:155:GLY:O	1:A:156:SER:C	2.46	0.58
2:B:333:GLY:O	2:B:336:GLN:HG2	2.03	0.58
2:B:215:TYR:HE2	2:B:225:PRO:HG3	1.68	0.58
1:A:56:TYR:O	1:A:143:ARG:NH2	2.36	0.58
1:A:115:TYR:N	1:A:115:TYR:CD2	2.70	0.58
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.39	0.58
1:A:92:LEU:H	1:A:92:LEU:CD1	2.07	0.58
1:A:95:PRO:HG3	4:A:999:U05:O2	2.04	0.58
1:A:253:THR:O	1:A:256:ASP:N	2.36	0.58
2:B:197:GLN:O	2:B:200:THR:HB	2.03	0.58
2:B:317:VAL:HG11	2:B:348:ASN:O	2.03	0.57
2:B:365:VAL:O	2:B:369:THR:HG23	2.04	0.57
1:A:311:LYS:HD2	1:A:312:GLU:HG3	1.85	0.57
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.85	0.57
1:A:442:VAL:CG1	1:A:481:ALA:CB	2.81	0.57
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.04	0.57
1:A:142:ILE:H	1:A:142:ILE:CD1	2.12	0.57
1:A:473:THR:HG22	1:A:475:GLN:H	1.70	0.57
2:B:8:VAL:HG13	2:B:159:ILE:HD13	1.87	0.57
2:B:167:ILE:HG12	2:B:214:LEU:HD21	1.85	0.57
2:B:229:TRP:HA	2:B:229:TRP:CE3	2.40	0.57
1:A:342:TYR:CA	1:A:349:LEU:HD12	2.35	0.57
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.86	0.57
2:B:40:GLU:O	2:B:44:GLU:HG3	2.05	0.56
2:B:215:TYR:OH	2:B:225:PRO:HA	2.05	0.56
1:A:51:GLY:C	1:A:53:GLU:H	2.14	0.56
1:A:161:GLN:HG2	1:A:182:GLN:HE22	1.70	0.56
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.39	0.56
2:B:420:PRO:C	2:B:422:LEU:H	2.14	0.56
2:B:296:THR:O	2:B:297:GLU:C	2.49	0.56
2:B:277:ARG:HB2	2:B:277:ARG:NH1	2.19	0.56
1:A:307:ARG:HH11	1:A:307:ARG:CG	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:HB2	2:B:177:ASP:OD1	2.05	0.56
2:B:30:LYS:NZ	2:B:404:GLU:OE2	2.38	0.56
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.40	0.56
1:A:332:GLN:HE21	1:A:338:THR:CG2	2.19	0.56
1:A:390:LYS:HE2	1:A:415:GLU:OE2	2.05	0.56
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.06	0.56
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.06	0.56
1:A:28:GLU:HB3	1:A:32:LYS:NZ	2.20	0.55
1:A:90:VAL:C	1:A:91:GLN:HG2	2.31	0.55
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.87	0.55
1:A:253:THR:O	1:A:254:VAL:C	2.49	0.55
2:B:65:LYS:HB2	2:B:68:SER:HB3	1.87	0.55
1:A:113:ASP:O	1:A:114:ALA:C	2.49	0.55
2:B:178:ILE:CD1	2:B:201:LYS:HG2	2.36	0.55
2:B:85:GLN:O	2:B:85:GLN:HG3	2.07	0.55
1:A:193:LEU:O	1:A:194:GLU:C	2.48	0.55
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.42	0.55
2:B:247:PRO:HB2	2:B:249:LYS:HD3	1.88	0.55
2:B:332:GLN:CG	2:B:338:THR:HG23	2.37	0.55
1:A:172:ARG:HH12	1:A:180:ILE:HB	1.72	0.55
1:A:225:PRO:HA	1:A:226:PRO:C	2.30	0.55
1:A:90:VAL:O	1:A:91:GLN:HG2	2.06	0.54
1:A:328:GLU:O	1:A:339:TYR:HA	2.08	0.54
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.89	0.54
2:B:104:LYS:HD2	2:B:192:ASP:O	2.07	0.54
2:B:131:THR:HG22	2:B:132:ILE:N	2.22	0.54
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.42	0.54
2:B:317:VAL:CG1	2:B:349:LEU:HD23	2.37	0.54
1:A:356:ARG:HH21	1:A:358:ARG:NH1	2.05	0.54
2:B:163:SER:O	2:B:167:ILE:HG13	2.08	0.54
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.90	0.54
2:B:202:ILE:CG2	2:B:203:GLU:N	2.68	0.54
2:B:284:ARG:O	2:B:284:ARG:HG3	2.07	0.54
1:A:94:ILE:HD12	1:A:230:MET:HE3	1.88	0.54
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.42	0.54
2:B:103:LYS:CE	2:B:179:VAL:HG23	2.38	0.54
1:A:276:VAL:HG12	1:A:276:VAL:O	2.07	0.54
2:B:282:LEU:HD11	2:B:296:THR:HG23	1.90	0.54
1:A:473:THR:HG22	1:A:474:ASN:N	2.23	0.53
1:A:432:GLU:OE1	1:A:432:GLU:HA	2.08	0.53
1:A:457:TYR:CD1	1:A:457:TYR:C	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:HG3	1:A:227:PHE:HE2	1.72	0.53
2:B:150:PRO:HG2	2:B:153:TRP:HB2	1.90	0.53
2:B:362:THR:CG2	2:B:363:ASN:N	2.70	0.53
1:A:28:GLU:CG	1:A:135:ILE:HG23	2.39	0.53
1:A:279:LEU:O	1:A:280:CSD:C	2.56	0.53
1:A:177:ASP:N	1:A:177:ASP:OD2	2.42	0.53
1:A:480:GLN:O	1:A:483:TYR:HB3	2.08	0.53
2:B:31:ILE:HD13	2:B:133:PRO:O	2.08	0.53
1:A:363:ASN:HA	1:A:511:ASP:CG	2.34	0.52
2:B:171:PHE:HB2	2:B:208:HIS:ND1	2.24	0.52
2:B:344:GLU:OE1	2:B:344:GLU:HA	2.08	0.52
1:A:103:LYS:O	1:A:236:PRO:HB3	2.09	0.52
1:A:22:LYS:CE	1:A:24:TRP:HD1	2.20	0.52
2:B:229:TRP:CZ3	2:B:407:GLN:HG3	2.45	0.52
2:B:295:LEU:HB3	2:B:300:GLU:HG2	1.91	0.52
1:A:393:ILE:HG23	1:A:414:TRP:CH2	2.43	0.52
2:B:380:ILE:O	2:B:384:GLY:N	2.43	0.52
1:A:106:VAL:HG13	1:A:236:PRO:HG3	1.92	0.52
1:A:159:ILE:O	1:A:162:SER:HB3	2.10	0.52
1:A:183:TYR:CD1	1:A:184:MET:HG3	2.45	0.52
1:A:368:LEU:HD22	1:A:423:VAL:HG11	1.92	0.52
1:A:523:GLU:O	1:A:527:LYS:HG2	2.09	0.52
2:B:142:ILE:H	2:B:142:ILE:CD1	2.16	0.52
2:B:167:ILE:HD12	2:B:167:ILE:C	2.35	0.52
2:B:199:ARG:O	2:B:202:ILE:HG22	2.09	0.52
1:A:41:MET:HB2	1:A:47:ILE:HD11	1.91	0.51
2:B:230:MET:C	2:B:232:TYR:N	2.66	0.51
1:A:160:PHE:O	1:A:161:GLN:C	2.54	0.51
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.46	0.51
1:A:460:ASN:ND2	3:A:1301:PO4:O4	2.32	0.51
1:A:487:GLN:HA	1:A:524:GLN:HE21	1.74	0.51
1:A:113:ASP:HB3	1:A:117:SER:HG	1.74	0.51
1:A:255:ASN:HD22	1:A:289:LEU:HB3	1.74	0.51
1:A:432:GLU:CG	1:A:433:PRO:HD2	2.39	0.51
2:B:420:PRO:HG2	2:B:423:VAL:HG23	1.92	0.51
2:B:420:PRO:O	2:B:422:LEU:N	2.42	0.51
1:A:136:ASN:HB3	1:A:139:THR:HG22	1.92	0.51
2:B:171:PHE:HB2	2:B:208:HIS:CE1	2.45	0.51
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.38	0.51
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.26	0.51
1:A:372:VAL:CG1	1:A:411:ILE:HD12	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:NH1	1:A:218:ASP:HB3	2.12	0.50
1:A:215:TYR:CD1	1:A:216:THR:N	2.80	0.50
1:A:245:VAL:HG13	1:A:245:VAL:O	2.09	0.50
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.41	0.50
1:A:276:VAL:O	1:A:277:ARG:C	2.52	0.50
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.46	0.50
1:A:253:THR:CG2	1:A:256:ASP:H	2.25	0.50
2:B:215:TYR:CE2	2:B:225:PRO:HG3	2.46	0.50
2:B:333:GLY:O	2:B:334:GLN:HB2	2.11	0.50
1:A:115:TYR:CD1	1:A:156:SER:HB3	2.46	0.50
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.41	0.50
2:B:168:LEU:O	2:B:172:ARG:HB2	2.10	0.50
2:B:205:LEU:O	2:B:209:LEU:HG	2.12	0.50
1:A:249:LYS:HD2	1:A:251:SER:O	2.11	0.50
1:A:480:GLN:CG	1:A:517:LEU:HD11	2.34	0.50
2:B:167:ILE:HG21	2:B:214:LEU:CD1	2.21	0.50
2:B:378:GLU:O	2:B:379:SER:C	2.55	0.50
1:A:28:GLU:HB3	1:A:32:LYS:HZ2	1.77	0.49
1:A:136:ASN:HB3	1:A:139:THR:CG2	2.42	0.49
1:A:198:HIS:O	1:A:202:ILE:HG12	2.12	0.49
2:B:201:LYS:NZ	2:B:204:GLU:OE2	2.38	0.49
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.47	0.49
1:A:54:ASN:HB3	1:A:143:ARG:NH1	2.27	0.49
2:B:131:THR:CG2	2:B:132:ILE:N	2.75	0.49
1:A:115:TYR:N	1:A:115:TYR:HD2	2.11	0.49
2:B:334:GLN:HB3	2:B:336:GLN:OE1	2.12	0.49
1:A:108:VAL:HG13	1:A:108:VAL:O	2.11	0.49
2:B:278:GLN:HB2	2:B:302:GLU:CD	2.38	0.49
1:A:324:ASP:O	1:A:343:GLN:HG2	2.13	0.49
2:B:326:ILE:CG2	2:B:327:ALA:N	2.76	0.49
1:A:148:VAL:O	1:A:150:PRO:CD	2.61	0.49
1:A:233:GLU:O	1:A:234:LEU:HD23	2.13	0.49
1:A:274:ILE:O	1:A:353:LYS:NZ	2.45	0.49
1:A:57:ASN:HA	1:A:129:ALA:O	2.13	0.49
1:A:89:GLU:CD	1:A:92:LEU:HA	2.38	0.49
1:A:433:PRO:HA	1:A:532:TYR:CG	2.47	0.49
2:B:139:THR:CB	2:B:140:PRO:HD2	2.40	0.49
1:A:281:LYS:O	1:A:284:ARG:HG3	2.13	0.49
2:B:195:ILE:HG23	2:B:196:GLY:N	2.26	0.49
1:A:326:ILE:O	1:A:341:ILE:HA	2.13	0.48
1:A:344:GLU:HG3	1:A:345:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:LEU:HD11	2:B:377:THR:HG21	1.94	0.48
1:A:24:TRP:O	1:A:25:PRO:O	2.31	0.48
1:A:270:ILE:HG23	1:A:271:TYR:N	2.27	0.48
2:B:51:GLY:C	2:B:53:GLU:OE1	2.56	0.48
2:B:206:ARG:HB3	2:B:224:GLU:CG	2.43	0.48
1:A:399:GLU:HG2	1:A:402:TRP:CZ3	2.48	0.48
2:B:86:ASP:HA	2:B:154:LYS:HZ1	1.78	0.48
1:A:320:ASP:OD1	1:A:323:LYS:HG3	2.13	0.48
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.94	0.48
1:A:356:ARG:NE	1:A:358:ARG:HG2	2.29	0.48
1:A:474:ASN:O	1:A:478:GLU:HG3	2.14	0.48
1:A:47:ILE:HG22	1:A:146:TYR:HA	1.95	0.48
2:B:372:VAL:HG13	2:B:389:PHE:CZ	2.49	0.48
2:B:120:LEU:O	2:B:121:ASP:C	2.57	0.47
2:B:339:TYR:C	2:B:339:TYR:CD2	2.91	0.47
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.49	0.47
1:A:198:HIS:O	1:A:199:ARG:C	2.57	0.47
1:A:265:ASN:O	1:A:266:TRP:C	2.56	0.47
1:A:476:LYS:HG3	1:A:517:LEU:HD12	1.96	0.47
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.50	0.47
1:A:24:TRP:HZ3	1:A:61:PHE:CD2	2.32	0.47
1:A:118:VAL:HB	1:A:149:LEU:HG	1.97	0.47
1:A:149:LEU:HD11	1:A:159:ILE:HG22	1.96	0.47
1:A:346:PHE:N	1:A:346:PHE:CD1	2.80	0.47
2:B:106:VAL:HA	2:B:189:VAL:O	2.14	0.47
1:A:167:ILE:O	1:A:170:PRO:HD2	2.15	0.47
2:B:282:LEU:CD1	2:B:296:THR:HG23	2.45	0.47
1:A:171:PHE:C	1:A:171:PHE:CD2	2.93	0.47
1:A:426:TRP:H	1:A:426:TRP:CD1	2.33	0.47
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.96	0.47
2:B:160:PHE:O	2:B:161:GLN:C	2.57	0.47
2:B:227:PHE:CB	2:B:231:GLY:HA2	2.42	0.47
1:A:60:VAL:HG12	1:A:61:PHE:N	2.30	0.47
1:A:354:TYR:CE1	1:A:356:ARG:HB3	2.49	0.47
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.11	0.47
2:B:281:LYS:C	2:B:283:LEU:N	2.72	0.47
1:A:507:GLN:O	1:A:509:GLN:HG3	2.15	0.47
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.30	0.47
1:A:370:GLU:O	1:A:371:ALA:C	2.57	0.47
1:A:522:ILE:O	1:A:526:ILE:HG13	2.14	0.47
2:B:350:LYS:NZ	2:B:378:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:HG23	1:A:30:LYS:HG2	1.96	0.46
2:B:207:GLN:HG2	2:B:224:GLU:OE2	2.15	0.46
1:A:210:LEU:HD23	1:A:210:LEU:C	2.41	0.46
2:B:21:VAL:HG12	2:B:22:LYS:N	2.29	0.46
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.51	0.46
1:A:100:LEU:HD23	2:B:138:GLU:OE2	2.15	0.46
1:A:24:TRP:CH2	1:A:59:PRO:HB2	2.50	0.46
2:B:27:THR:O	2:B:28:GLU:C	2.58	0.46
2:B:242:GLN:HE21	2:B:353:LYS:HG2	1.80	0.46
2:B:330:GLN:OE1	2:B:338:THR:OG1	2.24	0.46
2:B:264:LEU:O	2:B:265:ASN:C	2.58	0.46
1:A:113:ASP:O	1:A:114:ALA:O	2.33	0.46
1:A:208:HIS:CD2	1:A:208:HIS:C	2.94	0.46
1:A:319:TYR:CE1	1:A:321:PRO:HG3	2.51	0.46
1:A:332:GLN:HE21	1:A:338:THR:HG21	1.80	0.46
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.50	0.46
2:B:87:PHE:O	2:B:88:TRP:C	2.59	0.46
2:B:200:THR:C	2:B:202:ILE:N	2.73	0.46
2:B:297:GLU:O	2:B:301:LEU:HG	2.16	0.46
1:A:178:ILE:CG2	1:A:179:VAL:N	2.77	0.46
1:A:317:VAL:HG22	1:A:318:TYR:H	1.80	0.46
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.16	0.46
2:B:378:GLU:O	2:B:381:VAL:N	2.49	0.46
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.96	0.46
1:A:503:LEU:O	1:A:507:GLN:HB2	2.16	0.46
1:A:325:LEU:HB3	1:A:387:PRO:HB3	1.98	0.46
2:B:57:ASN:HA	2:B:129:ALA:O	2.16	0.46
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.98	0.45
1:A:461:ARG:NH1	3:A:1300:PO4:O2	2.42	0.45
1:A:377:THR:O	1:A:381:VAL:HG23	2.16	0.45
1:A:503:LEU:HD12	1:A:533:LEU:HD23	1.98	0.45
2:B:225:PRO:HA	2:B:226:PRO:HD2	1.78	0.45
2:B:228:LEU:HD23	2:B:228:LEU:HA	1.79	0.45
2:B:229:TRP:HA	2:B:229:TRP:HE3	1.82	0.45
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.51	0.45
1:A:303:LEU:HD23	1:A:303:LEU:O	2.16	0.45
2:B:329:ILE:HG22	2:B:330:GLN:N	2.31	0.45
1:A:206:ARG:NH2	1:A:216:THR:O	2.48	0.45
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.98	0.45
2:B:52:PRO:C	2:B:54:ASN:N	2.75	0.45
2:B:67:ASP:HB2	2:B:230:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:ARG:O	2:B:82:LYS:HG3	2.17	0.45
2:B:228:LEU:O	2:B:229:TRP:HB2	2.17	0.45
1:A:157:PRO:HB2	1:A:158:ALA:H	1.54	0.45
1:A:369:THR:O	1:A:372:VAL:HB	2.17	0.45
2:B:214:LEU:C	2:B:216:THR:H	2.21	0.45
2:B:253:THR:O	2:B:254:VAL:C	2.59	0.45
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.98	0.45
1:A:126:LYS:HE3	1:A:127:TYR:CE2	2.51	0.45
1:A:491:LEU:HD13	1:A:529:GLU:HG2	1.97	0.45
2:B:178:ILE:HG23	2:B:190:GLY:O	2.17	0.45
1:A:24:TRP:O	1:A:25:PRO:C	2.58	0.45
2:B:84:THR:O	2:B:85:GLN:C	2.59	0.45
2:B:198:HIS:C	2:B:200:THR:N	2.75	0.45
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.80	0.45
2:B:374:LYS:O	2:B:378:GLU:HG3	2.16	0.45
1:A:181:TYR:OH	1:A:183:TYR:HD2	2.00	0.45
1:A:239:TRP:CD1	1:A:316:GLY:C	2.95	0.45
1:A:428:GLN:HG3	1:A:428:GLN:O	2.17	0.45
1:A:340:GLN:HA	1:A:351:THR:HA	1.98	0.45
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.31	0.45
1:A:215:TYR:CD1	1:A:215:TYR:C	2.95	0.45
1:A:344:GLU:CB	1:A:347:LYS:HE3	2.45	0.45
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.52	0.45
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.99	0.44
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	2.52	0.44
2:B:342:TYR:CD1	2:B:342:TYR:C	2.95	0.44
1:A:94:ILE:HD13	1:A:230:MET:HE3	1.98	0.44
1:A:166:LYS:O	1:A:169:GLU:HB3	2.17	0.44
1:A:270:ILE:HG13	1:A:314:VAL:CG1	2.48	0.44
2:B:170:PRO:O	2:B:174:GLN:HG2	2.17	0.44
1:A:199:ARG:O	1:A:202:ILE:HB	2.18	0.44
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.99	0.44
1:A:332:GLN:HG2	1:A:338:THR:HG23	1.99	0.44
2:B:342:TYR:CB	2:B:348:ASN:HA	2.45	0.44
1:A:76:ASP:CG	1:A:78:ARG:HE	2.26	0.44
1:A:381:VAL:O	1:A:381:VAL:HG12	2.17	0.44
2:B:362:THR:CG2	2:B:363:ASN:H	2.29	0.44
1:A:27:THR:HG23	1:A:30:LYS:HG3	2.00	0.44
1:A:300:GLU:OE2	1:A:300:GLU:HA	2.17	0.44
1:A:342:TYR:CD1	1:A:342:TYR:C	2.96	0.44
2:B:118:VAL:HA	2:B:119:PRO:HD3	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:HIS:O	2:B:212:TRP:HB2	2.18	0.44
1:A:183:TYR:O	1:A:184:MET:HB2	2.17	0.44
2:B:293:ILE:HG23	2:B:294:PRO:HD2	2.00	0.44
1:A:92:LEU:CD1	1:A:93:GLY:H	2.28	0.43
1:A:80:LEU:O	1:A:83:ARG:N	2.45	0.43
1:A:402:TRP:CG	1:A:403:THR:N	2.85	0.43
2:B:86:ASP:HA	2:B:154:LYS:NZ	2.33	0.43
1:A:8:VAL:HG12	2:B:53:GLU:HB3	2.00	0.43
1:A:28:GLU:HG3	1:A:135:ILE:CG1	2.45	0.43
1:A:77:PHE:CE1	1:A:150:PRO:HB2	2.54	0.43
1:A:122:GLU:HG3	1:A:125:ARG:NH1	2.33	0.43
1:A:196:GLY:O	1:A:197:GLN:C	2.62	0.43
2:B:64:LYS:HG2	2:B:65:LYS:N	2.33	0.43
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.35	0.43
1:A:465:LYS:HD2	1:A:484:LEU:HD22	2.00	0.43
2:B:121:ASP:C	2:B:121:ASP:OD1	2.61	0.43
2:B:210:LEU:CG	2:B:223:LYS:O	2.66	0.43
1:A:253:THR:HG23	1:A:256:ASP:H	1.84	0.43
2:B:72:ARG:CZ	2:B:409:THR:HG22	2.48	0.43
1:A:307:ARG:CG	1:A:307:ARG:NH1	2.76	0.43
1:A:434:ILE:H	1:A:434:ILE:HG13	1.61	0.43
1:A:439:THR:HG21	2:B:289:LEU:HD13	2.01	0.43
2:B:173:LYS:O	2:B:176:PRO:HD3	2.18	0.43
1:A:118:VAL:HG13	1:A:119:PRO:HD2	2.00	0.43
1:A:168:LEU:O	1:A:169:GLU:C	2.61	0.43
1:A:180:ILE:HG22	1:A:181:TYR:N	2.34	0.43
1:A:219:LYS:NZ	1:A:224:GLU:OE2	2.52	0.43
1:A:89:GLU:OE1	1:A:92:LEU:HB3	2.19	0.43
1:A:92:LEU:N	1:A:92:LEU:CD1	2.62	0.43
1:A:435:VAL:HG22	2:B:290:THR:HG21	2.00	0.43
2:B:281:LYS:C	2:B:283:LEU:H	2.26	0.43
1:A:209:LEU:C	1:A:211:ARG:N	2.76	0.43
1:A:247:PRO:O	1:A:307:ARG:NH2	2.39	0.43
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.54	0.43
2:B:242:GLN:NE2	2:B:352:GLY:HA2	2.34	0.43
2:B:305:GLU:O	2:B:309:ILE:HG13	2.18	0.43
2:B:281:LYS:O	2:B:283:LEU:N	2.51	0.42
1:A:371:ALA:O	1:A:372:VAL:C	2.62	0.42
1:A:393:ILE:CB	1:A:423:VAL:HG13	2.49	0.42
2:B:150:PRO:HG2	2:B:153:TRP:CB	2.49	0.42
2:B:266:TRP:O	2:B:269:GLN:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:HA	1:A:55:PRO:HD2	1.89	0.42
1:A:242:GLN:HG3	1:A:243:PRO:HD2	2.02	0.42
2:B:365:VAL:O	2:B:366:LYS:C	2.61	0.42
1:A:17:ASP:CG	1:A:18:GLY:N	2.78	0.42
2:B:21:VAL:CG1	2:B:22:LYS:N	2.82	0.42
2:B:46:LYS:HE2	2:B:116:PHE:HB3	2.01	0.42
2:B:207:GLN:O	2:B:208:HIS:C	2.63	0.42
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.01	0.42
1:A:54:ASN:HB3	1:A:143:ARG:HH12	1.82	0.42
1:A:102:LYS:HG3	1:A:237:ASP:HA	2.01	0.42
1:A:170:PRO:O	1:A:171:PHE:C	2.63	0.42
1:A:516:GLU:O	1:A:517:LEU:C	2.63	0.42
2:B:24:TRP:HA	2:B:25:PRO:HD3	1.91	0.42
2:B:422:LEU:O	2:B:425:LEU:HG	2.19	0.42
1:A:108:VAL:HG23	1:A:188:TYR:CE1	2.55	0.42
1:A:311:LYS:HB3	1:A:311:LYS:HE3	1.81	0.42
2:B:262:GLY:O	2:B:263:LYS:C	2.62	0.42
1:A:169:GLU:OE1	1:A:169:GLU:HA	2.20	0.42
1:A:393:ILE:HG23	1:A:414:TRP:CZ3	2.55	0.42
2:B:242:GLN:HG2	2:B:353:LYS:HZ1	1.85	0.42
2:B:316:GLY:HA2	2:B:318:TYR:CE2	2.55	0.42
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.55	0.42
1:A:194:GLU:O	1:A:194:GLU:HG3	2.18	0.42
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.20	0.42
2:B:327:ALA:HA	2:B:340:GLN:O	2.19	0.42
1:A:28:GLU:HG3	1:A:135:ILE:HG23	1.99	0.42
1:A:195:ILE:O	1:A:198:HIS:CB	2.66	0.42
1:A:266:TRP:HA	1:A:266:TRP:CE3	2.55	0.42
1:A:287:LYS:N	1:A:291:GLU:OE2	2.43	0.42
1:A:170:PRO:CG	1:A:171:PHE:H	2.31	0.41
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.50	0.41
2:B:43:LYS:HB2	2:B:43:LYS:HE3	1.86	0.41
2:B:254:VAL:O	2:B:258:GLN:HG3	2.20	0.41
1:A:103:LYS:O	1:A:236:PRO:CB	2.68	0.41
1:A:303:LEU:C	1:A:303:LEU:CD2	2.92	0.41
1:A:402:TRP:O	1:A:403:THR:C	2.62	0.41
1:A:53:GLU:O	1:A:55:PRO:HD3	2.20	0.41
1:A:232:TYR:HB3	1:A:240:THR:O	2.20	0.41
2:B:77:PHE:O	2:B:78:ARG:C	2.61	0.41
2:B:185:ASP:OD2	2:B:185:ASP:N	2.51	0.41
2:B:327:ALA:O	2:B:389:PHE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:O	1:A:94:ILE:HG13	2.18	0.41
1:A:194:GLU:O	1:A:195:ILE:C	2.63	0.41
1:A:211:ARG:HE	1:A:211:ARG:HB2	1.71	0.41
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.55	0.41
2:B:254:VAL:HG23	2:B:291:GLU:O	2.20	0.41
2:B:306:ASN:HA	2:B:309:ILE:HD12	2.02	0.41
1:A:136:ASN:CB	1:A:139:THR:HG22	2.50	0.41
2:B:57:ASN:HD21	2:B:131:THR:N	2.19	0.41
2:B:87:PHE:CE1	2:B:154:LYS:HE2	2.55	0.41
1:A:108:VAL:O	1:A:109:LEU:HD12	2.20	0.41
1:A:194:GLU:HG2	1:A:197:GLN:NE2	2.14	0.41
1:A:233:GLU:HB3	1:A:240:THR:HG22	2.02	0.41
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.81	0.41
2:B:260:LEU:O	2:B:264:LEU:HG	2.21	0.41
2:B:350:LYS:C	2:B:351:THR:HG23	2.46	0.41
1:A:17:ASP:O	1:A:83:ARG:NH1	2.52	0.41
1:A:171:PHE:CE2	1:A:175:ASN:ND2	2.89	0.41
1:A:426:TRP:CD1	1:A:426:TRP:N	2.87	0.41
1:A:38:CYS:O	1:A:47:ILE:HD11	2.21	0.41
1:A:356:ARG:HG2	1:A:358:ARG:HG3	2.03	0.41
1:A:373:GLN:O	1:A:374:LYS:C	2.63	0.41
1:A:488:ASP:OD2	1:A:488:ASP:N	2.49	0.41
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.85	0.41
2:B:84:THR:O	2:B:154:LYS:NZ	2.52	0.41
2:B:170:PRO:C	2:B:174:GLN:HG2	2.45	0.41
2:B:401:TRP:O	2:B:404:GLU:HB2	2.20	0.41
1:A:153:TRP:CZ3	1:A:155:GLY:HA3	2.56	0.41
1:A:206:ARG:NH1	1:A:218:ASP:CA	2.82	0.41
1:A:221:HIS:CD2	1:A:221:HIS:N	2.89	0.41
1:A:362:THR:HG22	1:A:366:LYS:CD	2.31	0.41
1:A:497:THR:O	1:A:535:TRP:HA	2.21	0.41
2:B:195:ILE:CG2	2:B:196:GLY:N	2.84	0.41
2:B:230:MET:O	2:B:232:TYR:N	2.54	0.41
1:A:169:GLU:OE1	1:A:169:GLU:CA	2.69	0.40
1:A:368:LEU:O	1:A:372:VAL:HG23	2.21	0.40
1:A:495:ILE:HB	1:A:533:LEU:HD12	2.02	0.40
1:A:511:ASP:OD1	1:A:511:ASP:C	2.64	0.40
1:A:525:LEU:HD23	1:A:525:LEU:HA	1.91	0.40
2:B:198:HIS:O	2:B:200:THR:N	2.54	0.40
2:B:364:ASP:O	2:B:367:GLN:HB2	2.21	0.40
2:B:169:GLU:N	2:B:170:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:TYR:CD1	1:A:183:TYR:O	2.74	0.40
2:B:230:MET:CE	2:B:230:MET:HA	2.51	0.40
2:B:257:ILE:O	2:B:260:LEU:HB3	2.22	0.40
2:B:372:VAL:HA	2:B:389:PHE:CE2	2.56	0.40
1:A:12:LEU:O	1:A:13:LYS:C	2.63	0.40
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.56	0.40
1:A:473:THR:CG2	1:A:474:ASN:N	2.84	0.40
2:B:42:GLU:O	2:B:43:LYS:C	2.63	0.40
2:B:194:GLU:O	2:B:195:ILE:C	2.65	0.40
1:A:121:ASP:O	1:A:122:GLU:C	2.64	0.40
1:A:343:GLN:HG3	1:A:349:LEU:CD1	2.32	0.40
2:B:203:GLU:O	2:B:206:ARG:HB2	2.21	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	512/560 (91%)	447 (87%)	44 (9%)	21 (4%)	2	13
2	B	398/440 (90%)	334 (84%)	54 (14%)	10 (2%)	4	23
All	All	910/1000 (91%)	781 (86%)	98 (11%)	31 (3%)	3	17

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	114	ALA
1	A	157	PRO
1	A	195	ILE
1	A	219	LYS
1	A	402	TRP

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Mol	Chain	Res	Type
2	B	193	LEU
1	A	25	PRO
1	A	268	SER
2	B	85	GLN
2	B	213	GLY
1	A	156	SER
1	A	198	HIS
1	A	345	PRO
1	A	412	PRO
2	B	162	SER
2	B	232	TYR
2	B	282	LEU
2	B	421	PRO
1	A	92	LEU
1	A	117	SER
1	A	121	ASP
1	A	162	SER
2	B	170	PRO
1	A	254	VAL
2	B	225	PRO
1	A	170	PRO
1	A	169	GLU
1	A	52	PRO
1	A	247	PRO
2	B	176	PRO

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	467/499 (94%)	425 (91%)	42 (9%)	9	34
2	B	371/400 (93%)	338 (91%)	33 (9%)	9	34
All	All	838/899 (93%)	763 (91%)	75 (9%)	9	34

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	PRO
1	A	26	LEU
1	A	27	THR
1	A	28	GLU
1	A	44	GLU
1	A	58	THR
1	A	92	LEU
1	A	94	ILE
1	A	97	PRO
1	A	104	LYS
1	A	106	VAL
1	A	122	GLU
1	A	142	ILE
1	A	148	VAL
1	A	161	GLN
1	A	165	THR
1	A	168	LEU
1	A	184	MET
1	A	189	VAL
1	A	194	GLU
1	A	212	TRP
1	A	216	THR
1	A	218	ASP
1	A	250	ASP
1	A	305	GLU
1	A	307	ARG
1	A	314	VAL
1	A	340	GLN
1	A	344	GLU
1	A	345	PRO
1	A	362	THR
1	A	373	GLN
1	A	405	TYR
1	A	423	VAL
1	A	432	GLU
1	A	434	ILE
1	A	459	THR
1	A	465	LYS
1	A	488	ASP
1	A	495	ILE
1	A	500	GLN
1	A	517	LEU
2	B	8	VAL

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Mol	Chain	Res	Type
2	B	11	LYS
2	B	28	GLU
2	B	31	ILE
2	B	48	SER
2	B	55	PRO
2	B	66	LYS
2	B	73	LYS
2	B	88	TRP
2	B	134	SER
2	B	172	ARG
2	B	185	ASP
2	B	201	LYS
2	B	202	ILE
2	B	210	LEU
2	B	230	MET
2	B	242	GLN
2	B	277	ARG
2	B	280	CYS
2	B	283	LEU
2	B	286	THR
2	B	289	LEU
2	B	298	GLU
2	B	314	VAL
2	B	323	LYS
2	B	334	GLN
2	B	336	GLN
2	B	344	GLU
2	B	368	LEU
2	B	379	SER
2	B	394	GLN
2	B	418	ASN
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	136	ASN
1	A	161	GLN
1	A	182	GLN
1	A	197	GLN
1	A	208	HIS

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Mol	Chain	Res	Type
1	A	221	HIS
1	A	222	GLN
1	A	255	ASN
1	A	258	GLN
1	A	332	GLN
1	A	373	GLN
1	A	475	GLN
1	A	480	GLN
1	A	487	GLN
1	A	509	GLN
1	A	512	GLN
1	A	520	GLN
2	B	57	ASN
2	B	147	ASN
2	B	151	GLN
2	B	235	HIS
2	B	242	GLN
2	B	278	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSD	A	280	1	4,7,8	1.56	1 (25%)	1,8,10	7.96	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	2.66	1.50	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	7.96	120.26	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
4	U05	A	999	-	22,24,24	1.97	6 (27%)	26,35,35	1.79	7 (26%)
3	PO4	A	1301	-	4,4,4	1.72	1 (25%)	6,6,6	0.50	0
3	PO4	A	1300	-	4,4,4	1.73	1 (25%)	6,6,6	0.45	0

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
4	U05	A	999	-	-	2/4/6/6	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	U05	C12-N6	5.00	1.54	1.46
4	A	999	U05	C14-N11	3.67	1.57	1.47
4	A	999	U05	C4A-C5	3.18	1.54	1.50
4	A	999	U05	C8-C7	2.22	1.42	1.38
4	A	999	U05	C7-C6A	2.15	1.43	1.39
3	A	1300	PO4	P-O2	-2.14	1.48	1.54
3	A	1301	PO4	P-O4	-2.08	1.48	1.54
4	A	999	U05	C3-C4	2.07	1.42	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	U05	N1-C1A-N11	4.82	121.03	114.94
4	A	999	U05	C4A-C1A-N11	-3.11	117.21	120.93
4	A	999	U05	C6A-C11-N11	-3.10	118.20	121.47
4	A	999	U05	C12-N6-C6A	-3.01	113.66	118.38
4	A	999	U05	C15-C14-N11	2.65	122.38	112.40
4	A	999	U05	O13-C5-C4A	-2.17	116.32	119.94
4	A	999	U05	C2-N1-C1A	2.09	119.78	115.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

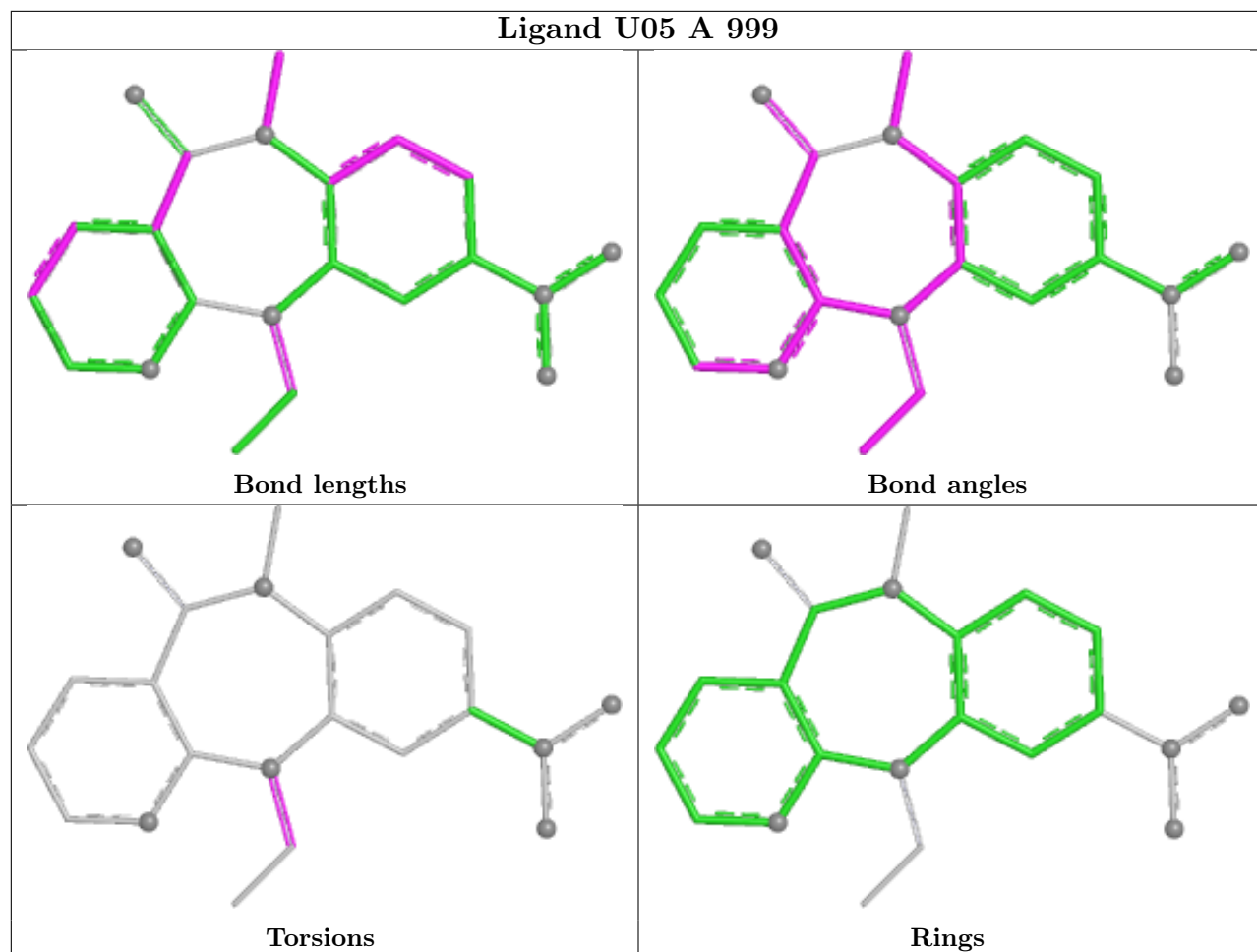
Mol	Chain	Res	Type	Atoms
4	A	999	U05	C15-C14-N11-C1A
4	A	999	U05	C15-C14-N11-C11

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	U05	1	0
3	A	1301	PO4	1	0
3	A	1300	PO4	1	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 than 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.



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	518/560 (92%)	-0.57	0 100 100	18, 58, 109, 145	0
2	B	406/440 (92%)	-0.60	2 (0%) 87 72	18, 55, 107, 141	0
All	All	924/1000 (92%)	-0.58	2 (0%) 91 83	18, 57, 108, 145	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	LEU	2.5
2	B	419	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	A	280	8/9	0.96	0.07	30,37,83,85	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

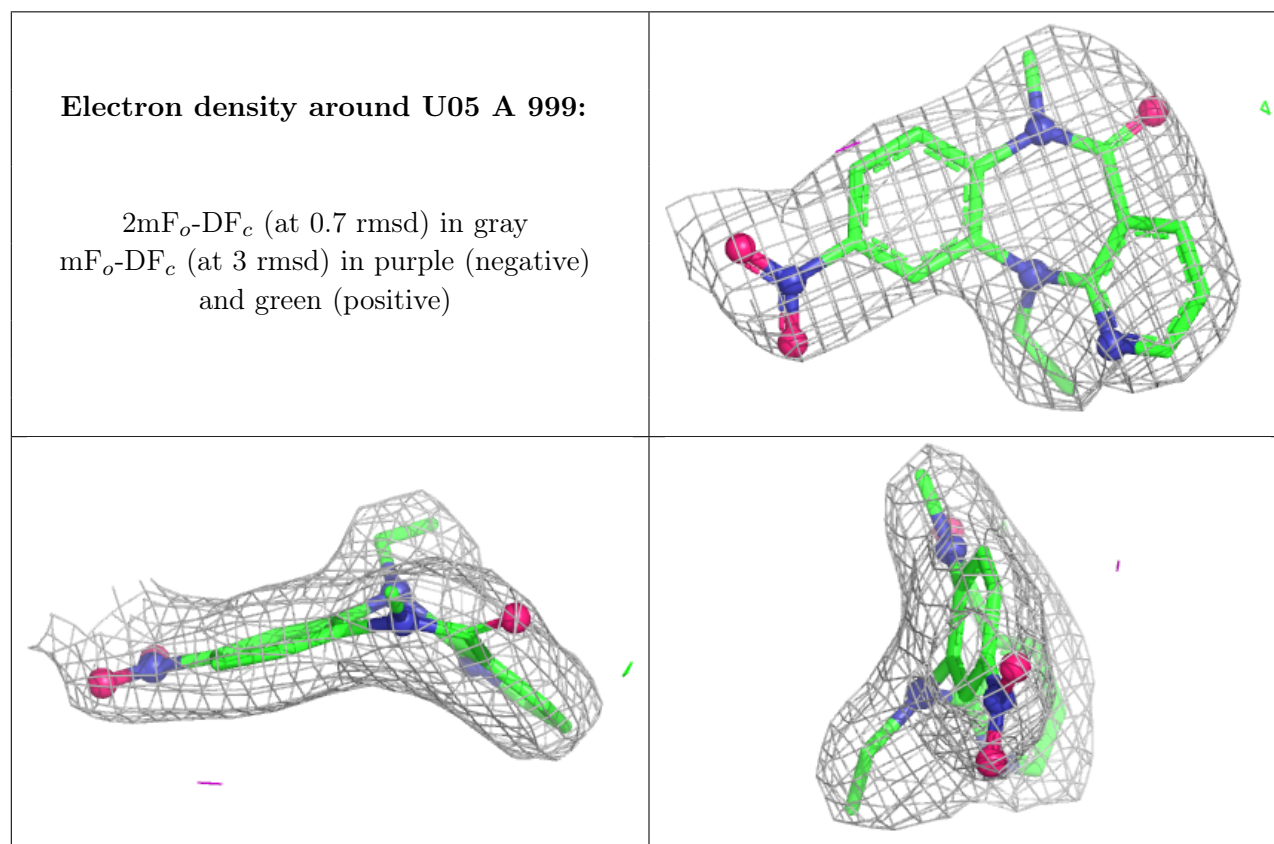
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	A	1300	5/5	0.52	0.10	125,126,133,133	0
3	PO4	A	1301	5/5	0.85	0.11	120,120,124,125	0
4	U05	A	999	22/22	0.97	0.06	21,48,69,75	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.