



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:21 PM UTC

PDB ID : 3I0R / pdb_00003i0r
Title : crystal structure of HIV reverse transcriptase in complex with inhibitor 3
Authors : Yan, Y.; Prasad, S.
Deposited on : 2009-06-25
Resolution : 2.98 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

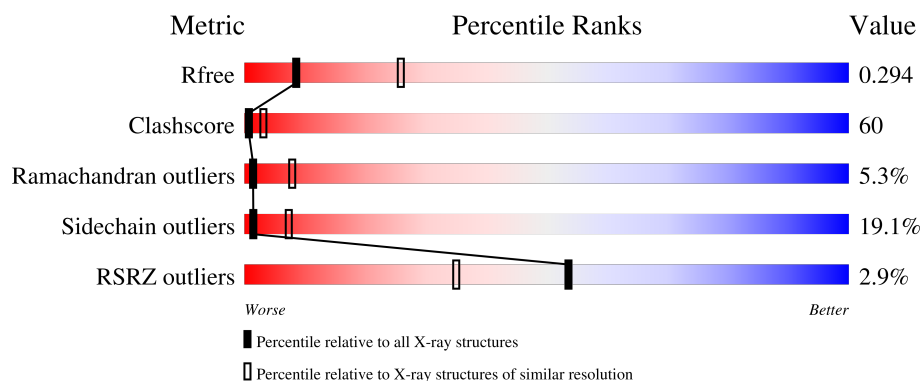
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	563	2% 31%48%16% . .
2	B	443	4% 34%41%15% . 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	RT3	A	601	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7823 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4442	2874	741	819	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP P04585
A	-1	ASN	-	expression tag	UNP P04585
A	0	SER	-	expression tag	UNP P04585

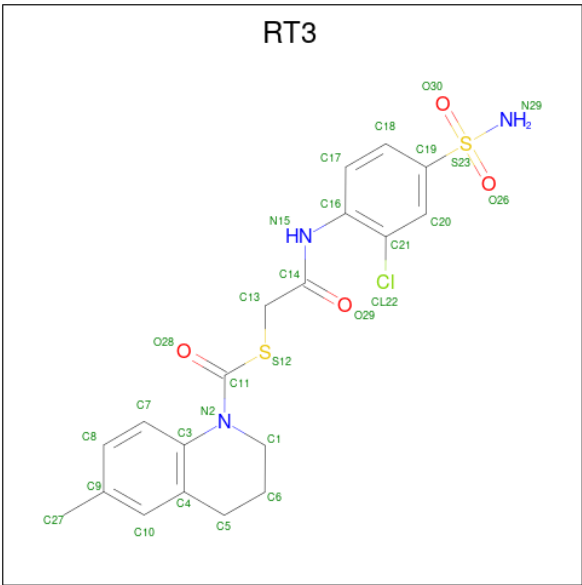
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3352	2182	555	609	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP P04585
B	-1	ASN	-	expression tag	UNP P04585
B	0	SER	-	expression tag	UNP P04585

- Molecule 3 is S-{2-[(2-chloro-4-sulfamoylphenyl)amino]-2-oxoethyl} 6-methyl-3,4-dihydroquinoline-1(2H)-carbothioate (CCD ID: RT3) (formula: C₁₉H₂₀ClN₃O₄S₂).

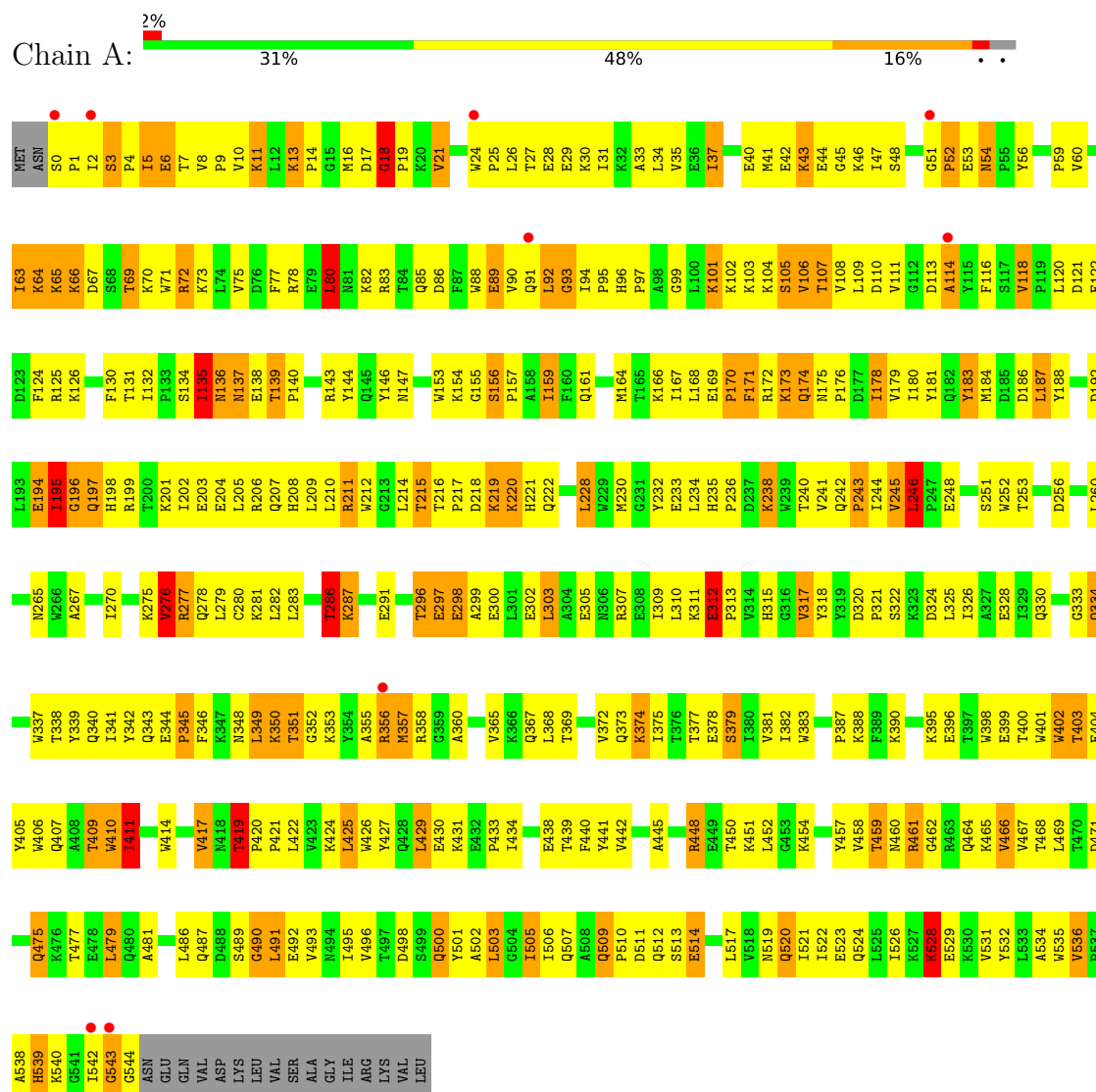


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	Cl	N	O	S	0	0
			29	19	1	3	4	2		

3 Residue-property plots

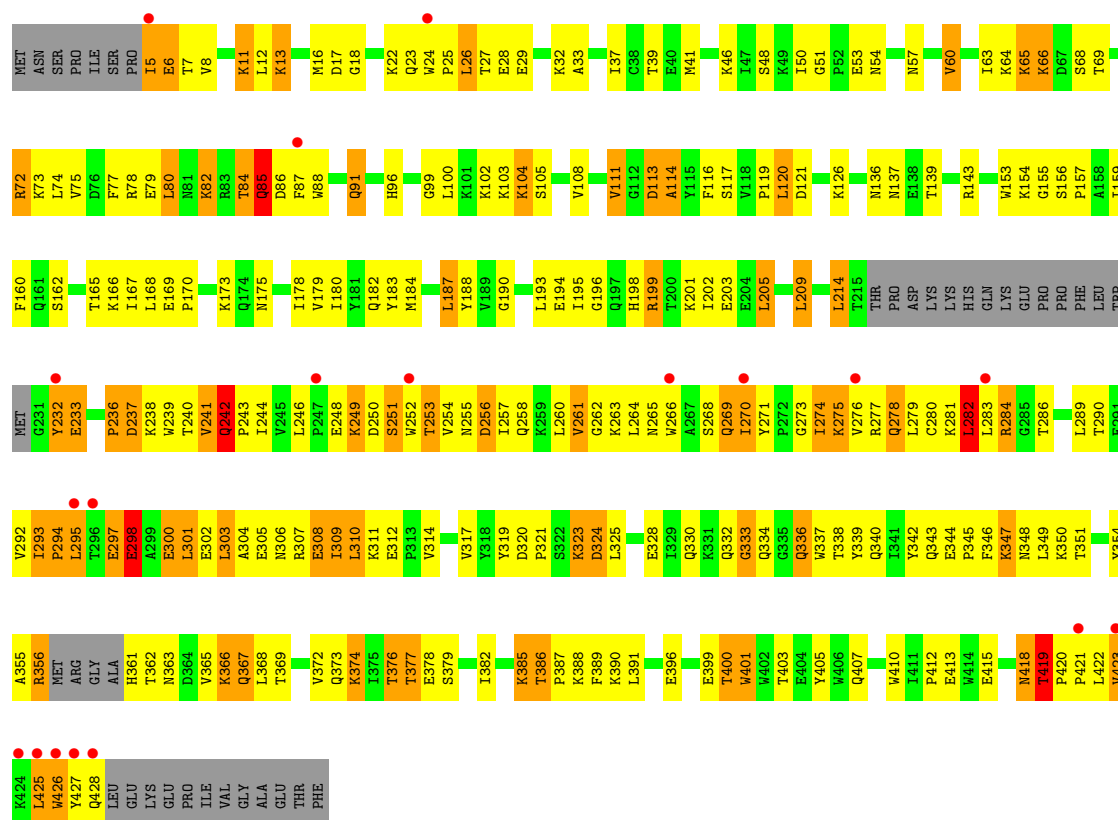
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: p51 RT





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.33Å 155.31Å 154.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.98 50.00 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.98) 99.3 (50.00-2.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.220 , 0.295 0.222 , 0.294	Depositor DCC
R_{free} test set	1494 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	76.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7823	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RT3

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	0.76	0/4559	1.12	24/6196 (0.4%)
2	B	0.77	0/3446	1.04	15/4682 (0.3%)
All	All	0.76	0/8005	1.08	39/10878 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	GLU	CA-C-N	10.62	130.58	119.85
1	A	312	GLU	C-N-CA	10.62	130.58	119.85
1	A	118	VAL	CA-C-N	8.28	128.78	119.92
1	A	118	VAL	C-N-CA	8.28	128.78	119.92
1	A	382	ILE	N-CA-C	7.66	117.77	110.42
1	A	419	THR	CA-C-N	6.83	124.65	119.66
1	A	419	THR	C-N-CA	6.83	124.65	119.66
1	A	18	GLY	CA-C-N	-6.81	113.24	120.66
1	A	18	GLY	C-N-CA	-6.81	113.24	120.66
1	A	118	VAL	N-CA-C	6.35	115.17	107.61
2	B	309	ILE	CB-CA-C	-6.32	103.76	112.04
2	B	401	TRP	N-CA-C	6.05	120.73	113.23
1	A	156	SER	CA-C-N	5.98	125.69	119.05
1	A	156	SER	C-N-CA	5.98	125.69	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	THR	N-CA-C	5.90	119.44	109.76
1	A	529	GLU	N-CA-C	-5.90	107.89	114.62
1	A	350	LYS	N-CA-C	5.81	116.98	108.14
1	A	411	ILE	N-CA-C	5.73	113.56	108.63
2	B	298	GLU	N-CA-C	-5.68	105.12	112.68
1	A	52	PRO	N-CA-C	-5.67	107.43	114.68
2	B	418	ASN	N-CA-C	5.60	117.06	109.11
2	B	96	HIS	CA-C-N	5.56	126.79	119.84
2	B	96	HIS	C-N-CA	5.56	126.79	119.84
1	A	183	TYR	N-CA-C	5.46	117.52	108.13
1	A	93	GLY	N-CA-C	-5.43	101.55	110.56
1	A	80	LEU	N-CA-C	-5.41	105.04	111.69
2	B	13	LYS	CA-C-N	5.36	126.54	119.84
2	B	13	LYS	C-N-CA	5.36	126.54	119.84
1	A	13	LYS	CA-C-N	5.24	126.39	119.84
1	A	13	LYS	C-N-CA	5.24	126.39	119.84
1	A	381	VAL	CB-CA-C	-5.24	104.99	111.70
2	B	139	THR	CA-C-N	-5.15	114.48	119.78
2	B	139	THR	C-N-CA	-5.15	114.48	119.78
2	B	376	THR	N-CA-C	-5.10	105.73	111.28
2	B	57	ASN	N-CA-C	5.06	116.75	108.55
2	B	293	ILE	CA-C-N	5.05	126.15	119.84
2	B	293	ILE	C-N-CA	5.05	126.15	119.84
2	B	282	LEU	N-CA-C	-5.04	105.92	111.71
1	A	505	ILE	CB-CA-C	-5.03	105.45	112.04

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	539	HIS	Peptide

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	4442	0	4489	573	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3352	0	3380	398	0
3	A	29	0	20	17	0
All	All	7823	0	7889	937	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 60.

All (937) 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:244:ILE:CD1	2:B:266:TRP:CZ3	2.03	1.41
2:B:244:ILE:CD1	2:B:266:TRP:CH2	2.21	1.23
1:A:1:PRO:O	1:A:2:ILE:HD13	1.36	1.21
1:A:206:ARG:NH2	1:A:218:ASP:HB3	1.57	1.19
1:A:220:LYS:HD3	1:A:220:LYS:C	1.67	1.18
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	1.69	1.18
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.21	1.17
2:B:244:ILE:CD1	2:B:266:TRP:HZ3	1.47	1.17
1:A:355:ALA:O	1:A:356:ARG:O	1.62	1.15
1:A:195:ILE:HD13	1:A:199:ARG:NH2	1.63	1.14
1:A:220:LYS:HE2	1:A:221:HIS:CE1	1.84	1.13
1:A:194:GLU:CD	1:A:194:GLU:H	1.53	1.11
2:B:344:GLU:HB3	2:B:347:LYS:HE2	1.28	1.11
1:A:406:TRP:HZ2	2:B:418:ASN:OD1	1.34	1.10
2:B:241:VAL:CG2	2:B:243:PRO:HD3	1.80	1.10
2:B:66:LYS:HG3	2:B:407:GLN:HE22	1.10	1.09
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.22	1.09
2:B:244:ILE:HD12	2:B:266:TRP:HZ3	1.15	1.09
2:B:298:GLU:CD	2:B:298:GLU:H	1.53	1.09
2:B:283:LEU:O	2:B:284:ARG:HG3	1.53	1.08
1:A:220:LYS:CE	1:A:221:HIS:CD2	2.37	1.08
1:A:107:THR:HG21	1:A:202:ILE:CD1	1.84	1.08
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.35	1.08
1:A:3:SER:OG	1:A:5:ILE:HG23	1.53	1.07
1:A:107:THR:HG21	1:A:202:ILE:HD11	1.14	1.07
1:A:220:LYS:HE2	1:A:221:HIS:CG	1.90	1.06
1:A:406:TRP:CZ2	2:B:418:ASN:OD1	2.09	1.06
2:B:366:LYS:HD3	2:B:405:TYR:CE1	1.91	1.05
1:A:298:GLU:OE2	1:A:298:GLU:N	1.89	1.05
1:A:498:ASP:OD2	1:A:538:ALA:HB2	1.55	1.05
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.39	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:HD12	1:A:94:ILE:O	1.57	1.04
2:B:244:ILE:HD11	2:B:266:TRP:CH2	1.88	1.04
2:B:242:GLN:H	2:B:243:PRO:HD3	1.20	1.04
1:A:197:GLN:N	1:A:197:GLN:OE1	1.90	1.03
1:A:489:SER:HB2	1:A:493:VAL:CG2	1.89	1.02
2:B:420:PRO:HG2	2:B:423:VAL:CG2	1.89	1.02
2:B:253:THR:HG22	2:B:255:ASN:N	1.74	1.01
1:A:3:SER:OG	1:A:5:ILE:CG2	2.10	1.00
2:B:253:THR:HG23	2:B:289:LEU:O	1.61	1.00
1:A:220:LYS:HE2	1:A:221:HIS:ND1	1.77	1.00
1:A:107:THR:CG2	1:A:202:ILE:HD11	1.91	0.99
2:B:344:GLU:HB3	2:B:347:LYS:CE	1.92	0.99
2:B:268:SER:O	2:B:269:GLN:HB2	1.58	0.98
2:B:271:TYR:HB3	2:B:274:ILE:HD11	1.46	0.98
2:B:244:ILE:HD12	2:B:266:TRP:CZ3	1.88	0.98
1:A:27:THR:O	1:A:31:ILE:HG13	1.63	0.98
1:A:183:TYR:CZ	1:A:230:MET:HE1	1.98	0.98
2:B:420:PRO:HG2	2:B:423:VAL:HG21	1.46	0.97
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	1.99	0.97
2:B:260:LEU:CD1	2:B:264:LEU:CD1	2.42	0.97
2:B:298:GLU:CD	2:B:298:GLU:N	2.22	0.97
2:B:241:VAL:HG23	2:B:243:PRO:HD3	1.44	0.96
1:A:460:ASN:HB2	2:B:286:THR:O	1.64	0.95
1:A:175:ASN:HB3	1:A:178:ILE:CD1	1.95	0.95
1:A:357:MET:HE3	1:A:514:GLU:OE2	1.67	0.95
2:B:260:LEU:HD13	2:B:264:LEU:HD12	1.48	0.95
1:A:220:LYS:CE	1:A:221:HIS:NE2	2.31	0.94
1:A:296:THR:HG22	1:A:299:ALA:H	1.31	0.94
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.46	0.94
1:A:277:ARG:HH12	1:A:334:GLN:HE21	0.97	0.94
1:A:220:LYS:HE3	1:A:221:HIS:CD2	2.02	0.94
2:B:66:LYS:HG3	2:B:407:GLN:NE2	1.82	0.94
1:A:51:GLY:HA3	1:A:53:GLU:OE1	1.65	0.93
2:B:65:LYS:HA	2:B:407:GLN:HG2	1.50	0.93
2:B:356:ARG:HH11	2:B:356:ARG:HB2	1.30	0.93
1:A:277:ARG:NH1	1:A:334:GLN:HE21	1.67	0.92
1:A:372:VAL:HG11	1:A:411:ILE:CG2	1.99	0.92
2:B:420:PRO:CG	2:B:423:VAL:HG21	1.99	0.92
1:A:199:ARG:O	1:A:203:GLU:HG2	1.70	0.92
2:B:242:GLN:H	2:B:243:PRO:CD	1.83	0.92
1:A:10:VAL:O	1:A:11:LYS:HG2	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LYS:HE3	1:A:221:HIS:NE2	1.85	0.92
2:B:297:GLU:HA	2:B:300:GLU:HB2	1.49	0.91
1:A:194:GLU:OE1	1:A:194:GLU:N	2.03	0.91
2:B:260:LEU:CD1	2:B:264:LEU:HD11	2.00	0.91
2:B:373:GLN:NE2	2:B:407:GLN:H	1.69	0.91
1:A:433:PRO:HB2	2:B:290:THR:HG22	1.52	0.91
2:B:244:ILE:HD11	2:B:266:TRP:HH2	1.26	0.91
1:A:543:GLY:HA2	2:B:284:ARG:CA	2.00	0.91
1:A:195:ILE:HG23	1:A:199:ARG:NE	1.87	0.90
2:B:373:GLN:HE22	2:B:407:GLN:H	1.07	0.90
2:B:373:GLN:O	2:B:377:THR:HG22	1.70	0.90
1:A:233:GLU:HG2	1:A:235:HIS:CE1	2.07	0.89
2:B:244:ILE:HD13	2:B:266:TRP:CH2	1.95	0.89
1:A:183:TYR:OH	1:A:230:MET:HE1	1.73	0.89
2:B:356:ARG:HH11	2:B:356:ARG:CB	1.86	0.89
1:A:220:LYS:CE	1:A:221:HIS:CE1	2.55	0.89
2:B:271:TYR:O	2:B:274:ILE:HG12	1.73	0.88
1:A:220:LYS:HE2	1:A:221:HIS:CD2	2.01	0.88
2:B:268:SER:HB3	2:B:274:ILE:HB	1.55	0.88
1:A:357:MET:O	1:A:357:MET:HG2	1.74	0.88
2:B:160:PHE:O	2:B:160:PHE:CD2	2.27	0.87
1:A:173:LYS:HA	1:A:173:LYS:CE	2.05	0.87
3:A:601:RT3:O28	3:A:601:RT3:H7	1.71	0.87
1:A:220:LYS:HD3	1:A:221:HIS:N	1.89	0.87
2:B:11:LYS:HB3	2:B:11:LYS:NZ	1.89	0.87
1:A:228:LEU:CD2	1:A:228:LEU:N	2.37	0.87
2:B:253:THR:HG22	2:B:255:ASN:H	1.38	0.86
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.57	0.86
2:B:236:PRO:O	2:B:238:LYS:N	2.08	0.86
1:A:186:ASP:O	1:A:187:LEU:HD23	1.74	0.86
1:A:489:SER:HB2	1:A:493:VAL:HG21	1.58	0.86
2:B:270:ILE:HB	2:B:346:PHE:O	1.74	0.86
1:A:489:SER:CB	1:A:493:VAL:HG21	2.06	0.85
1:A:194:GLU:CD	1:A:194:GLU:N	2.33	0.85
1:A:206:ARG:HH22	1:A:218:ASP:HB3	1.37	0.85
1:A:220:LYS:C	1:A:220:LYS:CD	2.43	0.85
1:A:498:ASP:OD2	1:A:538:ALA:CB	2.25	0.85
2:B:308:GLU:O	2:B:311:LYS:HG2	1.78	0.84
1:A:233:GLU:C	1:A:234:LEU:HD23	2.02	0.84
1:A:287:LYS:HD3	1:A:291:GLU:OE2	1.77	0.84
1:A:51:GLY:CA	1:A:53:GLU:OE1	2.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PRO:HB2	2:B:290:THR:CG2	2.08	0.83
1:A:296:THR:CG2	1:A:299:ALA:H	1.92	0.83
1:A:103:LYS:O	3:A:601:RT3:H17	1.79	0.82
1:A:195:ILE:CD1	1:A:199:ARG:NH2	2.42	0.82
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.27	0.82
2:B:271:TYR:CB	2:B:274:ILE:HD11	2.08	0.82
2:B:283:LEU:O	2:B:284:ARG:CG	2.28	0.82
2:B:396:GLU:O	2:B:400:THR:HG22	1.78	0.82
1:A:206:ARG:NH2	1:A:218:ASP:CB	2.41	0.82
2:B:260:LEU:CD1	2:B:264:LEU:HD12	2.05	0.82
2:B:344:GLU:HB2	2:B:347:LYS:HD3	1.61	0.81
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.62	0.81
1:A:489:SER:HB2	1:A:493:VAL:HG22	1.62	0.81
1:A:10:VAL:HG12	1:A:11:LYS:N	1.96	0.81
2:B:422:LEU:CD2	2:B:425:LEU:HD11	2.10	0.81
2:B:260:LEU:HD11	2:B:264:LEU:HD11	1.62	0.81
1:A:197:GLN:H	1:A:197:GLN:CD	1.88	0.81
1:A:500:GLN:HG3	2:B:422:LEU:HD12	1.60	0.81
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.44	0.80
1:A:298:GLU:H	1:A:298:GLU:CD	1.87	0.80
2:B:242:GLN:O	2:B:242:GLN:HG3	1.78	0.80
2:B:374:LYS:HD3	2:B:378:GLU:OE2	1.81	0.80
1:A:457:TYR:CD1	1:A:457:TYR:C	2.60	0.80
2:B:257:ILE:O	2:B:261:VAL:HG12	1.79	0.80
2:B:260:LEU:HD13	2:B:264:LEU:CD1	2.06	0.80
2:B:420:PRO:CG	2:B:423:VAL:CG2	2.55	0.80
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.12	0.80
1:A:175:ASN:CB	1:A:178:ILE:HD12	2.11	0.80
2:B:344:GLU:CB	2:B:347:LYS:HD3	2.12	0.80
1:A:0:SER:CB	1:A:113:ASP:OD2	2.30	0.80
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.64	0.80
1:A:464:GLN:HG2	1:A:465:LYS:N	1.95	0.80
1:A:543:GLY:HA2	2:B:284:ARG:HA	1.63	0.79
1:A:303:LEU:O	1:A:307:ARG:HG3	1.82	0.79
2:B:65:LYS:CA	2:B:407:GLN:HG2	2.13	0.79
1:A:104:LYS:N	1:A:192:ASP:OD2	2.15	0.79
1:A:277:ARG:HH12	1:A:334:GLN:NE2	1.80	0.79
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.08	0.78
2:B:241:VAL:HG23	2:B:242:GLN:H	1.48	0.78
1:A:210:LEU:C	1:A:212:TRP:H	1.89	0.78
1:A:93:GLY:HA3	2:B:137:ASN:ND2	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLN:NE2	1:A:338:THR:HG23	1.98	0.78
1:A:424:LYS:HE3	1:A:426:TRP:CE2	2.18	0.78
2:B:373:GLN:O	2:B:377:THR:CG2	2.32	0.78
1:A:10:VAL:HG12	1:A:11:LYS:H	1.47	0.78
1:A:410:TRP:CZ3	2:B:363:ASN:HB3	2.19	0.78
2:B:209:LEU:HB3	2:B:214:LEU:HB2	1.63	0.78
1:A:194:GLU:O	1:A:196:GLY:N	2.17	0.77
1:A:195:ILE:HG23	1:A:199:ARG:CZ	2.15	0.77
2:B:366:LYS:CD	2:B:405:TYR:CD1	2.67	0.77
1:A:175:ASN:ND2	1:A:178:ILE:HD11	2.00	0.77
1:A:72:ARG:HB3	1:A:72:ARG:NH1	2.01	0.76
1:A:424:LYS:HE3	1:A:426:TRP:NE1	2.00	0.76
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.10	0.76
2:B:162:SER:O	2:B:166:LYS:HE3	1.85	0.76
2:B:274:ILE:C	2:B:275:LYS:HG2	2.11	0.76
1:A:51:GLY:C	1:A:53:GLU:OE1	2.28	0.76
1:A:95:PRO:HA	2:B:136:ASN:OD1	1.85	0.76
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.20	0.76
2:B:12:LEU:HD23	2:B:17:ASP:HA	1.68	0.75
2:B:209:LEU:HG	2:B:214:LEU:HD12	1.68	0.75
1:A:356:ARG:HH21	1:A:358:ARG:HG3	1.50	0.75
1:A:228:LEU:H	1:A:228:LEU:HD23	1.50	0.75
1:A:296:THR:HG22	1:A:299:ALA:N	2.01	0.75
1:A:402:TRP:CD1	1:A:402:TRP:C	2.65	0.75
1:A:475:GLN:HG2	1:A:501:TYR:CE2	2.21	0.75
1:A:210:LEU:O	1:A:212:TRP:N	2.20	0.75
2:B:253:THR:CG2	2:B:255:ASN:H	1.99	0.75
2:B:344:GLU:O	2:B:347:LYS:HD2	1.87	0.75
2:B:356:ARG:CB	2:B:356:ARG:NH1	2.50	0.75
1:A:468:THR:C	1:A:469:LEU:HG	2.10	0.75
2:B:268:SER:O	2:B:269:GLN:CB	2.35	0.74
1:A:220:LYS:HE2	1:A:221:HIS:NE2	1.96	0.74
2:B:241:VAL:CB	2:B:243:PRO:HD3	2.17	0.74
1:A:51:GLY:HA3	1:A:53:GLU:CD	2.13	0.74
1:A:64:LYS:HD2	1:A:70:LYS:O	1.87	0.74
2:B:104:LYS:HA	2:B:237:ASP:OD2	1.88	0.74
2:B:319:TYR:O	2:B:321:PRO:HD3	1.88	0.74
1:A:45:GLY:O	1:A:147:ASN:OD1	2.06	0.74
1:A:228:LEU:N	1:A:228:LEU:HD22	2.01	0.74
2:B:5:ILE:N	2:B:5:ILE:HD12	2.02	0.74
1:A:430:GLU:HG2	1:A:531:VAL:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:HD22	1:A:507:GLN:HG3	1.70	0.74
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.70	0.74
1:A:173:LYS:HA	1:A:173:LYS:HE3	1.68	0.73
1:A:403:THR:HG22	1:A:404:GLU:HG3	1.69	0.73
1:A:125:ARG:HD3	1:A:146:TYR:O	1.88	0.73
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.23	0.73
2:B:388:LYS:HE3	2:B:415:GLU:HG3	1.70	0.73
1:A:430:GLU:HB2	1:A:532:TYR:HB2	1.70	0.73
2:B:254:VAL:O	2:B:258:GLN:HG3	1.89	0.73
2:B:330:GLN:OE1	2:B:338:THR:OG1	2.07	0.73
2:B:278:GLN:HE21	2:B:278:GLN:HA	1.54	0.73
2:B:298:GLU:HA	2:B:301:LEU:HD12	1.71	0.73
2:B:280:CYS:O	2:B:283:LEU:N	2.19	0.72
2:B:361:HIS:CD2	2:B:361:HIS:O	2.42	0.72
2:B:366:LYS:HD3	2:B:405:TYR:CD1	2.23	0.72
1:A:233:GLU:HG2	1:A:235:HIS:HE1	1.54	0.72
2:B:332:GLN:O	2:B:333:GLY:O	2.08	0.72
1:A:543:GLY:HA2	2:B:284:ARG:N	2.04	0.72
2:B:266:TRP:HE1	2:B:346:PHE:HE2	1.36	0.72
1:A:441:TYR:CD2	1:A:544:GLY:CA	2.73	0.72
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.71	0.72
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.71	0.72
1:A:10:VAL:O	1:A:11:LYS:CG	2.38	0.72
2:B:209:LEU:CD1	2:B:214:LEU:HD12	2.19	0.72
1:A:278:GLN:HB3	1:A:299:ALA:HA	1.72	0.72
2:B:366:LYS:HD2	2:B:405:TYR:CD1	2.24	0.72
2:B:345:PRO:O	2:B:347:LYS:HD2	1.89	0.71
2:B:373:GLN:HE22	2:B:407:GLN:N	1.86	0.71
1:A:139:THR:HG22	1:A:140:PRO:CD	2.16	0.71
2:B:13:LYS:HB3	2:B:16:MET:HE3	1.70	0.71
2:B:274:ILE:HA	2:B:306:ASN:HD21	1.55	0.71
2:B:422:LEU:HD22	2:B:425:LEU:HD11	1.73	0.71
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.70	0.71
3:A:601:RT3:O28	3:A:601:RT3:C7	2.38	0.71
2:B:239:TRP:O	2:B:240:THR:HG23	1.91	0.71
1:A:17:ASP:O	1:A:83:ARG:NH1	2.23	0.70
2:B:11:LYS:HB3	2:B:11:LYS:HZ3	1.54	0.70
2:B:344:GLU:HB3	2:B:347:LYS:CD	2.20	0.70
2:B:362:THR:HG23	2:B:366:LYS:HG2	1.71	0.70
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.26	0.70
1:A:173:LYS:HE3	1:A:173:LYS:CA	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:CB	1:A:178:ILE:CD1	2.66	0.70
1:A:175:ASN:HD21	1:A:201:LYS:CE	2.04	0.70
1:A:220:LYS:CE	1:A:221:HIS:CG	2.64	0.70
1:A:489:SER:OG	1:A:493:VAL:HG21	1.92	0.70
1:A:64:LYS:O	1:A:65:LYS:CB	2.38	0.70
1:A:467:VAL:HG12	1:A:468:THR:N	2.07	0.70
2:B:242:GLN:N	2:B:243:PRO:HD3	2.02	0.70
1:A:134:SER:OG	1:A:138:GLU:O	2.08	0.70
1:A:175:ASN:CG	1:A:178:ILE:HD11	2.17	0.70
1:A:53:GLU:OE1	1:A:53:GLU:N	2.23	0.70
1:A:173:LYS:CE	1:A:173:LYS:CA	2.69	0.69
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.27	0.69
2:B:250:ASP:O	2:B:251:SER:HB2	1.90	0.69
1:A:197:GLN:O	1:A:201:LYS:HB2	1.91	0.69
1:A:350:LYS:HE3	1:A:378:GLU:OE2	1.91	0.69
1:A:406:TRP:CH2	1:A:407:GLN:HB2	2.27	0.69
1:A:277:ARG:NH1	1:A:334:GLN:NE2	2.40	0.69
1:A:195:ILE:CD1	1:A:199:ARG:HH21	2.04	0.69
2:B:46:LYS:HA	2:B:46:LYS:HE2	1.74	0.69
2:B:253:THR:CG2	2:B:289:LEU:O	2.37	0.69
1:A:369:THR:CG2	1:A:398:TRP:CZ3	2.75	0.69
1:A:500:GLN:CG	2:B:422:LEU:HD12	2.23	0.69
2:B:244:ILE:CD1	2:B:266:TRP:HH2	1.85	0.69
1:A:63:ILE:HD11	1:A:72:ARG:HD3	1.75	0.68
1:A:330:GLN:HE21	1:A:338:THR:HG23	1.58	0.68
2:B:241:VAL:O	2:B:242:GLN:CB	2.42	0.68
1:A:1:PRO:O	1:A:2:ILE:CD1	2.28	0.68
1:A:445:ALA:O	1:A:477:THR:HG21	1.93	0.68
1:A:138:GLU:CD	1:A:138:GLU:H	2.01	0.68
2:B:243:PRO:HB3	2:B:311:LYS:HA	1.76	0.68
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.20	0.68
1:A:64:LYS:O	1:A:65:LYS:HB2	1.92	0.67
2:B:11:LYS:HG3	2:B:12:LEU:O	1.94	0.67
1:A:355:ALA:O	1:A:356:ARG:C	2.34	0.67
1:A:458:VAL:HG23	1:A:458:VAL:O	1.94	0.67
1:A:342:TYR:HA	1:A:349:LEU:CD1	2.23	0.67
1:A:406:TRP:CZ3	1:A:407:GLN:CB	2.76	0.67
2:B:366:LYS:CD	2:B:405:TYR:CE1	2.72	0.67
1:A:175:ASN:CG	1:A:178:ILE:CD1	2.67	0.67
2:B:344:GLU:O	2:B:347:LYS:CD	2.42	0.67
2:B:356:ARG:NH1	2:B:356:ARG:HB3	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ILE:HD12	1:A:116:PHE:O	1.95	0.67
2:B:308:GLU:HA	2:B:311:LYS:CE	2.25	0.67
1:A:175:ASN:ND2	1:A:201:LYS:CE	2.58	0.67
1:A:458:VAL:HG23	2:B:286:THR:HG21	1.76	0.67
2:B:420:PRO:HG2	2:B:423:VAL:CB	2.24	0.67
1:A:125:ARG:HB3	1:A:146:TYR:O	1.94	0.67
1:A:137:ASN:C	1:A:137:ASN:ND2	2.50	0.67
1:A:513:SER:N	1:A:519:ASN:HD21	1.94	0.66
1:A:360:ALA:HA	1:A:514:GLU:OE1	1.96	0.66
2:B:66:LYS:CG	2:B:407:GLN:NE2	2.55	0.66
1:A:82:LYS:O	1:A:82:LYS:HG2	1.95	0.66
1:A:410:TRP:CE3	2:B:363:ASN:CB	2.79	0.66
2:B:298:GLU:O	2:B:301:LEU:HB2	1.95	0.66
1:A:24:TRP:CD2	1:A:25:PRO:HD2	2.31	0.66
1:A:41:MET:HE2	1:A:47:ILE:HD13	1.76	0.66
2:B:305:GLU:O	2:B:309:ILE:HG13	1.96	0.66
2:B:86:ASP:O	2:B:91:GLN:HB2	1.96	0.66
2:B:103:LYS:HE3	2:B:179:VAL:CG2	2.26	0.66
1:A:137:ASN:C	1:A:137:ASN:HD22	2.04	0.66
2:B:344:GLU:CB	2:B:347:LYS:CD	2.74	0.65
1:A:181:TYR:HB2	3:A:601:RT3:H15	1.79	0.65
1:A:406:TRP:CE3	1:A:407:GLN:HB2	2.31	0.65
2:B:241:VAL:HB	2:B:243:PRO:HD3	1.78	0.65
1:A:1:PRO:C	1:A:2:ILE:HD13	2.18	0.65
2:B:308:GLU:HA	2:B:311:LYS:HE2	1.79	0.65
1:A:460:ASN:CB	2:B:286:THR:O	2.43	0.65
1:A:369:THR:CG2	1:A:398:TRP:HZ3	2.10	0.65
1:A:43:LYS:HE2	1:A:43:LYS:HA	1.78	0.65
2:B:241:VAL:CG2	2:B:243:PRO:CD	2.67	0.65
1:A:24:TRP:CG	1:A:25:PRO:HD2	2.32	0.65
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.79	0.65
2:B:156:SER:N	2:B:157:PRO:HD2	2.12	0.65
2:B:355:ALA:O	2:B:356:ARG:C	2.40	0.65
1:A:173:LYS:HE3	1:A:173:LYS:N	2.11	0.64
1:A:175:ASN:HD21	1:A:201:LYS:NZ	1.95	0.64
1:A:395:LYS:HZ3	1:A:414:TRP:NE1	1.94	0.64
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.78	0.64
1:A:406:TRP:CE3	1:A:407:GLN:CA	2.81	0.64
2:B:425:LEU:O	2:B:428:GLN:N	2.29	0.64
1:A:77:PHE:O	1:A:78:ARG:C	2.41	0.64
1:A:105:SER:OG	1:A:198:HIS:CD2	2.50	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:HD13	1:A:199:ARG:HH22	1.60	0.64
1:A:173:LYS:HA	1:A:173:LYS:HE2	1.78	0.64
2:B:303:LEU:HD22	2:B:307:ARG:NH2	2.13	0.64
1:A:131:THR:OG1	1:A:143:ARG:HD2	1.98	0.64
1:A:238:LYS:HB2	1:A:315:HIS:HB3	1.79	0.64
1:A:66:LYS:O	1:A:67:ASP:HB3	1.97	0.64
1:A:535:TRP:CE3	2:B:422:LEU:HD13	2.33	0.64
2:B:425:LEU:O	2:B:427:TYR:N	2.32	0.63
1:A:219:LYS:O	1:A:220:LYS:HB3	1.98	0.63
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.34	0.63
1:A:398:TRP:CH2	1:A:411:ILE:HD11	2.33	0.63
1:A:520:GLN:HA	1:A:523:GLU:HG2	1.81	0.63
2:B:244:ILE:HG22	2:B:263:LYS:NZ	2.14	0.63
1:A:245:VAL:HG22	1:A:245:VAL:O	1.98	0.63
2:B:209:LEU:CG	2:B:214:LEU:HD12	2.28	0.63
2:B:241:VAL:HG23	2:B:243:PRO:CD	2.23	0.63
1:A:29:GLU:HG3	1:A:30:LYS:N	2.14	0.63
1:A:102:LYS:HG3	3:A:601:RT3:O29	1.98	0.63
1:A:441:TYR:HD2	1:A:544:GLY:HA3	1.60	0.63
1:A:486:LEU:O	1:A:528:LYS:NZ	2.32	0.63
2:B:113:ASP:O	2:B:114:ALA:C	2.39	0.63
1:A:104:LYS:O	3:A:601:RT3:H18	1.98	0.63
1:A:228:LEU:N	1:A:228:LEU:HD23	2.11	0.63
2:B:102:LYS:O	2:B:237:ASP:HB3	1.99	0.63
1:A:28:GLU:HG2	1:A:135:ILE:HG23	1.80	0.62
2:B:361:HIS:O	2:B:361:HIS:CG	2.53	0.62
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.82	0.62
1:A:28:GLU:HG2	1:A:135:ILE:CG2	2.30	0.62
1:A:134:SER:O	1:A:136:ASN:O	2.17	0.62
1:A:234:LEU:HD23	1:A:234:LEU:N	2.13	0.62
2:B:13:LYS:CB	2:B:16:MET:HE3	2.30	0.62
1:A:60:VAL:CG2	1:A:130:PHE:CD2	2.82	0.62
1:A:441:TYR:CD2	1:A:544:GLY:HA2	2.34	0.62
1:A:543:GLY:H	2:B:283:LEU:HB3	1.64	0.62
2:B:268:SER:HB3	2:B:274:ILE:CB	2.28	0.62
1:A:41:MET:HB3	1:A:47:ILE:HG12	1.80	0.62
1:A:311:LYS:O	1:A:312:GLU:OE1	2.17	0.62
1:A:168:LEU:HD22	1:A:180:ILE:HD13	1.81	0.62
1:A:369:THR:HG22	1:A:398:TRP:CZ3	2.35	0.62
1:A:475:GLN:HG2	1:A:501:TYR:CD2	2.35	0.62
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:HD22	1:A:507:GLN:CG	2.30	0.62
2:B:11:LYS:HB3	2:B:11:LYS:HZ2	1.62	0.62
1:A:2:ILE:HG22	1:A:2:ILE:O	1.98	0.62
1:A:10:VAL:CG1	1:A:11:LYS:H	2.13	0.62
1:A:69:THR:HG23	1:A:69:THR:O	1.99	0.62
1:A:457:TYR:CD1	1:A:457:TYR:O	2.53	0.61
2:B:236:PRO:O	2:B:237:ASP:C	2.43	0.61
2:B:253:THR:CG2	2:B:254:VAL:N	2.62	0.61
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.30	0.61
2:B:108:VAL:HG22	2:B:188:TYR:CE2	2.35	0.61
1:A:219:LYS:O	1:A:220:LYS:HD2	2.00	0.61
1:A:410:TRP:O	1:A:410:TRP:CD1	2.54	0.61
1:A:54:ASN:OD1	1:A:54:ASN:C	2.42	0.61
1:A:542:ILE:CG2	1:A:543:GLY:N	2.63	0.61
1:A:60:VAL:CG2	1:A:130:PHE:HD2	2.14	0.61
2:B:236:PRO:O	2:B:239:TRP:N	2.32	0.61
2:B:309:ILE:O	2:B:312:GLU:HG2	2.01	0.61
2:B:420:PRO:HG3	2:B:423:VAL:HG21	1.80	0.61
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.30	0.60
1:A:365:VAL:O	1:A:369:THR:HG23	2.00	0.60
1:A:94:ILE:HD12	1:A:94:ILE:C	2.26	0.60
1:A:175:ASN:ND2	1:A:201:LYS:HE2	2.15	0.60
1:A:10:VAL:CG1	1:A:11:LYS:N	2.65	0.60
1:A:356:ARG:HH21	1:A:358:ARG:CG	2.13	0.60
1:A:458:VAL:O	1:A:458:VAL:CG2	2.49	0.60
2:B:121:ASP:OD2	2:B:121:ASP:C	2.45	0.60
1:A:369:THR:HG21	1:A:398:TRP:CH2	2.36	0.60
1:A:369:THR:HG21	1:A:398:TRP:CZ3	2.36	0.60
1:A:395:LYS:NZ	1:A:414:TRP:CE2	2.67	0.60
2:B:344:GLU:O	2:B:345:PRO:C	2.44	0.60
1:A:233:GLU:HB3	1:A:240:THR:HG23	1.84	0.60
2:B:241:VAL:O	2:B:242:GLN:HB3	2.02	0.60
2:B:425:LEU:C	2:B:427:TYR:N	2.58	0.60
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.37	0.60
1:A:246:LEU:CD1	1:A:310:LEU:HD12	2.14	0.59
2:B:256:ASP:O	2:B:260:LEU:HB2	2.02	0.59
1:A:520:GLN:O	1:A:523:GLU:HG2	2.03	0.59
2:B:111:VAL:O	2:B:111:VAL:CG1	2.50	0.59
1:A:511:ASP:OD2	1:A:511:ASP:C	2.45	0.59
1:A:433:PRO:HG3	2:B:255:ASN:ND2	2.17	0.59
2:B:24:TRP:O	2:B:26:LEU:HD13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:LEU:HB3	2:B:426:TRP:CZ2	2.37	0.59
1:A:195:ILE:CG1	1:A:199:ARG:HH21	2.16	0.59
1:A:406:TRP:CE3	1:A:406:TRP:C	2.81	0.59
2:B:111:VAL:O	2:B:111:VAL:HG13	2.02	0.59
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.37	0.59
1:A:205:LEU:CD1	1:A:209:LEU:HD11	2.33	0.59
2:B:162:SER:O	2:B:166:LYS:HG2	2.02	0.59
2:B:274:ILE:HA	2:B:306:ASN:ND2	2.18	0.59
1:A:430:GLU:HG2	1:A:531:VAL:C	2.28	0.59
1:A:70:LYS:NZ	1:A:72:ARG:HH12	2.00	0.58
1:A:417:VAL:HG22	1:A:419:THR:CG2	2.30	0.58
2:B:66:LYS:CB	2:B:407:GLN:NE2	2.67	0.58
1:A:72:ARG:NH1	1:A:72:ARG:CB	2.65	0.58
1:A:107:THR:HG22	1:A:198:HIS:HE1	1.68	0.58
1:A:113:ASP:O	1:A:114:ALA:C	2.44	0.58
1:A:156:SER:N	1:A:157:PRO:CD	2.65	0.58
2:B:425:LEU:C	2:B:427:TYR:H	2.12	0.58
1:A:17:ASP:OD2	1:A:56:TYR:OH	2.18	0.58
1:A:424:LYS:CE	1:A:426:TRP:CE2	2.86	0.58
1:A:513:SER:H	1:A:519:ASN:HD21	1.50	0.58
2:B:248:GLU:O	2:B:249:LYS:HB3	2.03	0.58
2:B:260:LEU:HD13	2:B:260:LEU:C	2.29	0.58
2:B:425:LEU:N	2:B:425:LEU:HD23	2.19	0.58
1:A:70:LYS:HZ3	1:A:72:ARG:HH12	1.52	0.58
2:B:64:LYS:HD2	2:B:69:THR:O	2.03	0.58
1:A:70:LYS:NZ	1:A:72:ARG:NH1	2.51	0.57
1:A:195:ILE:HD13	1:A:199:ARG:HH21	1.54	0.57
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.39	0.57
1:A:406:TRP:CE3	1:A:407:GLN:N	2.73	0.57
2:B:396:GLU:O	2:B:400:THR:CG2	2.49	0.57
1:A:409:THR:O	1:A:410:TRP:HB2	2.05	0.57
2:B:214:LEU:N	2:B:214:LEU:HD23	2.18	0.57
1:A:216:THR:HB	1:A:217:PRO:HD2	1.86	0.57
2:B:344:GLU:CB	2:B:347:LYS:CE	2.77	0.57
2:B:420:PRO:HG2	2:B:423:VAL:HB	1.87	0.57
2:B:422:LEU:HD23	2:B:425:LEU:HD11	1.84	0.57
2:B:50:ILE:HD12	2:B:54:ASN:HB3	1.87	0.57
1:A:64:LYS:NZ	1:A:69:THR:HA	2.19	0.57
2:B:241:VAL:CG2	2:B:242:GLN:H	2.13	0.57
2:B:280:CYS:O	2:B:282:LEU:N	2.38	0.56
1:A:170:PRO:O	1:A:172:ARG:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:C	1:A:212:TRP:N	2.52	0.56
1:A:398:TRP:CZ2	1:A:411:ILE:HG13	2.39	0.56
1:A:420:PRO:HA	1:A:421:PRO:C	2.30	0.56
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.20	0.56
2:B:242:GLN:O	2:B:243:PRO:C	2.49	0.56
2:B:256:ASP:O	2:B:260:LEU:N	2.38	0.56
1:A:5:ILE:HG12	1:A:6:GLU:N	2.14	0.56
1:A:104:LYS:HG3	1:A:192:ASP:HB3	1.88	0.56
2:B:203:GLU:OE1	2:B:203:GLU:HA	2.05	0.56
1:A:430:GLU:CB	1:A:532:TYR:HB2	2.36	0.56
2:B:277:ARG:HB3	2:B:277:ARG:NH1	2.20	0.56
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.41	0.56
1:A:246:LEU:O	1:A:307:ARG:NH2	2.39	0.56
1:A:535:TRP:O	1:A:536:VAL:HG12	2.06	0.56
2:B:209:LEU:HD12	2:B:214:LEU:HD12	1.88	0.56
2:B:314:VAL:CG1	2:B:317:VAL:HG23	2.36	0.56
1:A:175:ASN:HB3	1:A:178:ILE:CG1	2.35	0.56
1:A:5:ILE:HG12	1:A:6:GLU:O	2.06	0.55
1:A:183:TYR:CZ	1:A:230:MET:CE	2.83	0.55
2:B:277:ARG:HA	2:B:280:CYS:HB2	1.88	0.55
1:A:63:ILE:HD12	1:A:72:ARG:HG3	1.89	0.55
1:A:134:SER:OG	1:A:139:THR:HB	2.05	0.55
1:A:377:THR:O	1:A:378:GLU:C	2.49	0.55
1:A:410:TRP:CE2	2:B:363:ASN:ND2	2.72	0.55
2:B:183:TYR:OH	2:B:386:THR:HG23	2.06	0.55
2:B:253:THR:HB	2:B:256:ASP:OD2	2.05	0.55
1:A:138:GLU:CD	1:A:138:GLU:N	2.63	0.55
1:A:543:GLY:CA	2:B:284:ARG:N	2.69	0.55
1:A:195:ILE:HG23	1:A:199:ARG:HE	1.67	0.55
1:A:305:GLU:O	1:A:309:ILE:HG13	2.06	0.55
1:A:233:GLU:O	1:A:234:LEU:HD23	2.06	0.55
1:A:519:ASN:O	1:A:522:ILE:HB	2.07	0.55
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.42	0.55
2:B:266:TRP:NE1	2:B:346:PHE:HE2	2.03	0.55
2:B:350:LYS:C	2:B:351:THR:CG2	2.79	0.55
1:A:542:ILE:CG2	2:B:283:LEU:HD13	2.37	0.55
2:B:257:ILE:HG23	2:B:279:LEU:HD11	1.89	0.55
1:A:457:TYR:C	1:A:457:TYR:HD1	2.14	0.55
2:B:256:ASP:OD2	2:B:256:ASP:N	2.39	0.55
1:A:218:ASP:O	1:A:219:LYS:C	2.50	0.55
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:LEU:O	2:B:121:ASP:C	2.50	0.55
2:B:241:VAL:HG23	2:B:242:GLN:N	2.18	0.55
2:B:273:GLY:O	2:B:274:ILE:O	2.25	0.55
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.08	0.54
1:A:110:ASP:C	1:A:111:VAL:HG23	2.32	0.54
1:A:542:ILE:O	1:A:544:GLY:N	2.40	0.54
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.89	0.54
2:B:254:VAL:C	2:B:258:GLN:HG3	2.32	0.54
2:B:24:TRP:O	2:B:25:PRO:C	2.49	0.54
2:B:37:ILE:O	2:B:41:MET:HG3	2.07	0.54
2:B:283:LEU:O	2:B:284:ARG:CB	2.56	0.54
1:A:88:TRP:NE1	2:B:143:ARG:HD3	2.23	0.54
1:A:296:THR:HG23	1:A:298:GLU:OE2	2.07	0.54
1:A:220:LYS:HD3	1:A:220:LYS:O	2.04	0.54
1:A:409:THR:HG23	1:A:410:TRP:N	2.21	0.54
2:B:350:LYS:C	2:B:351:THR:HG23	2.32	0.54
1:A:410:TRP:CD2	2:B:363:ASN:ND2	2.76	0.54
2:B:379:SER:OG	2:B:387:PRO:HD3	2.08	0.54
1:A:155:GLY:O	1:A:159:ILE:HG13	2.08	0.54
2:B:120:LEU:HD22	2:B:121:ASP:N	2.23	0.54
1:A:86:ASP:HA	1:A:154:LYS:NZ	2.23	0.54
1:A:324:ASP:O	1:A:343:GLN:HG2	2.08	0.54
1:A:330:GLN:HE21	1:A:338:THR:CG2	2.20	0.54
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.89	0.54
2:B:277:ARG:HB3	2:B:277:ARG:HH11	1.73	0.54
1:A:19:PRO:O	1:A:56:TYR:HD1	1.90	0.54
1:A:467:VAL:HG12	1:A:468:THR:H	1.70	0.54
1:A:101:LYS:HD3	1:A:321:PRO:HD3	1.89	0.53
2:B:199:ARG:NH1	2:B:233:GLU:OE2	2.41	0.53
2:B:306:ASN:O	2:B:310:LEU:N	2.34	0.53
1:A:104:LYS:CB	1:A:192:ASP:HA	2.34	0.53
2:B:46:LYS:HA	2:B:46:LYS:CE	2.39	0.53
2:B:332:GLN:O	2:B:333:GLY:C	2.49	0.53
1:A:48:SER:O	1:A:144:TYR:HD1	1.91	0.53
1:A:186:ASP:C	1:A:187:LEU:HD23	2.34	0.53
2:B:80:LEU:O	2:B:84:THR:OG1	2.25	0.53
2:B:302:GLU:O	2:B:303:LEU:C	2.51	0.53
1:A:17:ASP:O	1:A:83:ARG:HD3	2.09	0.53
1:A:208:HIS:O	1:A:212:TRP:HD1	1.91	0.53
2:B:78:ARG:NH1	2:B:412:PRO:O	2.39	0.53
2:B:309:ILE:HA	2:B:312:GLU:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:CG1	3:A:601:RT3:C20	2.87	0.53
1:A:207:GLN:O	1:A:208:HIS:C	2.51	0.53
1:A:296:THR:HG23	1:A:298:GLU:CD	2.34	0.53
2:B:274:ILE:HG22	2:B:275:LYS:H	1.74	0.53
2:B:298:GLU:O	2:B:301:LEU:N	2.37	0.53
1:A:29:GLU:HG3	1:A:30:LYS:H	1.73	0.53
1:A:106:VAL:CG1	3:A:601:RT3:C21	2.87	0.53
1:A:72:ARG:CB	1:A:72:ARG:CZ	2.87	0.53
1:A:467:VAL:CG1	1:A:468:THR:N	2.71	0.53
2:B:418:ASN:O	2:B:419:THR:C	2.51	0.53
1:A:406:TRP:CE3	1:A:407:GLN:HA	2.44	0.53
2:B:274:ILE:HG22	2:B:275:LYS:N	2.24	0.53
1:A:277:ARG:O	1:A:281:LYS:HG3	2.09	0.52
1:A:517:LEU:HA	1:A:520:GLN:HG3	1.90	0.52
2:B:428:GLN:O	2:B:428:GLN:HG3	2.08	0.52
2:B:252:TRP:HE3	2:B:256:ASP:HB2	1.74	0.52
1:A:325:LEU:HD11	1:A:383:TRP:CE3	2.45	0.52
2:B:273:GLY:O	2:B:275:LYS:HG2	2.09	0.52
1:A:439:THR:CG2	1:A:441:TYR:CE1	2.92	0.52
2:B:199:ARG:HD3	2:B:233:GLU:OE1	2.09	0.52
2:B:362:THR:HG21	2:B:367:GLN:HG3	1.91	0.52
2:B:421:PRO:O	2:B:425:LEU:HD21	2.10	0.52
1:A:320:ASP:O	1:A:322:SER:N	2.43	0.52
1:A:398:TRP:CZ3	1:A:411:ILE:HD11	2.45	0.52
2:B:160:PHE:O	2:B:160:PHE:CG	2.60	0.52
2:B:242:GLN:O	2:B:242:GLN:CG	2.53	0.52
1:A:96:HIS:N	2:B:136:ASN:OD1	2.39	0.52
1:A:265:ASN:OD1	1:A:353:LYS:NZ	2.34	0.52
2:B:262:GLY:O	2:B:265:ASN:HB3	2.09	0.52
1:A:194:GLU:O	1:A:195:ILE:C	2.52	0.52
2:B:84:THR:O	2:B:86:ASP:N	2.42	0.52
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.45	0.51
1:A:3:SER:HG	1:A:5:ILE:CG2	2.22	0.51
1:A:51:GLY:HA3	1:A:53:GLU:OE2	2.10	0.51
1:A:326:ILE:CD1	1:A:388:LYS:HE3	2.40	0.51
1:A:349:LEU:HD12	1:A:349:LEU:H	1.74	0.51
1:A:349:LEU:O	1:A:350:LYS:HB3	2.11	0.51
1:A:466:VAL:O	1:A:467:VAL:CG2	2.57	0.51
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.93	0.51
1:A:172:ARG:HH21	1:A:180:ILE:HB	1.74	0.51
1:A:104:LYS:HG3	1:A:192:ASP:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TYR:CD1	1:A:342:TYR:C	2.89	0.51
2:B:266:TRP:CZ2	2:B:427:TYR:CE1	2.98	0.51
1:A:103:LYS:O	3:A:601:RT3:C17	2.56	0.51
1:A:175:ASN:CG	1:A:178:ILE:HD12	2.35	0.51
1:A:438:GLU:HG2	1:A:459:THR:HB	1.93	0.51
1:A:532:TYR:C	1:A:532:TYR:CD2	2.88	0.51
2:B:72:ARG:O	2:B:72:ARG:HG3	2.11	0.51
1:A:63:ILE:CD1	1:A:72:ARG:HD3	2.41	0.51
1:A:498:ASP:HB2	1:A:536:VAL:O	2.11	0.51
2:B:169:GLU:N	2:B:170:PRO:HD2	2.25	0.51
2:B:337:TRP:N	2:B:337:TRP:CD1	2.79	0.51
1:A:134:SER:O	1:A:135:ILE:C	2.54	0.51
2:B:297:GLU:CA	2:B:300:GLU:HB2	2.31	0.51
2:B:378:GLU:O	2:B:382:ILE:HG13	2.11	0.51
1:A:106:VAL:HG13	3:A:601:RT3:C20	2.41	0.50
1:A:170:PRO:C	1:A:174:GLN:NE2	2.69	0.50
1:A:487:GLN:HA	1:A:524:GLN:HE22	1.77	0.50
1:A:535:TRP:CD2	2:B:422:LEU:CD1	2.94	0.50
2:B:88:TRP:CH2	2:B:154:LYS:HD3	2.46	0.50
2:B:242:GLN:N	2:B:243:PRO:CD	2.55	0.50
1:A:33:ALA:O	1:A:37:ILE:HG13	2.11	0.50
1:A:466:VAL:C	1:A:467:VAL:HG23	2.36	0.50
1:A:538:ALA:C	1:A:540:LYS:N	2.70	0.50
2:B:314:VAL:CG1	2:B:317:VAL:CG2	2.89	0.50
2:B:300:GLU:HA	2:B:303:LEU:HD12	1.93	0.50
1:A:395:LYS:HE2	1:A:414:TRP:CH2	2.47	0.50
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.94	0.50
2:B:165:THR:HB	2:B:166:LYS:HE2	1.92	0.50
2:B:240:THR:O	2:B:241:VAL:O	2.30	0.50
2:B:314:VAL:HG11	2:B:317:VAL:CG2	2.42	0.50
2:B:339:TYR:CD1	2:B:339:TYR:C	2.89	0.50
2:B:236:PRO:C	2:B:238:LYS:N	2.70	0.50
1:A:240:THR:OG1	1:A:241:VAL:N	2.44	0.49
1:A:296:THR:HG22	1:A:298:GLU:N	2.27	0.49
1:A:31:ILE:O	1:A:35:VAL:HG23	2.11	0.49
1:A:302:GLU:O	1:A:303:LEU:C	2.53	0.49
1:A:296:THR:O	1:A:300:GLU:HG2	2.12	0.49
2:B:328:GLU:OE2	2:B:342:TYR:OH	2.22	0.49
2:B:5:ILE:N	2:B:5:ILE:CD1	2.72	0.49
2:B:195:ILE:O	2:B:198:HIS:HB3	2.12	0.49
1:A:320:ASP:C	1:A:322:SER:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:CYS:C	2:B:282:LEU:N	2.70	0.49
1:A:43:LYS:HA	1:A:43:LYS:CE	2.38	0.49
1:A:252:TRP:CE3	1:A:256:ASP:HB3	2.47	0.49
1:A:464:GLN:CG	1:A:465:LYS:N	2.72	0.49
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.47	0.49
1:A:120:LEU:O	1:A:121:ASP:C	2.55	0.49
1:A:277:ARG:NH1	1:A:334:GLN:HB2	2.26	0.49
1:A:280:CYS:O	1:A:281:LYS:C	2.54	0.49
1:A:109:LEU:HB2	1:A:187:LEU:HB2	1.96	0.48
1:A:181:TYR:CD2	3:A:601:RT3:H10	2.48	0.48
1:A:195:ILE:HG12	1:A:199:ARG:HH21	1.78	0.48
1:A:424:LYS:NZ	1:A:426:TRP:CE2	2.81	0.48
1:A:424:LYS:NZ	1:A:426:TRP:CZ2	2.80	0.48
2:B:85:GLN:HA	2:B:88:TRP:CD1	2.48	0.48
2:B:273:GLY:C	2:B:274:ILE:O	2.55	0.48
2:B:422:LEU:O	2:B:423:VAL:C	2.56	0.48
1:A:11:LYS:HE2	1:A:11:LYS:HB3	1.47	0.48
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.95	0.48
1:A:170:PRO:O	1:A:173:LYS:N	2.46	0.48
1:A:219:LYS:O	1:A:220:LYS:CB	2.61	0.48
1:A:344:GLU:O	1:A:345:PRO:C	2.56	0.48
2:B:301:LEU:HD23	2:B:305:GLU:OE1	2.12	0.48
2:B:362:THR:CG2	2:B:367:GLN:OE1	2.61	0.48
1:A:13:LYS:O	1:A:16:MET:HB2	2.13	0.48
1:A:350:LYS:CE	1:A:378:GLU:OE2	2.58	0.48
2:B:175:ASN:HD21	2:B:201:LYS:HZ2	1.61	0.48
2:B:246:LEU:CD2	2:B:260:LEU:HD21	2.43	0.48
1:A:43:LYS:HE2	1:A:43:LYS:CA	2.41	0.48
1:A:278:GLN:HB2	1:A:302:GLU:CG	2.44	0.48
1:A:109:LEU:O	1:A:187:LEU:N	2.41	0.48
1:A:454:LYS:HA	1:A:467:VAL:O	2.14	0.48
1:A:542:ILE:HG22	1:A:543:GLY:N	2.29	0.48
2:B:389:PHE:HB3	2:B:391:LEU:HD21	1.95	0.48
1:A:72:ARG:HH11	1:A:72:ARG:CG	2.27	0.48
2:B:304:ALA:O	2:B:308:GLU:N	2.35	0.48
1:A:52:PRO:N	1:A:53:GLU:OE1	2.47	0.48
2:B:65:LYS:NZ	2:B:72:ARG:HE	2.12	0.48
2:B:324:ASP:O	2:B:343:GLN:HG2	2.14	0.48
2:B:334:GLN:O	2:B:336:GLN:HG3	2.13	0.48
1:A:70:LYS:HZ3	1:A:72:ARG:NH1	2.11	0.48
1:A:337:TRP:NE1	1:A:367:GLN:OE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:LYS:NZ	2:B:85:GLN:HG2	2.29	0.47
2:B:82:LYS:HE3	2:B:413:GLU:OE2	2.14	0.47
1:A:93:GLY:HA3	2:B:137:ASN:CG	2.39	0.47
1:A:205:LEU:HD13	1:A:209:LEU:CD1	2.44	0.47
1:A:467:VAL:CG1	1:A:468:THR:H	2.27	0.47
2:B:376:THR:HG21	2:B:410:TRP:CH2	2.49	0.47
2:B:307:ARG:O	2:B:308:GLU:C	2.56	0.47
1:A:88:TRP:O	1:A:89:GLU:C	2.57	0.47
1:A:369:THR:CG2	1:A:398:TRP:CH2	2.96	0.47
1:A:466:VAL:CG1	1:A:467:VAL:N	2.77	0.47
1:A:296:THR:O	1:A:300:GLU:CG	2.62	0.47
2:B:54:ASN:HD21	2:B:126:LYS:CA	2.28	0.47
2:B:209:LEU:HD12	2:B:209:LEU:HA	1.76	0.47
1:A:170:PRO:C	1:A:174:GLN:HE21	2.23	0.47
1:A:357:MET:O	1:A:357:MET:CG	2.57	0.47
1:A:401:TRP:HB2	1:A:425:LEU:HD21	1.96	0.47
1:A:426:TRP:HE3	1:A:526:ILE:HD13	1.79	0.47
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.50	0.47
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.61	0.47
1:A:75:VAL:HG11	1:A:77:PHE:CZ	2.50	0.47
1:A:283:LEU:O	1:A:286:THR:HB	2.14	0.47
1:A:410:TRP:O	1:A:410:TRP:CG	2.63	0.47
2:B:271:TYR:HB2	2:B:274:ILE:HD11	1.94	0.47
1:A:320:ASP:C	1:A:320:ASP:OD1	2.57	0.47
2:B:344:GLU:O	2:B:347:LYS:HD3	2.15	0.47
1:A:520:GLN:C	1:A:522:ILE:N	2.72	0.47
2:B:199:ARG:HH11	2:B:233:GLU:CD	2.23	0.47
1:A:24:TRP:CG	1:A:25:PRO:CD	2.98	0.46
1:A:110:ASP:C	1:A:111:VAL:CG2	2.88	0.46
1:A:270:ILE:HA	1:A:351:THR:HG23	1.95	0.46
2:B:306:ASN:O	2:B:310:LEU:HB2	2.15	0.46
2:B:354:TYR:HD2	2:B:374:LYS:HZ2	1.60	0.46
1:A:94:ILE:C	1:A:94:ILE:CD1	2.89	0.46
1:A:234:LEU:HD12	3:A:601:RT3:H8	1.98	0.46
2:B:253:THR:HG23	2:B:254:VAL:N	2.29	0.46
2:B:309:ILE:C	2:B:312:GLU:HG2	2.40	0.46
2:B:65:LYS:C	2:B:407:GLN:HG2	2.40	0.46
1:A:63:ILE:HD12	1:A:72:ARG:CG	2.45	0.46
1:A:175:ASN:HD21	1:A:201:LYS:HE2	1.72	0.46
1:A:438:GLU:HG3	1:A:461:ARG:HG2	1.98	0.46
2:B:238:LYS:HB2	2:B:238:LYS:HE2	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PHE:O	1:A:171:PHE:CD1	2.69	0.46
1:A:450:THR:O	1:A:451:LYS:CB	2.63	0.46
1:A:479:LEU:HD12	1:A:479:LEU:HA	1.57	0.46
2:B:273:GLY:O	2:B:274:ILE:C	2.57	0.46
2:B:314:VAL:HG12	2:B:317:VAL:HG23	1.97	0.46
1:A:107:THR:CG2	1:A:202:ILE:CD1	2.69	0.46
1:A:121:ASP:C	1:A:121:ASP:OD1	2.57	0.46
1:A:122:GLU:C	1:A:124:PHE:N	2.71	0.46
1:A:406:TRP:CE3	1:A:407:GLN:CB	2.96	0.46
2:B:330:GLN:CD	2:B:340:GLN:HE22	2.24	0.46
1:A:176:PRO:C	1:A:178:ILE:H	2.24	0.46
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.50	0.46
1:A:468:THR:O	1:A:469:LEU:HG	2.16	0.46
1:A:194:GLU:C	1:A:196:GLY:N	2.74	0.46
2:B:266:TRP:CZ2	2:B:427:TYR:CZ	3.03	0.46
2:B:309:ILE:HA	2:B:312:GLU:CG	2.45	0.46
1:A:202:ILE:O	1:A:205:LEU:HB3	2.16	0.46
1:A:242:GLN:O	1:A:243:PRO:C	2.58	0.46
1:A:491:LEU:H	1:A:491:LEU:CD1	2.28	0.46
1:A:94:ILE:O	1:A:94:ILE:CD1	2.47	0.46
1:A:102:LYS:HA	3:A:601:RT3:O29	2.16	0.46
1:A:410:TRP:CZ3	2:B:363:ASN:CB	2.92	0.46
2:B:209:LEU:CB	2:B:214:LEU:HB2	2.41	0.45
2:B:305:GLU:HA	2:B:308:GLU:HB2	1.98	0.45
2:B:330:GLN:HE22	2:B:340:GLN:CD	2.22	0.45
1:A:5:ILE:HG22	1:A:212:TRP:HE3	1.80	0.45
1:A:168:LEU:O	1:A:169:GLU:C	2.58	0.45
1:A:296:THR:CG2	1:A:297:GLU:N	2.76	0.45
1:A:374:LYS:C	1:A:374:LYS:CD	2.88	0.45
2:B:23:GLN:OE1	2:B:60:VAL:N	2.49	0.45
1:A:64:LYS:HD3	1:A:71:TRP:CE2	2.52	0.45
1:A:99:GLY:HA3	2:B:136:ASN:ND2	2.32	0.45
1:A:244:ILE:HG22	1:A:246:LEU:HD23	1.98	0.45
2:B:423:VAL:O	2:B:427:TYR:HD2	2.00	0.45
1:A:5:ILE:HG22	1:A:212:TRP:CE3	2.52	0.45
1:A:105:SER:HG	1:A:198:HIS:CD2	2.34	0.45
1:A:538:ALA:C	1:A:540:LYS:H	2.24	0.45
2:B:85:GLN:O	2:B:85:GLN:HG3	2.13	0.45
2:B:243:PRO:CB	2:B:311:LYS:HA	2.45	0.45
2:B:277:ARG:NH1	2:B:277:ARG:CB	2.79	0.45
1:A:492:GLU:O	1:A:493:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:TRP:CD2	2:B:422:LEU:HD13	2.52	0.45
2:B:66:LYS:N	2:B:407:GLN:HG2	2.32	0.45
2:B:356:ARG:HG3	2:B:356:ARG:O	2.17	0.45
1:A:181:TYR:CB	3:A:601:RT3:H15	2.44	0.45
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.52	0.45
2:B:156:SER:N	2:B:157:PRO:CD	2.80	0.45
1:A:460:ASN:C	1:A:462:GLY:H	2.25	0.45
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.51	0.45
2:B:241:VAL:HG11	2:B:311:LYS:O	2.17	0.45
2:B:248:GLU:O	2:B:249:LYS:CB	2.64	0.45
1:A:296:THR:CG2	1:A:298:GLU:N	2.80	0.45
1:A:325:LEU:HB3	1:A:387:PRO:HB3	1.99	0.45
2:B:320:ASP:OD2	2:B:323:LYS:HG3	2.17	0.45
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.99	0.45
1:A:17:ASP:O	1:A:18:GLY:O	2.35	0.44
1:A:63:ILE:CD1	1:A:72:ARG:CD	2.94	0.44
1:A:172:ARG:O	1:A:175:ASN:N	2.47	0.44
1:A:228:LEU:CD2	1:A:228:LEU:H	2.07	0.44
1:A:330:GLN:HE22	1:A:340:GLN:NE2	2.07	0.44
1:A:489:SER:CB	1:A:493:VAL:CG2	2.68	0.44
2:B:120:LEU:HD23	2:B:120:LEU:HA	1.73	0.44
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.47	0.44
2:B:205:LEU:HD22	2:B:205:LEU:O	2.18	0.44
1:A:3:SER:HA	1:A:212:TRP:O	2.17	0.44
1:A:11:LYS:O	1:A:85:GLN:HB3	2.16	0.44
1:A:13:LYS:HA	1:A:14:PRO:HD2	1.79	0.44
1:A:41:MET:HE2	1:A:47:ILE:CD1	2.45	0.44
1:A:236:PRO:HA	3:A:601:RT3:C16	2.48	0.44
2:B:41:MET:HE3	2:B:116:PHE:CE1	2.52	0.44
2:B:65:LYS:HA	2:B:407:GLN:CG	2.33	0.44
2:B:298:GLU:N	2:B:298:GLU:OE2	2.39	0.44
2:B:365:VAL:O	2:B:366:LYS:C	2.61	0.44
2:B:422:LEU:HB3	2:B:426:TRP:CE2	2.52	0.44
1:A:195:ILE:HG23	1:A:199:ARG:NH2	2.32	0.44
1:A:466:VAL:C	1:A:467:VAL:CG2	2.91	0.44
1:A:40:GLU:O	1:A:43:LYS:HB2	2.17	0.44
1:A:96:HIS:O	1:A:97:PRO:C	2.58	0.44
1:A:122:GLU:C	1:A:124:PHE:H	2.26	0.44
1:A:171:PHE:O	1:A:175:ASN:HB2	2.18	0.44
2:B:278:GLN:HE21	2:B:278:GLN:CA	2.27	0.44
1:A:37:ILE:O	1:A:40:GLU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:O	1:A:543:GLY:C	2.60	0.44
2:B:309:ILE:CA	2:B:312:GLU:HG2	2.47	0.44
1:A:131:THR:HG23	1:A:143:ARG:HG2	2.00	0.44
1:A:277:ARG:HE	1:A:277:ARG:HB3	1.05	0.44
2:B:295:LEU:O	2:B:297:GLU:OE2	2.36	0.44
2:B:298:GLU:C	2:B:300:GLU:N	2.74	0.44
2:B:344:GLU:O	2:B:345:PRO:O	2.36	0.44
1:A:8:VAL:HB	1:A:159:ILE:HD13	1.99	0.44
1:A:89:GLU:HB2	1:A:92:LEU:HD22	2.00	0.44
1:A:439:THR:HG21	1:A:441:TYR:CE1	2.53	0.44
1:A:502:ALA:O	1:A:506:ILE:HD12	2.18	0.44
2:B:253:THR:HG21	2:B:255:ASN:HB2	2.00	0.44
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.99	0.44
1:A:236:PRO:HA	3:A:601:RT3:C21	2.48	0.44
2:B:246:LEU:HD22	2:B:260:LEU:HD21	1.99	0.44
2:B:330:GLN:HE22	2:B:340:GLN:NE2	2.16	0.44
1:A:103:LYS:HA	1:A:192:ASP:OD2	2.18	0.43
1:A:500:GLN:HE21	1:A:500:GLN:HB3	1.67	0.43
2:B:279:LEU:O	2:B:282:LEU:HB2	2.17	0.43
1:A:46:LYS:HE3	1:A:116:PHE:HB3	1.99	0.43
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.98	0.43
1:A:419:THR:HA	1:A:420:PRO:HD3	1.85	0.43
1:A:426:TRP:CE3	1:A:526:ILE:HD13	2.53	0.43
1:A:429:LEU:HD21	1:A:506:ILE:HG22	1.99	0.43
2:B:422:LEU:CB	2:B:426:TRP:CZ2	3.00	0.43
1:A:92:LEU:HD12	1:A:92:LEU:HA	1.51	0.43
1:A:170:PRO:O	1:A:171:PHE:C	2.61	0.43
1:A:303:LEU:O	1:A:303:LEU:HD23	2.18	0.43
1:A:375:ILE:O	1:A:379:SER:HB2	2.18	0.43
1:A:535:TRP:C	1:A:536:VAL:CG1	2.91	0.43
2:B:13:LYS:HE3	2:B:85:GLN:CB	2.48	0.43
2:B:400:THR:HG1	2:B:401:TRP:CD1	2.36	0.43
1:A:48:SER:O	1:A:144:TYR:HA	2.18	0.43
1:A:95:PRO:HA	2:B:136:ASN:O	2.19	0.43
1:A:542:ILE:HG23	1:A:543:GLY:H	1.84	0.43
2:B:88:TRP:CZ3	2:B:154:LYS:HD3	2.53	0.43
2:B:105:SER:O	2:B:190:GLY:HA2	2.18	0.43
2:B:310:LEU:HD12	2:B:310:LEU:HA	1.81	0.43
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.64	0.43
1:A:475:GLN:HG2	1:A:501:TYR:CZ	2.53	0.43
1:A:339:TYR:CE1	1:A:352:GLY:HA3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:THR:O	2:B:28:GLU:C	2.62	0.43
2:B:64:LYS:O	2:B:65:LYS:CB	2.66	0.43
2:B:420:PRO:HB2	2:B:423:VAL:HG23	2.01	0.43
1:A:153:TRP:CD1	1:A:154:LYS:H	2.37	0.43
1:A:206:ARG:CZ	1:A:218:ASP:CB	2.96	0.43
1:A:320:ASP:C	1:A:322:SER:N	2.77	0.43
2:B:274:ILE:HD13	2:B:274:ILE:N	2.33	0.43
1:A:44:GLU:C	1:A:46:LYS:H	2.26	0.43
1:A:175:ASN:HB3	1:A:178:ILE:HG13	2.01	0.43
2:B:6:GLU:OE1	2:B:6:GLU:O	2.37	0.43
2:B:330:GLN:NE2	2:B:340:GLN:HE22	2.17	0.43
2:B:425:LEU:HD23	2:B:425:LEU:H	1.81	0.43
1:A:171:PHE:CD1	1:A:171:PHE:C	2.97	0.43
2:B:202:ILE:HD13	2:B:202:ILE:HA	1.85	0.43
1:A:1:PRO:HD2	1:A:215:THR:CG2	2.49	0.42
1:A:48:SER:C	1:A:144:TYR:HD1	2.26	0.42
1:A:279:LEU:HD23	1:A:302:GLU:OE1	2.19	0.42
1:A:505:ILE:O	1:A:510:PRO:CG	2.67	0.42
2:B:325:LEU:HD12	2:B:385:LYS:HG2	2.01	0.42
1:A:325:LEU:HD11	1:A:383:TRP:CD2	2.54	0.42
2:B:368:LEU:O	2:B:372:VAL:HG23	2.19	0.42
1:A:70:LYS:HZ1	1:A:72:ARG:NH1	2.16	0.42
1:A:430:GLU:HB2	1:A:532:TYR:CB	2.44	0.42
1:A:34:LEU:O	1:A:35:VAL:C	2.62	0.42
2:B:54:ASN:HD21	2:B:126:LYS:HA	1.83	0.42
2:B:169:GLU:C	2:B:169:GLU:CD	2.87	0.42
2:B:261:VAL:O	2:B:262:GLY:C	2.63	0.42
2:B:332:GLN:O	2:B:336:GLN:OE1	2.37	0.42
1:A:8:VAL:CG1	1:A:159:ILE:HD13	2.50	0.42
1:A:108:VAL:HG22	1:A:188:TYR:CE2	2.53	0.42
2:B:87:PHE:HZ	2:B:159:ILE:HG13	1.83	0.42
2:B:298:GLU:C	2:B:301:LEU:H	2.27	0.42
2:B:308:GLU:O	2:B:311:LYS:HE3	2.19	0.42
1:A:1:PRO:HD3	1:A:215:THR:HG21	2.02	0.42
1:A:169:GLU:HB3	1:A:170:PRO:HD2	2.02	0.42
1:A:426:TRP:O	1:A:427:TYR:HB3	2.20	0.42
1:A:520:GLN:O	1:A:521:ILE:C	2.60	0.42
1:A:396:GLU:HA	1:A:399:GLU:HG2	2.02	0.42
2:B:276:VAL:HG13	2:B:277:ARG:N	2.35	0.42
1:A:5:ILE:CG1	1:A:6:GLU:N	2.82	0.42
1:A:183:TYR:CE2	1:A:184:MET:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLU:O	1:A:204:GLU:HG2	2.19	0.42
1:A:220:LYS:CD	1:A:221:HIS:CD2	3.01	0.42
1:A:395:LYS:HE2	1:A:414:TRP:CZ3	2.55	0.42
1:A:91:GLN:HG3	1:A:93:GLY:O	2.20	0.42
1:A:244:ILE:HG22	1:A:246:LEU:CD2	2.50	0.42
2:B:168:LEU:HD13	2:B:180:ILE:HG21	2.01	0.42
2:B:277:ARG:CB	2:B:277:ARG:CZ	2.98	0.42
2:B:374:LYS:O	2:B:377:THR:HG23	2.20	0.42
1:A:253:THR:HA	1:A:291:GLU:O	2.20	0.41
1:A:486:LEU:C	1:A:524:GLN:HE21	2.28	0.41
2:B:103:LYS:CE	2:B:179:VAL:HG23	2.46	0.41
2:B:293:ILE:HA	2:B:294:PRO:HD2	1.81	0.41
1:A:167:ILE:HD12	1:A:214:LEU:CD1	2.49	0.41
2:B:253:THR:HG22	2:B:254:VAL:N	2.35	0.41
1:A:8:VAL:HG11	1:A:159:ILE:HD13	2.02	0.41
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.56	0.41
1:A:72:ARG:HB3	1:A:72:ARG:HH11	1.79	0.41
1:A:170:PRO:C	1:A:172:ARG:N	2.77	0.41
1:A:424:LYS:CE	1:A:426:TRP:CZ2	3.03	0.41
1:A:528:LYS:HA	1:A:528:LYS:HD2	1.79	0.41
2:B:278:GLN:HB2	2:B:302:GLU:CD	2.44	0.41
1:A:121:ASP:OD1	1:A:122:GLU:N	2.54	0.41
1:A:395:LYS:HE2	1:A:414:TRP:CZ2	2.56	0.41
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.56	0.41
2:B:65:LYS:HZ3	2:B:72:ARG:HE	1.68	0.41
2:B:195:ILE:HG23	2:B:196:GLY:N	2.35	0.41
2:B:363:ASN:OD1	2:B:366:LYS:CB	2.68	0.41
1:A:3:SER:HA	1:A:4:PRO:HD2	1.86	0.41
1:A:317:VAL:HG23	1:A:318:TYR:O	2.20	0.41
1:A:487:GLN:HA	1:A:524:GLN:NE2	2.35	0.41
1:A:519:ASN:HA	1:A:522:ILE:HD12	2.03	0.41
1:A:21:VAL:CG1	1:A:59:PRO:CD	2.99	0.41
1:A:63:ILE:HD11	1:A:72:ARG:CD	2.47	0.41
1:A:406:TRP:C	1:A:406:TRP:HE3	2.27	0.41
1:A:509:GLN:O	1:A:510:PRO:C	2.61	0.41
2:B:7:THR:HG22	2:B:119:PRO:HB2	2.02	0.41
2:B:330:GLN:HE22	2:B:340:GLN:HE22	1.68	0.41
1:A:278:GLN:HB2	1:A:302:GLU:HG3	2.03	0.41
1:A:342:TYR:CA	1:A:349:LEU:HD12	2.44	0.41
2:B:183:TYR:OH	2:B:386:THR:CG2	2.68	0.41
2:B:239:TRP:O	2:B:240:THR:CG2	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:LYS:HG3	2:B:426:TRP:HA	2.01	0.41
1:A:276:VAL:O	1:A:276:VAL:CG1	2.69	0.41
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.47	0.41
1:A:512:GLN:O	1:A:512:GLN:HG2	2.19	0.41
1:A:522:ILE:O	1:A:526:ILE:HG13	2.21	0.41
1:A:103:LYS:HG3	3:A:601:RT3:H113	2.03	0.41
1:A:210:LEU:O	1:A:211:ARG:C	2.64	0.41
1:A:244:ILE:HD11	1:A:267:ALA:HB2	1.99	0.41
1:A:542:ILE:HG23	2:B:283:LEU:HB3	2.01	0.41
2:B:32:LYS:O	2:B:33:ALA:C	2.64	0.41
2:B:99:GLY:O	2:B:100:LEU:C	2.64	0.41
2:B:275:LYS:HB3	2:B:302:GLU:OE2	2.20	0.41
2:B:425:LEU:O	2:B:426:TRP:C	2.63	0.41
1:A:230:MET:HE2	1:A:230:MET:HB2	1.91	0.41
1:A:275:LYS:O	1:A:276:VAL:HG23	2.21	0.41
1:A:489:SER:O	1:A:490:GLY:O	2.38	0.41
2:B:63:ILE:HD13	2:B:74:LEU:CD2	2.44	0.41
1:A:21:VAL:HG13	1:A:59:PRO:CD	2.46	0.40
1:A:122:GLU:O	1:A:124:PHE:N	2.54	0.40
1:A:459:THR:OG1	1:A:460:ASN:N	2.54	0.40
2:B:253:THR:HG22	2:B:255:ASN:CA	2.48	0.40
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.75	0.40
1:A:233:GLU:HB3	1:A:240:THR:CG2	2.50	0.40
1:A:282:LEU:HA	1:A:282:LEU:HD23	1.85	0.40
1:A:479:LEU:HB3	1:A:517:LEU:HD21	2.02	0.40
2:B:65:LYS:NZ	2:B:72:ARG:NE	2.68	0.40
2:B:201:LYS:HA	2:B:201:LYS:HD3	1.90	0.40
2:B:261:VAL:HG23	2:B:276:VAL:HG21	2.03	0.40
1:A:40:GLU:OE1	1:A:40:GLU:HA	2.22	0.40
1:A:169:GLU:CB	1:A:170:PRO:CD	2.99	0.40
1:A:174:GLN:O	1:A:175:ASN:CG	2.65	0.40
1:A:333:GLY:O	1:A:334:GLN:C	2.65	0.40
2:B:13:LYS:CE	2:B:85:GLN:HG2	2.51	0.40
2:B:162:SER:O	2:B:166:LYS:CE	2.63	0.40
2:B:166:LYS:O	2:B:167:ILE:C	2.62	0.40
1:A:215:THR:C	1:A:216:THR:HG23	2.47	0.40
1:A:406:TRP:CH2	2:B:418:ASN:OD1	2.68	0.40
2:B:51:GLY:O	2:B:53:GLU:N	2.54	0.40
2:B:280:CYS:C	2:B:282:LEU:H	2.28	0.40
2:B:350:LYS:HG3	2:B:351:THR:H	1.87	0.40
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:CG	1:A:448:ARG:HH11	2.34	0.40
1:A:509:GLN:N	1:A:510:PRO:HD3	2.36	0.40
2:B:24:TRP:HE3	2:B:25:PRO:HD2	1.87	0.40
2:B:193:LEU:C	2:B:194:GLU:O	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	543/563 (96%)	442 (81%)	72 (13%)	29 (5%)	1	8
2	B	399/443 (90%)	331 (83%)	47 (12%)	21 (5%)	1	8
All	All	942/1006 (94%)	773 (82%)	119 (13%)	50 (5%)	1	8

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	90	VAL
1	A	195	ILE
1	A	345	PRO
1	A	356	ARG
1	A	410	TRP
1	A	491	LEU
2	B	85	GLN
2	B	237	ASP
2	B	241	VAL
2	B	242	GLN
2	B	269	GLN
2	B	274	ILE
2	B	284	ARG

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Mol	Chain	Res	Type
2	B	333	GLY
1	A	18	GLY
1	A	114	ALA
1	A	171	PHE
1	A	196	GLY
1	A	211	ARG
1	A	276	VAL
1	A	346	PHE
1	A	490	GLY
1	A	528	LYS
1	A	543	GLY
2	B	114	ALA
2	B	249	LYS
2	B	281	LYS
2	B	324	ASP
2	B	426	TRP
1	A	3	SER
1	A	6	GLU
1	A	135	ILE
1	A	539	HIS
2	B	236	PRO
2	B	308	GLU
1	A	66	LYS
1	A	89	GLU
1	A	243	PRO
1	A	312	GLU
1	A	334	GLN
2	B	294	PRO
2	B	423	VAL
2	B	214	LEU
2	B	303	LEU
1	A	170	PRO
1	A	287	LYS
2	B	419	THR
2	B	18	GLY
1	A	246	LEU

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	486/503 (97%)	391 (80%)	95 (20%)	1	7
2	B	369/403 (92%)	301 (82%)	68 (18%)	1	8
All	All	855/906 (94%)	692 (81%)	163 (19%)	1	7

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	7	THR
1	A	11	LYS
1	A	21	VAL
1	A	26	LEU
1	A	37	ILE
1	A	42	GLU
1	A	43	LYS
1	A	54	ASN
1	A	63	ILE
1	A	64	LYS
1	A	69	THR
1	A	72	ARG
1	A	73	LYS
1	A	80	LEU
1	A	92	LEU
1	A	101	LYS
1	A	105	SER
1	A	106	VAL
1	A	107	THR
1	A	118	VAL
1	A	126	LYS
1	A	132	ILE
1	A	135	ILE
1	A	136	ASN
1	A	137	ASN
1	A	139	THR
1	A	159	ILE
1	A	161	GLN
1	A	166	LYS
1	A	173	LYS
1	A	174	GLN
1	A	178	ILE

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Mol	Chain	Res	Type
1	A	179	VAL
1	A	187	LEU
1	A	194	GLU
1	A	195	ILE
1	A	197	GLN
1	A	215	THR
1	A	219	LYS
1	A	220	LYS
1	A	222	GLN
1	A	228	LEU
1	A	238	LYS
1	A	245	VAL
1	A	246	LEU
1	A	248	GLU
1	A	251	SER
1	A	260	LEU
1	A	276	VAL
1	A	277	ARG
1	A	286	THR
1	A	296	THR
1	A	297	GLU
1	A	298	GLU
1	A	303	LEU
1	A	312	GLU
1	A	317	VAL
1	A	341	ILE
1	A	349	LEU
1	A	351	THR
1	A	357	MET
1	A	368	LEU
1	A	373	GLN
1	A	374	LYS
1	A	379	SER
1	A	400	THR
1	A	402	TRP
1	A	403	THR
1	A	409	THR
1	A	411	ILE
1	A	417	VAL
1	A	419	THR
1	A	422	LEU
1	A	425	LEU

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Mol	Chain	Res	Type
1	A	429	LEU
1	A	431	LYS
1	A	434	ILE
1	A	448	ARG
1	A	452	LEU
1	A	459	THR
1	A	461	ARG
1	A	466	VAL
1	A	471	ASP
1	A	475	GLN
1	A	479	LEU
1	A	495	ILE
1	A	496	VAL
1	A	500	GLN
1	A	503	LEU
1	A	509	GLN
1	A	514	GLU
1	A	520	GLN
1	A	528	LYS
1	A	536	VAL
2	B	5	ILE
2	B	6	GLU
2	B	8	VAL
2	B	11	LYS
2	B	22	LYS
2	B	26	LEU
2	B	29	GLU
2	B	39	THR
2	B	48	SER
2	B	60	VAL
2	B	65	LYS
2	B	66	LYS
2	B	68	SER
2	B	72	ARG
2	B	73	LYS
2	B	79	GLU
2	B	80	LEU
2	B	82	LYS
2	B	84	THR
2	B	85	GLN
2	B	91	GLN
2	B	104	LYS

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Mol	Chain	Res	Type
2	B	111	VAL
2	B	113	ASP
2	B	117	SER
2	B	120	LEU
2	B	173	LYS
2	B	178	ILE
2	B	184	MET
2	B	187	LEU
2	B	199	ARG
2	B	205	LEU
2	B	209	LEU
2	B	232	TYR
2	B	233	GLU
2	B	242	GLN
2	B	251	SER
2	B	253	THR
2	B	256	ASP
2	B	261	VAL
2	B	270	ILE
2	B	275	LYS
2	B	278	GLN
2	B	282	LEU
2	B	292	VAL
2	B	295	LEU
2	B	297	GLU
2	B	298	GLU
2	B	300	GLU
2	B	301	LEU
2	B	310	LEU
2	B	323	LYS
2	B	336	GLN
2	B	347	LYS
2	B	349	LEU
2	B	356	ARG
2	B	366	LYS
2	B	367	GLN
2	B	374	LYS
2	B	377	THR
2	B	385	LYS
2	B	386	THR
2	B	390	LYS
2	B	399	GLU

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Mol	Chain	Res	Type
2	B	400	THR
2	B	403	THR
2	B	419	THR
2	B	425	LEU

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

Mol	Chain	Res	Type
1	A	57	ASN
1	A	136	ASN
1	A	147	ASN
1	A	161	GLN
1	A	174	GLN
1	A	175	ASN
1	A	198	HIS
1	A	221	HIS
1	A	235	HIS
1	A	242	GLN
1	A	258	GLN
1	A	330	GLN
1	A	334	GLN
1	A	336	GLN
1	A	407	GLN
1	A	480	GLN
1	A	509	GLN
1	A	512	GLN
1	A	519	ASN
1	A	524	GLN
2	B	96	HIS
2	B	137	ASN
2	B	147	ASN
2	B	161	GLN
2	B	175	ASN
2	B	242	GLN
2	B	278	GLN
2	B	306	ASN
2	B	361	HIS
2	B	373	GLN
2	B	394	GLN
2	B	407	GLN
2	B	418	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand 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$
3	RT3	A	601	-	29,31,31	2.42	6 (20%)	41,45,45	1.93	12 (29%)

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
3	RT3	A	601	-	-	12/18/29/29	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	RT3	C19-S23	-10.49	1.61	1.77
3	A	601	RT3	C3-C4	4.43	1.46	1.40
3	A	601	RT3	C16-C21	4.26	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	RT3	C16-N15	-2.55	1.36	1.41
3	A	601	RT3	C13-S12	-2.25	1.77	1.80
3	A	601	RT3	C21-CL22	2.21	1.78	1.73

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	RT3	O26-S23-O30	-6.39	108.97	118.80
3	A	601	RT3	C3-N2-C11	-4.32	112.96	122.86
3	A	601	RT3	C4-C3-N2	2.84	121.83	118.17
3	A	601	RT3	O26-S23-N29	2.79	111.37	107.35
3	A	601	RT3	O26-S23-C19	2.66	110.35	107.35
3	A	601	RT3	C17-C18-C19	2.64	122.01	119.44
3	A	601	RT3	C6-C5-C4	-2.53	106.39	112.43
3	A	601	RT3	C13-C14-N15	2.27	117.87	114.55
3	A	601	RT3	C16-C21-CL22	2.21	121.92	119.52
3	A	601	RT3	C21-C20-C19	2.20	120.26	118.80
3	A	601	RT3	C8-C9-C10	2.04	120.97	117.96
3	A	601	RT3	C1-N2-C11	2.03	126.08	119.43

There are no chirality outliers.

All (12) torsion outliers are listed below:

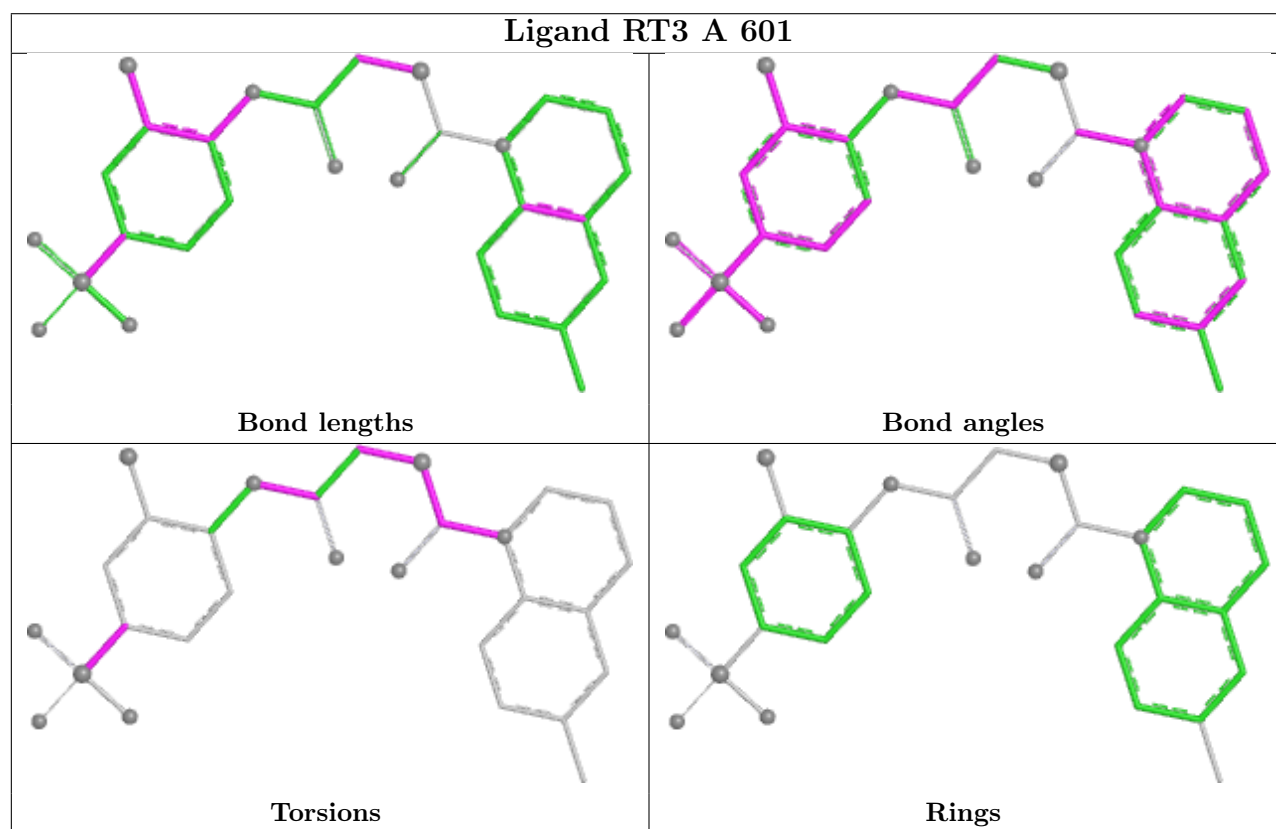
Mol	Chain	Res	Type	Atoms
3	A	601	RT3	O29-C14-N15-C16
3	A	601	RT3	C13-C14-N15-C16
3	A	601	RT3	O28-C11-S12-C13
3	A	601	RT3	N2-C11-S12-C13
3	A	601	RT3	S12-C11-N2-C1
3	A	601	RT3	O28-C11-N2-C3
3	A	601	RT3	C20-C19-S23-N29
3	A	601	RT3	C18-C19-S23-N29
3	A	601	RT3	C20-C19-S23-O30
3	A	601	RT3	C18-C19-S23-O30
3	A	601	RT3	C14-C13-S12-C11
3	A	601	RT3	O28-C11-N2-C1

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	RT3	17	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	545/563 (96%)	0.17	9 (1%) 69 50	44, 71, 91, 113	0
2	B	405/443 (91%)	0.22	19 (4%) 36 22	45, 64, 108, 114	0
All	All	950/1006 (94%)	0.19	28 (2%) 53 35	44, 69, 104, 114	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	426	TRP	3.8
2	B	295	LEU	3.3
2	B	425	LEU	3.1
2	B	5	ILE	3.0
1	A	114	ALA	3.0
2	B	270	ILE	2.9
2	B	428	GLN	2.8
1	A	542	ILE	2.7
2	B	276	VAL	2.7
2	B	24	TRP	2.6
1	A	24	TRP	2.4
1	A	91	GLN	2.4
1	A	0	SER	2.4
2	B	421	PRO	2.3
2	B	247	PRO	2.2
1	A	51	GLY	2.2
2	B	424	LYS	2.2
2	B	87	PHE	2.2
2	B	266	TRP	2.1
1	A	2	ILE	2.1
2	B	296	THR	2.1
2	B	423	VAL	2.1
2	B	232	TYR	2.1
2	B	283	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	543	GLY	2.1
2	B	252	TRP	2.1
1	A	356	ARG	2.0
2	B	427	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

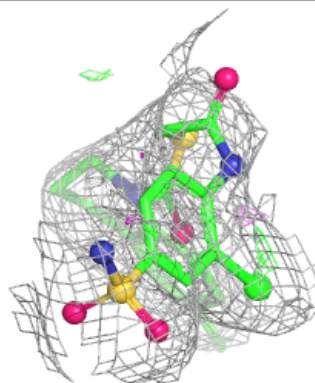
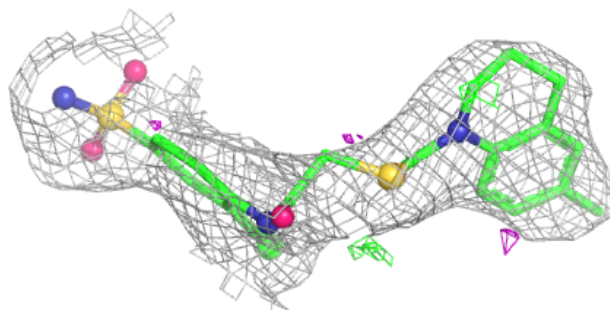
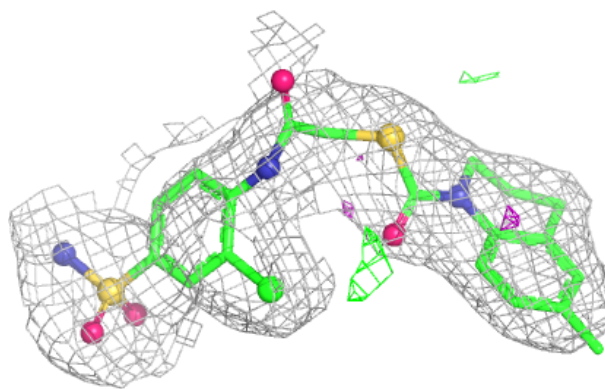
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	RT3	A	601	29/29	0.90	0.16	86,100,107,107	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 RT3 A 601:

$2mF_o-DF_c$ (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.