Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 10:23 AM EDT

PDB ID	:	3C6U
Title	:	Crystal Structure of HIV Reverse Transcriptase in complex with inhibitor 22
Authors	:	Yan, Y.; Prasad, S.
Deposited on	:	2008-02-05
Resolution	:	2.70 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.70 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	Percentile Ranks	Value
Rfree		0.276
Clashscore		40
Ramachandran outliers		2.5%
Sidechain outliers		23.0%
RSRZ outliers		4.7%

Worse   *Better*

▊ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
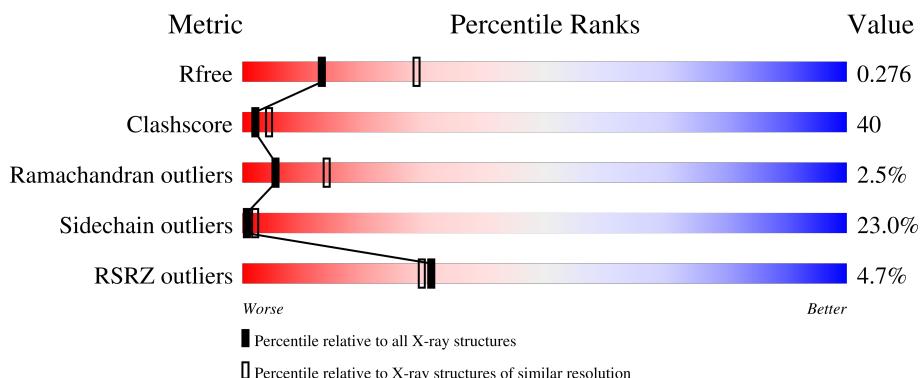
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	563	4% — 39% / 43% / 16% / ••
2	B	443	5% — 36% / 42% / 13% / • / 9%
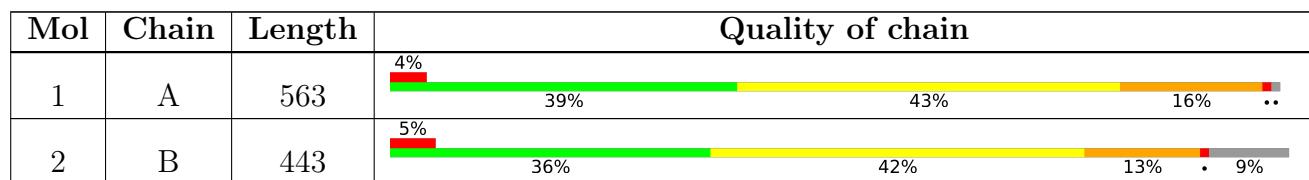
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8289 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total 4542	C 2934	N 760	O 840	S 8	0	0	0

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 Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total 3344	C 2176	N 554	O 608	S 6	0	0	0

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 3-chloro-5-[2-chloro-5-(1H-indazol-3-ylmethoxy)phenoxy]benzonitrile (three-letter code: M22) (formula: $C_{21}H_{13}Cl_2N_3O_2$).

M22
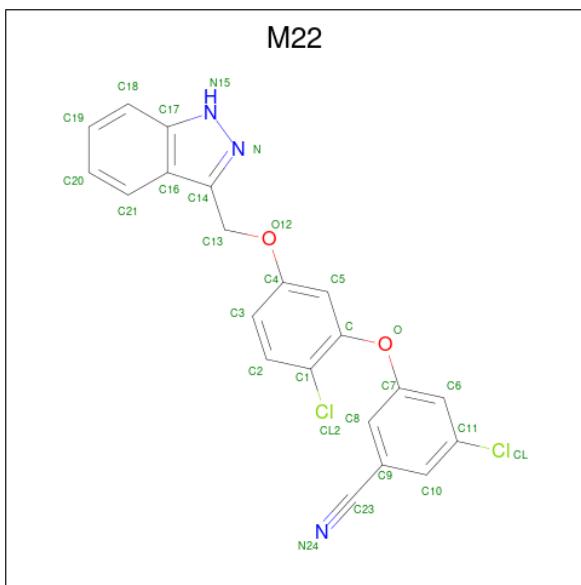
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			28	21	2	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	211	Total	O	0	0
			211	211		
4	B	164	Total	O	0	0
			164	164		

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

Chain A:
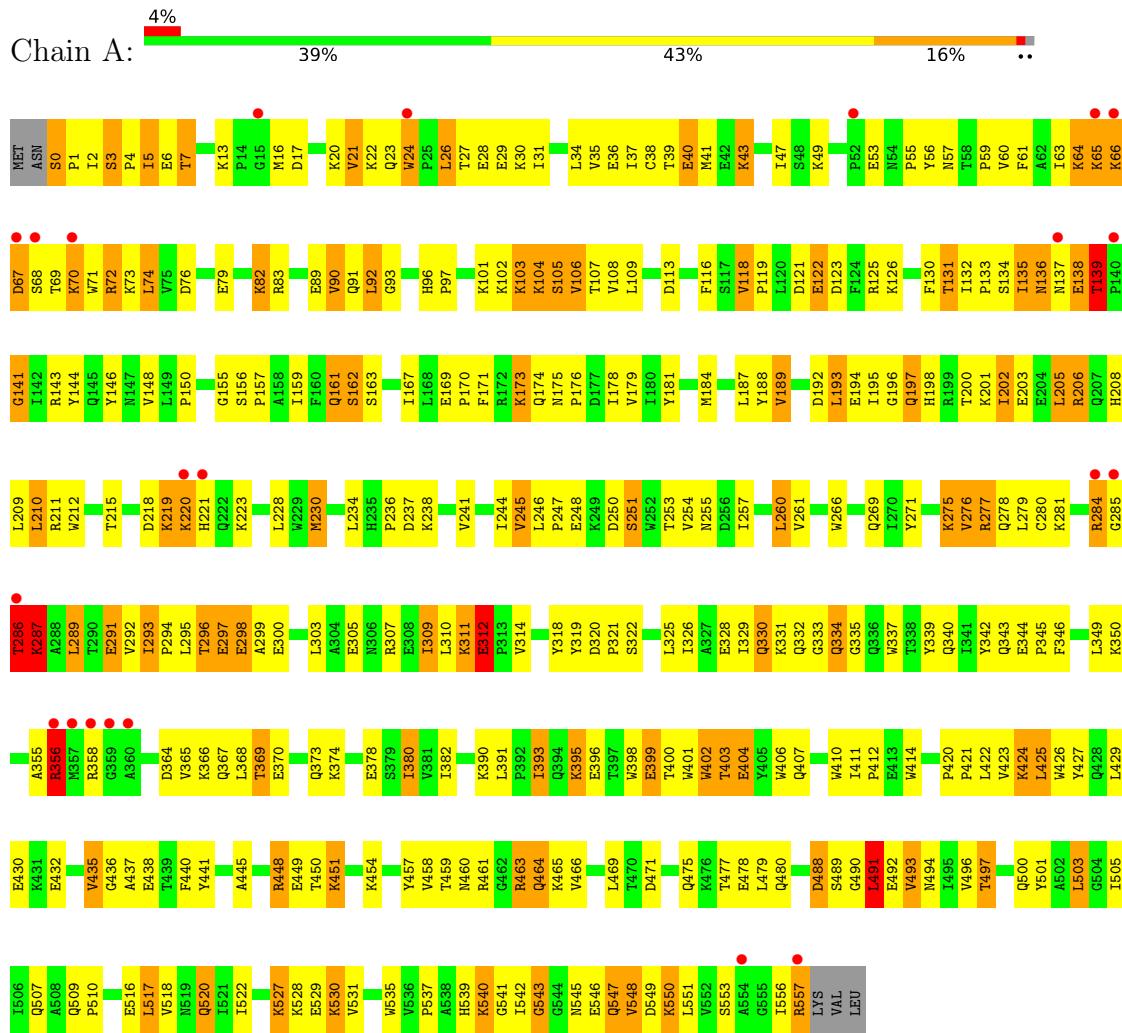
• Molecule 2: Reverse transcriptase

Chain B:
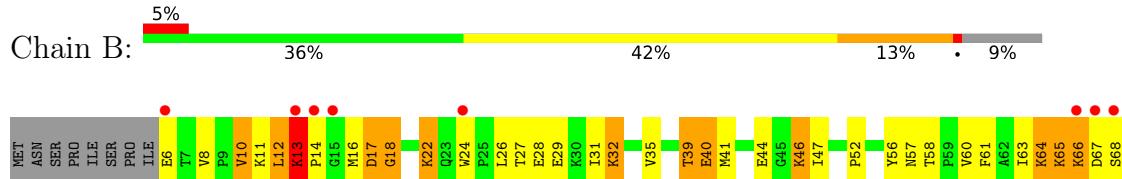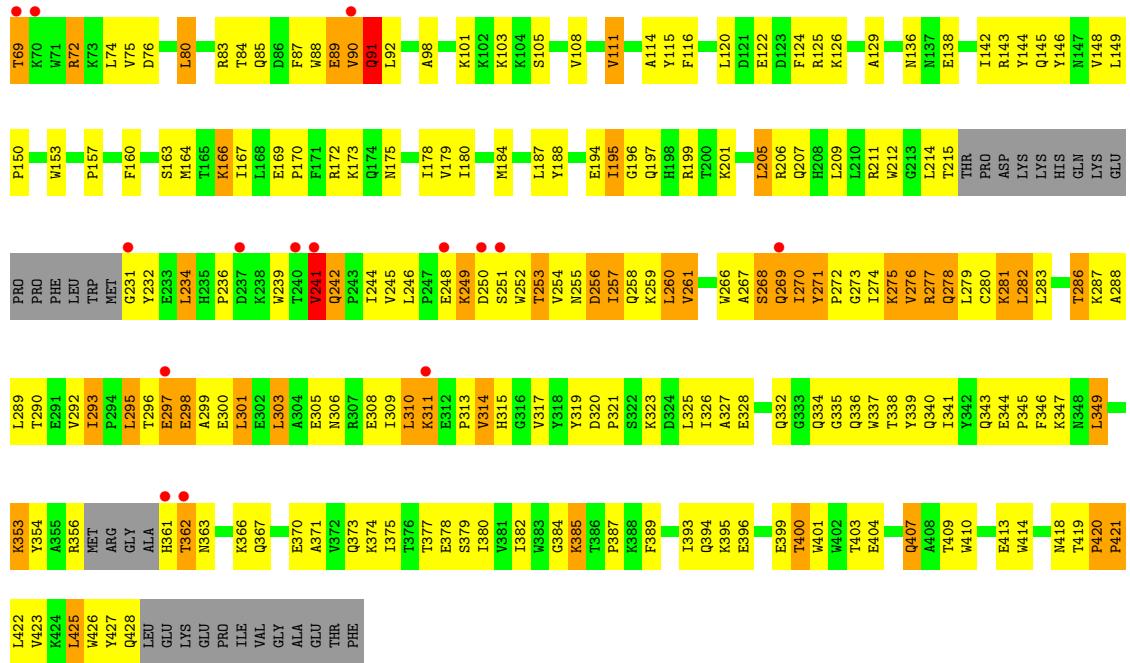
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	118.75Å 154.20Å 156.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.85 – 2.70 17.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	88.1 (17.85-2.70) 88.3 (17.85-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$<I/\sigma(I)>$ [1]	2.09 (at 2.70Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.194 , 0.275 0.200 , 0.276	Depositor DCC
R_{free} test set	1775 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 80.4	EDS
L-test for twinning[2]	$<|L|> = 0.53, <L^2> = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8289	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: M22

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	0.29	0/4659	0.56	0/6330
2	B	0.28	0/3438	0.61	4/4671 (0.1%)
All	All	0.29	0/8097	0.58	4/11001 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	13	LYS	C-N-CD	-11.22	95.91	120.60
2	B	271	TYR	C-N-CD	-5.97	107.47	120.60
2	B	420	PRO	C-N-CD	-5.25	109.05	120.60
2	B	419	THR	C-N-CD	-5.04	109.50	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4542	0	4595	384	0
2	B	3344	0	3369	270	0
3	A	28	0	13	5	0
4	A	211	0	0	14	0
4	B	164	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8289	0	7977	636	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 40.

All (636) 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:13:LYS:HE3	2:B:85:GLN:HB3	1.32	1.11
1:A:255:ASN:HB2	1:A:289:LEU:HD22	1.20	1.09
1:A:287:LYS:HB2	1:A:291:GLU:HG2	1.42	0.99
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.43	0.97
1:A:104:LYS:HG3	1:A:192:ASP:HA	1.48	0.96
1:A:131:THR:HG23	1:A:143:ARG:HD2	1.49	0.95
1:A:403:THR:HG22	1:A:404:GLU:HG2	1.51	0.92
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.53	0.91
1:A:255:ASN:HB2	1:A:289:LEU:CD2	2.02	0.90
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.53	0.88
1:A:143:ARG:HG3	1:A:143:ARG:HH11	1.39	0.87
2:B:125:ARG:HB3	2:B:145:GLN:NE2	1.89	0.87
1:A:5:ILE:HG22	1:A:212:TRP:CE3	2.10	0.87
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.11	0.86
2:B:420:PRO:HB2	2:B:423:VAL:CG2	2.05	0.86
1:A:104:LYS:HG3	1:A:192:ASP:CA	2.05	0.86
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	2.11	0.85
1:A:63:ILE:CG2	1:A:74:LEU:HD11	2.06	0.85
1:A:466:VAL:HG21	1:A:551:LEU:HG	1.58	0.85
1:A:500:GLN:HG3	2:B:422:LEU:HD11	1.60	0.84
2:B:362:THR:HG23	2:B:366:LYS:HG2	1.58	0.84
1:A:26:LEU:HD22	1:A:133:PRO:HG2	1.59	0.83
2:B:362:THR:HG23	2:B:366:LYS:HZ2	1.45	0.82
2:B:422:LEU:HA	2:B:425:LEU:CD2	2.09	0.82
1:A:64:LYS:HZ3	1:A:69:THR:HG23	1.44	0.82
2:B:184:MET:CE	2:B:410:TRP:HB3	2.10	0.82
1:A:287:LYS:HB2	1:A:291:GLU:CG	2.10	0.81
1:A:206:ARG:NH1	1:A:218:ASP:HA	1.96	0.81
1:A:296:THR:HG22	1:A:299:ALA:H	1.44	0.81
1:A:65:LYS:CG	1:A:68:SER:HB3	2.11	0.80
2:B:13:LYS:HE3	2:B:85:GLN:CB	2.11	0.80
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.64	0.80
2:B:371:ALA:O	2:B:375:ILE:HD12	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:LYS:CE	2:B:85:GLN:HB3	2.10	0.80
2:B:279:LEU:HD21	2:B:303:LEU:CD2	2.11	0.80
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.25	0.79
1:A:64:LYS:NZ	1:A:69:THR:HG23	1.98	0.79
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.18	0.78
2:B:125:ARG:HG2	2:B:146:TYR:O	1.82	0.78
2:B:66:LYS:HA	2:B:407:GLN:NE2	1.98	0.78
1:A:277:ARG:O	1:A:281:LYS:HG3	1.83	0.78
2:B:13:LYS:HB2	2:B:16:MET:HE3	1.66	0.78
2:B:373:GLN:O	2:B:377:THR:HG23	1.82	0.77
1:A:7:THR:HG21	1:A:121:ASP:HA	1.66	0.77
2:B:279:LEU:HD21	2:B:303:LEU:HD21	1.64	0.77
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.15	0.77
1:A:206:ARG:HH22	1:A:218:ASP:HB3	1.48	0.77
2:B:366:LYS:O	2:B:370:GLU:HG3	1.83	0.77
1:A:175:ASN:HD21	1:A:201:LYS:CE	1.97	0.77
1:A:70:LYS:NZ	1:A:72:ARG:NH2	2.32	0.76
2:B:362:THR:CG2	2:B:366:LYS:HG2	2.13	0.76
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.21	0.76
1:A:173:LYS:N	1:A:173:LYS:HD2	2.00	0.76
1:A:287:LYS:HD2	1:A:287:LYS:N	1.98	0.76
2:B:254:VAL:O	2:B:258:GLN:HG3	1.85	0.76
2:B:325:LEU:HD12	2:B:385:LYS:HG2	1.67	0.76
2:B:401:TRP:O	2:B:404:GLU:HG2	1.86	0.76
2:B:422:LEU:HA	2:B:425:LEU:HD21	1.67	0.75
1:A:161:GLN:HG3	4:A:643:HOH:O	1.87	0.75
2:B:253:THR:HG23	2:B:289:LEU:O	1.87	0.75
1:A:246:LEU:HD22	1:A:260:LEU:HD21	1.68	0.75
1:A:430:GLU:HG2	1:A:531:VAL:O	1.87	0.75
1:A:489:SER:HB2	1:A:493:VAL:HG11	1.69	0.74
1:A:35:VAL:O	1:A:39:THR:HG23	1.88	0.74
2:B:297:GLU:O	2:B:301:LEU:HD23	1.87	0.74
1:A:241:VAL:CG2	1:A:244:ILE:HD11	2.17	0.74
1:A:175:ASN:HD21	1:A:201:LYS:NZ	1.85	0.73
1:A:516:GLU:O	1:A:520:GLN:HG2	1.88	0.73
1:A:63:ILE:HG23	1:A:74:LEU:HD11	1.70	0.73
1:A:3:SER:OG	1:A:5:ILE:HG23	1.89	0.73
2:B:66:LYS:HA	2:B:407:GLN:HE22	1.51	0.73
1:A:366:LYS:O	1:A:370:GLU:HG3	1.88	0.73
1:A:70:LYS:HZ1	1:A:72:ARG:NH2	1.86	0.73
1:A:125:ARG:HG2	1:A:146:TYR:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:SER:HB2	4:A:758:HOH:O	1.89	0.72
1:A:489:SER:HB2	1:A:493:VAL:CG1	2.18	0.72
2:B:279:LEU:O	2:B:282:LEU:HG	1.89	0.72
1:A:266:TRP:O	1:A:269:GLN:HG3	1.89	0.72
1:A:296:THR:CG2	1:A:299:ALA:H	2.02	0.72
1:A:5:ILE:HG22	1:A:212:TRP:HE3	1.55	0.72
2:B:334:GLN:HG3	4:B:628:HOH:O	1.89	0.72
1:A:458:VAL:HG13	1:A:548:VAL:HG13	1.72	0.71
1:A:31:ILE:O	1:A:35:VAL:HG23	1.90	0.71
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.52	0.70
1:A:65:LYS:HD3	1:A:70:LYS:HG2	1.74	0.70
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.21	0.70
1:A:537:PRO:HB2	1:A:540:LYS:HG2	1.74	0.70
2:B:103:LYS:HE3	2:B:179:VAL:CG2	2.21	0.70
1:A:365:VAL:O	1:A:369:THR:HG23	1.92	0.70
2:B:80:LEU:O	2:B:84:THR:HG23	1.92	0.70
2:B:184:MET:HE2	2:B:410:TRP:HB3	1.73	0.70
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.73	0.69
1:A:466:VAL:CG2	1:A:551:LEU:HG	2.22	0.69
1:A:65:LYS:HG3	1:A:68:SER:HB3	1.73	0.69
1:A:296:THR:HG22	1:A:299:ALA:CB	2.22	0.69
1:A:489:SER:CB	1:A:493:VAL:HG11	2.23	0.69
2:B:298:GLU:O	2:B:301:LEU:HB2	1.93	0.69
1:A:63:ILE:HG21	1:A:74:LEU:HD11	1.73	0.68
2:B:31:ILE:O	2:B:35:VAL:HG23	1.93	0.68
2:B:323:LYS:HB2	2:B:343:GLN:NE2	2.09	0.68
1:A:492:GLU:HG2	1:A:530:LYS:HG3	1.75	0.68
2:B:378:GLU:O	2:B:382:ILE:HG13	1.93	0.68
1:A:65:LYS:HE2	1:A:72:ARG:HH11	1.56	0.68
2:B:184:MET:HE1	2:B:410:TRP:HB3	1.75	0.68
1:A:298:GLU:OE2	1:A:298:GLU:N	2.27	0.68
1:A:356:ARG:NH2	1:A:358:ARG:HD2	2.08	0.68
2:B:268:SER:C	2:B:269:GLN:HG3	2.13	0.68
2:B:344:GLU:HB2	2:B:347:LYS:HD3	1.74	0.68
2:B:395:LYS:HE3	2:B:399:GLU:OE1	1.94	0.68
1:A:175:ASN:HD22	1:A:178:ILE:HD12	1.58	0.68
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.24	0.67
2:B:111:VAL:HG21	2:B:187:LEU:HD22	1.75	0.67
2:B:257:ILE:O	2:B:261:VAL:HG13	1.93	0.67
1:A:369:THR:HG21	1:A:398:TRP:CZ3	2.30	0.67
1:A:134:SER:OG	1:A:139:THR:HB	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:TYR:HB2	1:A:188:TYR:HB2	1.75	0.67
1:A:90:VAL:HG12	1:A:91:GLN:N	2.10	0.67
1:A:70:LYS:HE2	1:A:72:ARG:NE	2.09	0.67
2:B:393:ILE:HG12	2:B:394:GLN:H	1.60	0.67
1:A:20:LYS:HE2	1:A:55:PRO:HB2	1.77	0.67
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.59	0.67
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.44	0.66
1:A:435:VAL:HG23	2:B:290:THR:HG21	1.76	0.66
1:A:441:TYR:O	1:A:548:VAL:HG21	1.95	0.66
1:A:556:ILE:HD13	1:A:556:ILE:N	2.11	0.66
2:B:395:LYS:HG3	2:B:399:GLU:OE1	1.96	0.66
1:A:540:LYS:O	1:A:542:ILE:N	2.26	0.66
2:B:125:ARG:HB3	2:B:145:GLN:HE21	1.60	0.66
1:A:28:GLU:HG2	1:A:135:ILE:CD1	2.26	0.66
1:A:211:ARG:O	1:A:211:ARG:HD3	1.96	0.66
1:A:63:ILE:HD11	1:A:72:ARG:HG3	1.78	0.65
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.26	0.65
2:B:22:LYS:HD3	4:B:554:HOH:O	1.94	0.65
1:A:529:GLU:C	1:A:530:LYS:HG2	2.15	0.65
1:A:104:LYS:CG	1:A:192:ASP:HA	2.25	0.65
1:A:540:LYS:CB	1:A:542:ILE:HD12	2.25	0.65
2:B:13:LYS:HB2	2:B:16:MET:CE	2.27	0.65
2:B:64:LYS:O	2:B:68:SER:HB3	1.96	0.65
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.11	0.65
1:A:319:TYR:O	1:A:321:PRO:HD3	1.96	0.65
2:B:422:LEU:HA	2:B:425:LEU:HD23	1.78	0.65
2:B:344:GLU:CB	2:B:347:LYS:HD3	2.27	0.64
2:B:195:ILE:O	2:B:199:ARG:HG3	1.97	0.64
1:A:448:ARG:HG2	1:A:448:ARG:HH11	1.61	0.64
2:B:66:LYS:HG2	2:B:407:GLN:NE2	2.12	0.64
2:B:245:VAL:HB	4:B:576:HOH:O	1.95	0.64
2:B:10:VAL:HB	2:B:124:PHE:CD1	2.33	0.64
1:A:26:LEU:HD22	1:A:133:PRO:CG	2.27	0.63
2:B:256:ASP:OD2	2:B:256:ASP:N	2.28	0.63
1:A:131:THR:CG2	1:A:143:ARG:HD2	2.24	0.63
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.33	0.63
2:B:377:THR:HG22	2:B:410:TRP:HZ2	1.62	0.63
1:A:175:ASN:ND2	1:A:178:ILE:HD12	2.13	0.63
1:A:500:GLN:HG3	2:B:422:LEU:CD1	2.29	0.63
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.29	0.63
1:A:241:VAL:HG23	1:A:244:ILE:HD11	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LYS:HB2	4:B:605:HOH:O	1.97	0.63
1:A:193:LEU:HB3	1:A:197:GLN:HG3	1.80	0.63
1:A:91:GLN:HG3	1:A:93:GLY:O	1.99	0.62
1:A:490:GLY:O	1:A:492:GLU:N	2.32	0.62
1:A:65:LYS:HB3	1:A:68:SER:C	2.19	0.62
1:A:325:LEU:C	1:A:326:ILE:HD13	2.20	0.62
1:A:325:LEU:O	1:A:326:ILE:HD13	1.99	0.62
1:A:403:THR:CG2	1:A:404:GLU:HG2	2.26	0.62
1:A:337:TRP:NE1	1:A:367:GLN:OE1	2.27	0.62
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.80	0.62
2:B:422:LEU:HB3	2:B:426:TRP:CZ2	2.34	0.62
1:A:63:ILE:CG1	1:A:72:ARG:HG3	2.30	0.62
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.82	0.62
1:A:449:GLU:O	1:A:451:LYS:HE2	1.99	0.62
1:A:436:GLY:HA2	4:A:803:HOH:O	1.98	0.62
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.30	0.62
1:A:400:THR:O	1:A:404:GLU:HG3	1.99	0.61
2:B:105:SER:HB2	4:B:445:HOH:O	2.00	0.61
1:A:437:ALA:HB3	1:A:494:ASN:HD21	1.65	0.61
1:A:143:ARG:HG3	1:A:143:ARG:NH1	2.12	0.61
2:B:250:ASP:O	2:B:251:SER:HB3	2.00	0.61
1:A:118:VAL:HG23	1:A:119:PRO:HD2	1.82	0.61
2:B:206:ARG:HH21	2:B:231:GLY:N	1.99	0.61
1:A:369:THR:HG21	1:A:398:TRP:HZ3	1.65	0.61
2:B:274:ILE:HG23	2:B:306:ASN:ND2	2.16	0.61
1:A:173:LYS:O	1:A:176:PRO:HD3	1.99	0.61
1:A:311:LYS:O	1:A:312:GLU:HB3	2.01	0.61
2:B:404:GLU:HB3	4:B:617:HOH:O	1.99	0.61
2:B:266:TRP:HZ2	2:B:427:TYR:CE2	2.19	0.61
1:A:2:ILE:HD12	1:A:116:PHE:O	2.00	0.60
1:A:13:LYS:O	1:A:16:MET:HB2	2.01	0.60
2:B:206:ARG:NH2	2:B:231:GLY:N	2.49	0.60
1:A:241:VAL:HG21	1:A:244:ILE:HD11	1.83	0.60
1:A:284:ARG:O	1:A:284:ARG:HG3	2.00	0.60
1:A:333:GLY:O	1:A:335:GLY:N	2.33	0.60
2:B:266:TRP:CE3	2:B:426:TRP:HB3	2.35	0.60
2:B:268:SER:O	2:B:270:ILE:N	2.30	0.60
2:B:175:ASN:HB3	2:B:178:ILE:HG13	1.84	0.60
2:B:13:LYS:O	2:B:16:MET:HE3	2.01	0.60
2:B:101:LYS:HG2	4:B:441:HOH:O	2.01	0.60
2:B:108:VAL:CG2	2:B:234:LEU:HD11	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:HB3	2:B:428:GLN:OE1	2.02	0.60
1:A:106:VAL:HA	1:A:189:VAL:O	2.02	0.60
1:A:70:LYS:HG3	1:A:71:TRP:N	2.15	0.60
2:B:260:LEU:O	2:B:260:LEU:HD22	2.02	0.59
1:A:131:THR:HG23	1:A:143:ARG:CD	2.29	0.59
1:A:206:ARG:NH2	1:A:218:ASP:HB3	2.17	0.59
1:A:330:GLN:HE22	1:A:340:GLN:NE2	2.00	0.59
2:B:65:LYS:HG2	4:B:599:HOH:O	2.01	0.59
2:B:114:ALA:HB2	2:B:214:LEU:CD2	2.31	0.59
1:A:37:ILE:O	1:A:41:MET:HG3	2.03	0.59
1:A:553:SER:OG	1:A:557:ARG:NH1	2.34	0.59
1:A:547:GLN:O	1:A:550:LYS:HG3	2.03	0.59
1:A:171:PHE:CD2	1:A:205:LEU:HD23	2.37	0.59
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.85	0.58
1:A:175:ASN:N	1:A:176:PRO:HD3	2.17	0.58
1:A:296:THR:HG21	4:A:565:HOH:O	2.03	0.58
1:A:356:ARG:CZ	1:A:358:ARG:HD2	2.33	0.58
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.38	0.58
2:B:296:THR:HB	2:B:298:GLU:OE2	2.03	0.58
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.85	0.58
1:A:230:MET:HA	1:A:230:MET:HE2	1.85	0.58
1:A:373:GLN:HE22	2:B:401:TRP:HE1	1.49	0.58
1:A:64:LYS:HZ3	1:A:69:THR:HA	1.67	0.58
1:A:102:LYS:HZ1	1:A:237:ASP:HB3	1.69	0.58
1:A:540:LYS:HB2	1:A:542:ILE:HD12	1.85	0.58
2:B:278:GLN:HE22	2:B:281:LYS:NZ	2.02	0.57
2:B:298:GLU:CD	2:B:298:GLU:H	2.05	0.57
1:A:53:GLU:H	1:A:53:GLU:CD	2.07	0.57
2:B:6:GLU:HG2	2:B:6:GLU:O	2.02	0.57
2:B:12:LEU:HD23	2:B:17:ASP:HA	1.86	0.57
2:B:64:LYS:O	2:B:65:LYS:HB2	2.03	0.57
1:A:296:THR:HG22	1:A:299:ALA:N	2.18	0.57
1:A:528:LYS:HG3	1:A:531:VAL:CG2	2.34	0.57
1:A:101:LYS:O	3:A:561:M22:H3	2.04	0.57
1:A:219:LYS:O	1:A:220:LYS:HB3	2.05	0.57
1:A:503:LEU:HD22	1:A:507:GLN:HG3	1.87	0.57
1:A:107:THR:HG21	1:A:202:ILE:HD13	1.87	0.57
1:A:445:ALA:O	1:A:477:THR:HG21	2.05	0.57
1:A:454:LYS:HB2	1:A:556:ILE:HG13	1.87	0.57
1:A:135:ILE:O	1:A:136:ASN:HB2	2.05	0.57
2:B:428:GLN:O	2:B:428:GLN:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:VAL:O	1:A:522:ILE:HD12	2.04	0.57
2:B:194:GLU:OE2	2:B:196:GLY:N	2.30	0.57
2:B:393:ILE:HG12	2:B:394:GLN:N	2.20	0.57
1:A:291:GLU:HG3	1:A:291:GLU:O	2.02	0.56
1:A:420:PRO:HA	1:A:421:PRO:C	2.23	0.56
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.40	0.56
1:A:535:TRP:CZ3	2:B:426:TRP:HZ2	2.23	0.56
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.87	0.56
1:A:63:ILE:CD1	1:A:72:ARG:HG3	2.36	0.56
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.87	0.56
2:B:268:SER:O	2:B:269:GLN:HG3	2.05	0.56
1:A:448:ARG:HH11	1:A:448:ARG:CG	2.19	0.56
1:A:69:THR:O	1:A:69:THR:HG22	2.05	0.56
1:A:193:LEU:HB3	1:A:197:GLN:CG	2.37	0.55
2:B:64:LYS:NZ	2:B:69:THR:O	2.39	0.55
2:B:422:LEU:HD13	2:B:426:TRP:CH2	2.42	0.55
1:A:492:GLU:CG	1:A:530:LYS:HG3	2.36	0.55
2:B:207:GLN:OE1	2:B:211:ARG:NH1	2.37	0.55
1:A:102:LYS:HE3	1:A:236:PRO:O	2.06	0.55
2:B:205:LEU:HD22	2:B:205:LEU:O	2.07	0.55
1:A:464:GLN:HG2	1:A:465:LYS:N	2.22	0.55
1:A:194:GLU:CD	1:A:194:GLU:H	2.10	0.55
2:B:28:GLU:O	2:B:32:LYS:HG3	2.07	0.55
2:B:253:THR:HG22	2:B:255:ASN:N	2.21	0.55
2:B:374:LYS:O	2:B:378:GLU:HG3	2.07	0.55
1:A:253:THR:HG22	1:A:292:VAL:HG23	1.89	0.55
1:A:102:LYS:NZ	1:A:237:ASP:HB3	2.22	0.55
2:B:293:ILE:HG13	2:B:293:ILE:O	2.07	0.55
2:B:254:VAL:HG21	2:B:288:ALA:O	2.07	0.54
1:A:1:PRO:O	1:A:2:ILE:HD13	2.06	0.54
1:A:396:GLU:HB2	4:A:621:HOH:O	2.08	0.54
1:A:318:TYR:CZ	3:A:561:M22:H13A	2.42	0.54
1:A:380:ILE:HG23	2:B:27:THR:HG22	1.89	0.54
2:B:303:LEU:HD23	2:B:303:LEU:N	2.23	0.54
1:A:298:GLU:H	1:A:298:GLU:CD	2.10	0.54
2:B:253:THR:O	2:B:257:ILE:HG13	2.08	0.54
2:B:278:GLN:HE22	2:B:281:LYS:HZ2	1.53	0.54
1:A:393:ILE:HD12	1:A:423:VAL:HG12	1.90	0.54
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.38	0.53
1:A:432:GLU:OE1	1:A:432:GLU:HA	2.08	0.53
1:A:70:LYS:HE2	1:A:72:ARG:CZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD23	1:A:210:LEU:O	2.08	0.53
1:A:540:LYS:HB3	1:A:542:ILE:HD12	1.89	0.53
2:B:362:THR:HG23	2:B:366:LYS:NZ	2.20	0.53
1:A:63:ILE:HG13	1:A:72:ARG:HG3	1.91	0.53
1:A:542:ILE:O	1:A:545:ASN:HB3	2.09	0.53
1:A:246:LEU:CD1	1:A:310:LEU:HD12	2.33	0.53
1:A:501:TYR:O	1:A:505:ILE:HG13	2.08	0.53
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.48	0.53
1:A:406:TRP:HZ2	2:B:418:ASN:OD1	1.90	0.53
1:A:331:LYS:HE3	1:A:364:ASP:OD1	2.08	0.53
1:A:169:GLU:N	1:A:170:PRO:HD2	2.23	0.53
2:B:282:LEU:HB3	2:B:293:ILE:CD1	2.39	0.53
2:B:335:GLY:HA3	2:B:356:ARG:HG2	1.91	0.53
2:B:345:PRO:O	2:B:346:PHE:HB2	2.08	0.53
1:A:155:GLY:O	1:A:159:ILE:HD12	2.10	0.52
1:A:346:PHE:N	1:A:346:PHE:CD1	2.74	0.52
1:A:64:LYS:HZ3	1:A:69:THR:CG2	2.19	0.52
2:B:18:GLY:HA3	2:B:56:TYR:CE1	2.44	0.52
2:B:393:ILE:CG1	2:B:394:GLN:H	2.23	0.52
1:A:253:THR:HA	1:A:292:VAL:HA	1.92	0.52
1:A:24:TRP:CD1	1:A:24:TRP:N	2.77	0.52
1:A:424:LYS:NZ	1:A:426:TRP:CE3	2.78	0.52
2:B:266:TRP:CG	2:B:426:TRP:CE3	2.98	0.52
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.92	0.52
2:B:194:GLU:HB3	2:B:197:GLN:HG3	1.91	0.52
1:A:65:LYS:CD	1:A:72:ARG:HD2	2.40	0.52
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.38	0.52
2:B:150:PRO:HD2	2:B:153:TRP:HE3	1.75	0.52
1:A:206:ARG:O	1:A:209:LEU:HB2	2.10	0.52
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.40	0.52
1:A:406:TRP:CH2	1:A:407:GLN:HB2	2.45	0.52
1:A:21:VAL:HG13	1:A:57:ASN:O	2.10	0.51
1:A:31:ILE:HD13	1:A:133:PRO:O	2.10	0.51
1:A:438:GLU:HG3	1:A:461:ARG:HD2	1.92	0.51
2:B:253:THR:CG2	2:B:255:ASN:H	2.23	0.51
2:B:271:TYR:HB3	2:B:274:ILE:HD11	1.92	0.51
2:B:320:ASP:OD2	2:B:323:LYS:HG3	2.11	0.51
1:A:27:THR:O	1:A:31:ILE:HG13	2.11	0.51
2:B:64:LYS:HB2	4:B:579:HOH:O	2.10	0.51
2:B:98:ALA:HB1	2:B:101:LYS:NZ	2.24	0.51
1:A:66:LYS:O	1:A:67:ASP:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:C	1:A:221:HIS:H	2.14	0.51
1:A:540:LYS:C	1:A:542:ILE:H	2.13	0.51
2:B:270:ILE:O	2:B:272:PRO:HD3	2.11	0.51
1:A:261:VAL:HG13	1:A:276:VAL:HG21	1.93	0.51
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.02	0.51
1:A:65:LYS:HE2	1:A:72:ARG:NH1	2.25	0.51
1:A:134:SER:O	1:A:136:ASN:N	2.44	0.51
1:A:245:VAL:O	1:A:247:PRO:HD3	2.11	0.51
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.92	0.51
1:A:424:LYS:NZ	1:A:426:TRP:CZ3	2.79	0.51
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.46	0.50
2:B:319:TYR:OH	2:B:385:LYS:HD2	2.11	0.50
2:B:332:GLN:NE2	2:B:338:THR:OG1	2.32	0.50
2:B:422:LEU:HB3	2:B:426:TRP:CE2	2.46	0.50
1:A:355:ALA:O	1:A:356:ARG:O	2.29	0.50
1:A:356:ARG:HH22	1:A:358:ARG:HD2	1.77	0.50
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.38	0.50
2:B:323:LYS:NZ	2:B:344:GLU:OE2	2.38	0.50
1:A:3:SER:OG	1:A:5:ILE:HD12	2.12	0.50
1:A:546:GLU:HG3	1:A:547:GLN:NE2	2.27	0.50
2:B:44:GLU:HB3	2:B:46:LYS:HE2	1.94	0.50
1:A:437:ALA:HB3	1:A:494:ASN:ND2	2.26	0.50
2:B:326:ILE:O	2:B:341:ILE:HA	2.12	0.50
1:A:56:TYR:O	1:A:57:ASN:HB2	2.12	0.50
1:A:63:ILE:HG13	1:A:72:ARG:CG	2.41	0.50
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.46	0.49
1:A:296:THR:HG22	1:A:299:ALA:HB2	1.93	0.49
1:A:311:LYS:O	1:A:312:GLU:OE2	2.29	0.49
1:A:411:ILE:HG22	1:A:412:PRO:O	2.12	0.49
1:A:27:THR:OG1	1:A:30:LYS:HG3	2.11	0.49
1:A:82:LYS:O	1:A:82:LYS:HG3	2.12	0.49
1:A:457:TYR:HA	1:A:548:VAL:HG11	1.93	0.49
1:A:287:LYS:HG2	1:A:291:GLU:CD	2.33	0.49
1:A:307:ARG:HD2	4:A:765:HOH:O	2.12	0.49
2:B:425:LEU:HG	2:B:426:TRP:N	2.28	0.49
2:B:98:ALA:HA	4:B:441:HOH:O	2.11	0.49
2:B:325:LEU:HD12	2:B:385:LYS:CG	2.39	0.49
1:A:395:LYS:HA	1:A:414:TRP:CH2	2.47	0.49
2:B:57:ASN:OD1	2:B:143:ARG:NH1	2.45	0.49
2:B:180:ILE:HA	2:B:188:TYR:O	2.13	0.49
1:A:28:GLU:HG2	1:A:135:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ASN:HA	2:B:286:THR:OG1	2.13	0.49
1:A:494:ASN:HB3	2:B:289:LEU:CD1	2.43	0.49
2:B:273:GLY:O	2:B:275:LYS:HD3	2.13	0.49
1:A:305:GLU:O	1:A:309:ILE:HG13	2.13	0.49
2:B:13:LYS:HE3	2:B:85:GLN:CA	2.42	0.49
2:B:150:PRO:HG2	2:B:153:TRP:HB3	1.95	0.49
1:A:171:PHE:CE2	1:A:205:LEU:HD23	2.48	0.48
2:B:259:LYS:HD3	4:B:570:HOH:O	2.12	0.48
2:B:296:THR:O	2:B:299:ALA:HB3	2.13	0.48
1:A:230:MET:HA	1:A:230:MET:CE	2.43	0.48
2:B:244:ILE:HG12	2:B:266:TRP:CZ3	2.48	0.48
2:B:266:TRP:CD1	2:B:426:TRP:CE3	3.01	0.48
2:B:66:LYS:HG2	2:B:407:GLN:HE21	1.77	0.48
1:A:318:TYR:CZ	3:A:561:M22:C13	2.97	0.48
2:B:266:TRP:CZ2	2:B:427:TYR:CE2	3.00	0.48
2:B:275:LYS:CD	2:B:275:LYS:N	2.77	0.48
1:A:223:LYS:HD2	4:A:670:HOH:O	2.13	0.48
2:B:244:ILE:HG12	2:B:266:TRP:HZ3	1.78	0.48
1:A:135:ILE:O	1:A:138:GLU:OE1	2.32	0.48
2:B:311:LYS:O	2:B:311:LYS:HG3	2.14	0.48
1:A:34:LEU:HD23	1:A:73:LYS:HB2	1.95	0.48
1:A:89:GLU:O	1:A:90:VAL:O	2.32	0.48
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.94	0.48
2:B:354:TYR:HA	2:B:374:LYS:NZ	2.29	0.48
2:B:323:LYS:HB2	2:B:343:GLN:HE22	1.76	0.48
1:A:237:ASP:OD2	1:A:237:ASP:N	2.46	0.47
1:A:402:TRP:CD2	1:A:403:THR:N	2.82	0.47
2:B:88:TRP:CZ3	2:B:89:GLU:HG3	2.49	0.47
2:B:354:TYR:HD2	2:B:374:LYS:HD2	1.79	0.47
1:A:458:VAL:HG22	1:A:548:VAL:HG22	1.96	0.47
1:A:492:GLU:CD	1:A:530:LYS:HG3	2.34	0.47
2:B:317:VAL:HG12	2:B:349:LEU:HD12	1.96	0.47
1:A:356:ARG:NH1	1:A:358:ARG:HD2	2.30	0.47
2:B:87:PHE:CZ	2:B:92:LEU:HD12	2.49	0.47
2:B:150:PRO:HG2	2:B:153:TRP:CB	2.45	0.47
2:B:267:ALA:O	2:B:271:TYR:HB2	2.14	0.47
2:B:341:ILE:HD11	2:B:375:ILE:HG23	1.96	0.47
1:A:220:LYS:HD3	1:A:221:HIS:CE1	2.49	0.47
2:B:66:LYS:CG	2:B:407:GLN:HE21	2.28	0.47
2:B:317:VAL:HG12	2:B:349:LEU:CD1	2.45	0.47
1:A:382:ILE:O	2:B:136:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:O	1:A:403:THR:HB	2.14	0.47
2:B:163:SER:O	2:B:167:ILE:HG13	2.15	0.47
1:A:30:LYS:HE2	1:A:61:PHE:CE1	2.50	0.47
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.96	0.47
1:A:281:LYS:O	1:A:284:ARG:HG2	2.15	0.47
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.50	0.47
1:A:395:LYS:HD2	1:A:414:TRP:CE2	2.50	0.47
1:A:454:LYS:HD2	1:A:556:ILE:HD11	1.96	0.47
1:A:463:ARG:NH2	1:A:488:ASP:O	2.47	0.47
2:B:252:TRP:O	2:B:292:VAL:HG13	2.15	0.47
2:B:420:PRO:HA	2:B:421:PRO:HD2	1.50	0.47
1:A:0:SER:N	4:A:633:HOH:O	2.48	0.47
1:A:60:VAL:HG23	1:A:130:PHE:HB2	1.96	0.47
1:A:102:LYS:O	1:A:103:LYS:NZ	2.40	0.47
1:A:277:ARG:NH1	1:A:278:GLN:HE21	2.13	0.46
1:A:278:GLN:HB3	1:A:299:ALA:HA	1.96	0.46
1:A:457:TYR:CD1	1:A:457:TYR:C	2.88	0.46
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.50	0.46
1:A:448:ARG:CG	1:A:448:ARG:NH1	2.78	0.46
2:B:41:MET:HB3	2:B:47:ILE:HG12	1.96	0.46
2:B:377:THR:HG22	2:B:410:TRP:CZ2	2.46	0.46
2:B:380:ILE:O	2:B:384:GLY:HA2	2.16	0.46
1:A:47:ILE:HG22	1:A:146:TYR:HA	1.96	0.46
2:B:276:VAL:HG13	2:B:276:VAL:O	2.14	0.46
1:A:162:SER:CB	2:B:52:PRO:HG3	2.46	0.46
1:A:104:LYS:HG3	1:A:192:ASP:C	2.35	0.46
1:A:136:ASN:HB2	1:A:138:GLU:OE1	2.16	0.46
1:A:228:LEU:N	1:A:228:LEU:CD1	2.79	0.46
1:A:460:ASN:HA	2:B:286:THR:HG1	1.80	0.46
2:B:303:LEU:HD23	2:B:303:LEU:H	1.81	0.46
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.97	0.46
1:A:234:LEU:O	3:A:561:M22:H20	2.15	0.46
2:B:172:ARG:HH21	2:B:180:ILE:HB	1.81	0.46
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.14	0.46
2:B:242:GLN:O	2:B:242:GLN:HG3	2.16	0.46
2:B:278:GLN:HA	2:B:281:LYS:HD2	1.97	0.46
2:B:353:LYS:HG2	2:B:353:LYS:O	2.16	0.46
1:A:285:GLY:O	1:A:286:THR:O	2.34	0.46
2:B:278:GLN:NE2	2:B:281:LYS:NZ	2.64	0.46
1:A:297:GLU:HA	1:A:300:GLU:HB2	1.98	0.46
1:A:399:GLU:O	1:A:402:TRP:HE3	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ARG:O	1:A:557:ARG:HG2	2.16	0.46
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.50	0.46
2:B:282:LEU:HD13	2:B:295:LEU:CD1	2.46	0.46
1:A:65:LYS:HD3	1:A:70:LYS:CG	2.44	0.46
1:A:7:THR:CG2	1:A:121:ASP:HA	2.39	0.46
1:A:175:ASN:HD22	1:A:178:ILE:CD1	2.25	0.46
2:B:26:LEU:HB3	2:B:31:ILE:HG13	1.97	0.46
1:A:92:LEU:N	1:A:92:LEU:CD2	2.79	0.45
1:A:393:ILE:HD12	1:A:423:VAL:CG1	2.46	0.45
2:B:396:GLU:O	2:B:400:THR:HG22	2.16	0.45
1:A:26:LEU:CD2	1:A:133:PRO:HG2	2.40	0.45
1:A:275:LYS:HZ2	1:A:332:GLN:NE2	2.14	0.45
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.97	0.45
1:A:491:LEU:HD12	1:A:491:LEU:HA	1.71	0.45
2:B:270:ILE:HB	2:B:346:PHE:O	2.16	0.45
2:B:172:ARG:NH2	2:B:180:ILE:O	2.49	0.45
2:B:253:THR:HG23	2:B:254:VAL:N	2.31	0.45
2:B:320:ASP:HA	2:B:321:PRO:HD3	1.75	0.45
1:A:63:ILE:HG23	1:A:74:LEU:CD1	2.42	0.45
2:B:157:PRO:HG3	2:B:184:MET:HA	1.97	0.45
1:A:89:GLU:CB	1:A:92:LEU:HD21	2.47	0.45
1:A:403:THR:CG2	1:A:404:GLU:N	2.80	0.45
2:B:24:TRP:CZ2	2:B:399:GLU:CG	3.00	0.45
2:B:72:ARG:NH2	2:B:409:THR:CG2	2.80	0.45
2:B:271:TYR:CD1	2:B:310:LEU:HD12	2.51	0.45
1:A:17:ASP:O	1:A:83:ARG:HD3	2.16	0.45
1:A:175:ASN:ND2	1:A:178:ILE:CD1	2.79	0.45
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.49	0.45
1:A:450:THR:O	1:A:451:LYS:HB2	2.16	0.45
1:A:546:GLU:HG3	1:A:547:GLN:HE21	1.82	0.45
2:B:61:PHE:HE2	2:B:76:ASP:HB2	1.82	0.45
2:B:422:LEU:CD1	2:B:426:TRP:CH2	3.00	0.45
1:A:90:VAL:HG12	1:A:91:GLN:H	1.78	0.45
1:A:246:LEU:HD22	1:A:260:LEU:CD2	2.44	0.45
2:B:166:LYS:HD3	2:B:166:LYS:HA	1.56	0.45
2:B:395:LYS:NZ	2:B:399:GLU:OE2	2.48	0.45
2:B:420:PRO:HB2	2:B:423:VAL:HG21	1.96	0.45
1:A:65:LYS:HG2	1:A:68:SER:HB3	1.97	0.45
2:B:297:GLU:O	2:B:300:GLU:HB2	2.17	0.45
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.52	0.45
2:B:197:GLN:O	2:B:201:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:THR:HG21	2:B:367:GLN:HG3	1.98	0.44
1:A:65:LYS:CE	1:A:72:ARG:NH1	2.79	0.44
1:A:278:GLN:HG3	1:A:298:GLU:CB	2.47	0.44
2:B:72:ARG:NH2	2:B:409:THR:HG22	2.33	0.44
2:B:167:ILE:HG23	2:B:212:TRP:CE3	2.52	0.44
1:A:293:ILE:HA	1:A:294:PRO:HD3	1.88	0.44
2:B:323:LYS:CB	2:B:343:GLN:NE2	2.80	0.44
1:A:131:THR:HG22	1:A:141:GLY:HA3	1.99	0.44
2:B:90:VAL:O	2:B:91:GLN:HB2	2.18	0.44
2:B:404:GLU:HG2	2:B:404:GLU:H	1.64	0.44
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.99	0.44
1:A:356:ARG:CZ	1:A:358:ARG:HG3	2.47	0.44
2:B:194:GLU:OE1	2:B:197:GLN:HG3	2.18	0.44
2:B:314:VAL:O	2:B:315:HIS:HB3	2.17	0.44
1:A:365:VAL:HG21	1:A:425:LEU:HD11	2.00	0.44
2:B:58:THR:HG23	4:B:454:HOH:O	2.16	0.44
2:B:91:GLN:HG3	4:B:521:HOH:O	2.17	0.44
2:B:422:LEU:HD13	2:B:426:TRP:CZ2	2.53	0.44
2:B:425:LEU:HG	2:B:426:TRP:H	1.83	0.44
1:A:161:GLN:HE21	1:A:161:GLN:HB3	1.60	0.44
1:A:424:LYS:HE3	1:A:426:TRP:CH2	2.53	0.44
1:A:460:ASN:ND2	2:B:288:ALA:HB2	2.33	0.44
2:B:66:LYS:CG	2:B:407:GLN:NE2	2.81	0.44
2:B:361:HIS:N	4:B:619:HOH:O	2.51	0.44
1:A:520:GLN:HG2	1:A:520:GLN:H	1.55	0.43
2:B:246:LEU:HD11	2:B:310:LEU:CD2	2.48	0.43
1:A:203:GLU:HA	1:A:203:GLU:OE1	2.17	0.43
1:A:320:ASP:OD1	1:A:322:SER:OG	2.36	0.43
1:A:369:THR:CG2	1:A:398:TRP:HZ3	2.31	0.43
1:A:489:SER:OG	1:A:493:VAL:HG11	2.18	0.43
1:A:65:LYS:HE2	1:A:72:ARG:CD	2.49	0.43
1:A:497:THR:O	1:A:535:TRP:HA	2.19	0.43
2:B:142:ILE:HG22	2:B:144:TYR:CE2	2.54	0.43
2:B:253:THR:CG2	2:B:254:VAL:N	2.81	0.43
2:B:422:LEU:CB	2:B:426:TRP:CZ2	3.00	0.43
1:A:200:THR:HG22	4:A:603:HOH:O	2.18	0.43
1:A:228:LEU:N	1:A:228:LEU:HD12	2.33	0.43
1:A:527:LYS:HZ2	1:A:527:LYS:HG3	1.64	0.43
2:B:44:GLU:HB3	2:B:46:LYS:CE	2.49	0.43
2:B:344:GLU:HA	2:B:345:PRO:HD3	1.87	0.43
1:A:369:THR:CG2	1:A:398:TRP:CZ3	3.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:GLU:CG	1:A:547:GLN:NE2	2.81	0.43
2:B:46:LYS:HD3	2:B:116:PHE:HB3	1.99	0.43
2:B:362:THR:HG22	2:B:367:GLN:HG3	2.00	0.43
1:A:70:LYS:CE	1:A:72:ARG:NH2	2.81	0.43
1:A:230:MET:CE	1:A:230:MET:CA	2.96	0.43
2:B:270:ILE:CG2	2:B:346:PHE:CD2	3.02	0.43
2:B:393:ILE:CG1	2:B:394:GLN:N	2.81	0.43
1:A:23:GLN:HG3	1:A:24:TRP:O	2.18	0.43
1:A:109:LEU:HB2	1:A:187:LEU:HB2	2.00	0.43
1:A:208:HIS:HA	4:A:778:HOH:O	2.18	0.43
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.85	0.43
1:A:277:ARG:HE	1:A:277:ARG:HB3	1.64	0.43
2:B:249:LYS:HB3	2:B:249:LYS:HE2	1.57	0.43
2:B:275:LYS:HD3	2:B:275:LYS:N	2.34	0.43
2:B:249:LYS:HG2	2:B:252:TRP:CE2	2.54	0.43
1:A:440:PHE:HZ	1:A:488:ASP:O	2.01	0.42
2:B:12:LEU:HD12	2:B:84:THR:HG22	2.01	0.42
2:B:60:VAL:HG23	2:B:75:VAL:HG22	2.00	0.42
1:A:197:GLN:H	1:A:197:GLN:CD	2.22	0.42
1:A:318:TYR:CE2	3:A:561:M22:H13	2.54	0.42
1:A:107:THR:CG2	1:A:202:ILE:HD13	2.48	0.42
2:B:24:TRP:CZ2	2:B:399:GLU:HG2	2.54	0.42
2:B:65:LYS:HB2	2:B:65:LYS:HE3	1.84	0.42
2:B:72:ARG:HH22	2:B:409:THR:CG2	2.32	0.42
2:B:241:VAL:O	2:B:242:GLN:HB2	2.19	0.42
1:A:542:ILE:O	1:A:543:GLY:O	2.37	0.42
2:B:116:PHE:HA	2:B:148:VAL:HG21	2.01	0.42
1:A:63:ILE:HG12	1:A:74:LEU:HD21	2.00	0.42
1:A:421:PRO:HG3	4:A:591:HOH:O	2.19	0.42
2:B:63:ILE:HG21	2:B:74:LEU:HD22	2.02	0.42
2:B:111:VAL:HG11	2:B:164:MET:HE3	2.02	0.42
1:A:406:TRP:CE3	1:A:407:GLN:HB2	2.51	0.42
1:A:539:HIS:C	1:A:540:LYS:HD3	2.40	0.42
1:A:138:GLU:HA	4:A:728:HOH:O	2.20	0.42
1:A:445:ALA:HB1	1:A:557:ARG:NE	2.35	0.42
2:B:116:PHE:N	2:B:116:PHE:CD2	2.87	0.42
2:B:298:GLU:CD	2:B:298:GLU:N	2.73	0.42
1:A:395:LYS:CD	1:A:414:TRP:CH2	3.03	0.42
1:A:466:VAL:CG2	1:A:551:LEU:CD2	2.98	0.42
2:B:129:ALA:HA	2:B:144:TYR:O	2.20	0.42
2:B:274:ILE:HD13	2:B:309:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:LEU:O	2:B:425:LEU:HG	2.19	0.42
1:A:107:THR:HG23	1:A:198:HIS:HE1	1.85	0.42
1:A:193:LEU:CB	1:A:197:GLN:HG2	2.50	0.42
1:A:296:THR:HG22	1:A:299:ALA:HB3	2.01	0.42
1:A:438:GLU:HG3	1:A:461:ARG:HB2	2.01	0.42
2:B:114:ALA:CB	2:B:214:LEU:CD2	2.97	0.42
2:B:270:ILE:HG21	2:B:346:PHE:CD2	2.55	0.42
1:A:3:SER:HA	1:A:4:PRO:HD2	1.82	0.41
2:B:236:PRO:O	2:B:239:TRP:N	2.52	0.41
2:B:379:SER:OG	2:B:387:PRO:HD3	2.20	0.41
1:A:197:GLN:O	1:A:201:LYS:HB2	2.20	0.41
1:A:480:GLN:HG2	1:A:517:LEU:HD21	2.01	0.41
1:A:163:SER:O	1:A:167:ILE:HG13	2.21	0.41
1:A:296:THR:HG23	1:A:298:GLU:H	1.85	0.41
1:A:403:THR:HG22	1:A:404:GLU:N	2.35	0.41
2:B:66:LYS:CA	2:B:407:GLN:NE2	2.79	0.41
2:B:253:THR:CG2	2:B:255:ASN:N	2.83	0.41
1:A:328:GLU:HG2	1:A:390:LYS:HB2	2.02	0.41
2:B:420:PRO:O	2:B:422:LEU:N	2.53	0.41
1:A:174:GLN:HB3	4:A:807:HOH:O	2.19	0.41
1:A:175:ASN:HD21	1:A:201:LYS:CD	2.34	0.41
1:A:466:VAL:CG2	1:A:551:LEU:CG	2.96	0.41
1:A:540:LYS:HB2	1:A:542:ILE:CD1	2.49	0.41
2:B:362:THR:CG2	2:B:366:LYS:HZ2	2.24	0.41
1:A:148:VAL:O	1:A:150:PRO:HD3	2.21	0.41
1:A:253:THR:HG22	1:A:292:VAL:CG2	2.50	0.41
1:A:261:VAL:HG13	1:A:276:VAL:CG2	2.50	0.41
1:A:517:LEU:HA	1:A:520:GLN:HG3	2.03	0.41
1:A:528:LYS:HG3	1:A:531:VAL:HG21	2.02	0.41
2:B:13:LYS:HD2	2:B:85:GLN:N	2.36	0.41
2:B:260:LEU:HD22	2:B:260:LEU:C	2.41	0.41
2:B:327:ALA:HA	2:B:340:GLN:O	2.20	0.41
2:B:328:GLU:O	2:B:339:TYR:HA	2.20	0.41
1:A:104:LYS:HG3	1:A:192:ASP:CB	2.51	0.41
1:A:138:GLU:O	1:A:139:THR:O	2.38	0.41
1:A:339:TYR:OH	1:A:378:GLU:OE2	2.29	0.41
2:B:277:ARG:O	2:B:281:LYS:HG3	2.21	0.41
1:A:175:ASN:ND2	1:A:201:LYS:CE	2.77	0.41
1:A:210:LEU:C	1:A:212:TRP:N	2.73	0.41
1:A:251:SER:HB3	1:A:292:VAL:HG11	2.02	0.41
1:A:257:ILE:O	1:A:261:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LYS:HD3	1:A:540:LYS:N	2.32	0.41
1:A:549:ASP:O	1:A:553:SER:HB2	2.20	0.41
2:B:271:TYR:HA	2:B:272:PRO:HD2	1.84	0.41
1:A:246:LEU:CD2	1:A:260:LEU:HD21	2.43	0.41
1:A:278:GLN:HG3	1:A:298:GLU:HB3	2.03	0.41
1:A:365:VAL:HG11	1:A:401:TRP:CD1	2.56	0.41
1:A:23:GLN:NE2	1:A:26:LEU:HD21	2.36	0.40
2:B:39:THR:HG22	2:B:40:GLU:N	2.37	0.40
2:B:72:ARG:HH22	2:B:409:THR:HG21	1.86	0.40
2:B:344:GLU:HB3	2:B:347:LYS:HD3	2.02	0.40
1:A:40:GLU:O	1:A:43:LYS:HB2	2.21	0.40
1:A:194:GLU:CD	1:A:194:GLU:N	2.75	0.40
1:A:276:VAL:O	1:A:276:VAL:HG13	2.21	0.40
1:A:398:TRP:CZ2	1:A:411:ILE:HG13	2.56	0.40
1:A:410:TRP:CE3	2:B:363:ASN:CB	3.04	0.40
1:A:509:GLN:N	1:A:510:PRO:CD	2.84	0.40
2:B:83:ARG:NH2	4:B:477:HOH:O	2.54	0.40
2:B:85:GLN:O	2:B:89:GLU:HB2	2.20	0.40
1:A:65:LYS:HA	1:A:65:LYS:HD2	1.68	0.40
1:A:193:LEU:HB2	1:A:197:GLN:HG2	2.04	0.40
1:A:284:ARG:HB3	4:A:704:HOH:O	2.21	0.40
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.56	0.40
1:A:61:PHE:HD2	1:A:74:LEU:HD12	1.87	0.40
1:A:426:TRP:O	1:A:427:TYR:HB3	2.20	0.40
1:A:438:GLU:HG3	1:A:461:ARG:CD	2.51	0.40
1:A:65:LYS:HB3	1:A:68:SER:O	2.21	0.40
1:A:406:TRP:CE3	1:A:406:TRP:C	2.95	0.40
1:A:491:LEU:H	1:A:491:LEU:HD13	1.86	0.40
1:A:535:TRP:CZ3	1:A:537:PRO:HD3	2.56	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	556/563 (99%)	487 (88%)	53 (10%)	16 (3%)	4	10
2	B	398/443 (90%)	357 (90%)	33 (8%)	8 (2%)	7	19
All	All	954/1006 (95%)	844 (88%)	86 (9%)	24 (2%)	5	14

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	90	VAL
1	A	136	ASN
1	A	139	THR
1	A	286	THR
1	A	287	LYS
1	A	334	GLN
1	A	356	ARG
1	A	491	LEU
1	A	543	GLY
2	B	14	PRO
2	B	241	VAL
2	B	242	GLN
1	A	135	ILE
1	A	196	GLY
1	A	541	GLY
2	B	91	GLN
2	B	421	PRO
1	A	345	PRO
2	B	65	LYS
1	A	141	GLY
1	A	312	GLU
2	B	18	GLY
2	B	313	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	498/503 (99%)	375 (75%)	123 (25%)		0	2
2	B	368/403 (91%)	292 (79%)	76 (21%)		1	3
All	All	866/906 (96%)	667 (77%)	199 (23%)		1	2

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	21	VAL
1	A	22	LYS
1	A	24	TRP
1	A	26	LEU
1	A	29	GLU
1	A	36	GLU
1	A	40	GLU
1	A	43	LYS
1	A	49	LYS
1	A	64	LYS
1	A	65	LYS
1	A	66	LYS
1	A	67	ASP
1	A	70	LYS
1	A	72	ARG
1	A	74	LEU
1	A	82	LYS
1	A	92	LEU
1	A	103	LYS
1	A	104	LYS
1	A	105	SER
1	A	106	VAL
1	A	108	VAL
1	A	113	ASP
1	A	118	VAL
1	A	122	GLU
1	A	123	ASP
1	A	126	LYS
1	A	131	THR
1	A	137	ASN
1	A	138	GLU

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Mol	Chain	Res	Type
1	A	139	THR
1	A	161	GLN
1	A	162	SER
1	A	173	LYS
1	A	179	VAL
1	A	184	MET
1	A	189	VAL
1	A	193	LEU
1	A	195	ILE
1	A	197	GLN
1	A	202	ILE
1	A	205	LEU
1	A	206	ARG
1	A	210	LEU
1	A	215	THR
1	A	219	LYS
1	A	220	LYS
1	A	230	MET
1	A	238	LYS
1	A	245	VAL
1	A	248	GLU
1	A	250	ASP
1	A	251	SER
1	A	260	LEU
1	A	275	LYS
1	A	276	VAL
1	A	277	ARG
1	A	279	LEU
1	A	280	CYS
1	A	284	ARG
1	A	286	THR
1	A	287	LYS
1	A	289	LEU
1	A	291	GLU
1	A	293	ILE
1	A	295	LEU
1	A	296	THR
1	A	297	GLU
1	A	298	GLU
1	A	303	LEU
1	A	309	ILE
1	A	311	LYS

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Mol	Chain	Res	Type
1	A	312	GLU
1	A	330	GLN
1	A	334	GLN
1	A	344	GLU
1	A	350	LYS
1	A	356	ARG
1	A	368	LEU
1	A	369	THR
1	A	374	LYS
1	A	380	ILE
1	A	393	ILE
1	A	395	LYS
1	A	399	GLU
1	A	402	TRP
1	A	403	THR
1	A	404	GLU
1	A	422	LEU
1	A	424	LYS
1	A	425	LEU
1	A	429	LEU
1	A	435	VAL
1	A	448	ARG
1	A	451	LYS
1	A	459	THR
1	A	463	ARG
1	A	464	GLN
1	A	469	LEU
1	A	471	ASP
1	A	475	GLN
1	A	478	GLU
1	A	479	LEU
1	A	488	ASP
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	497	THR
1	A	503	LEU
1	A	517	LEU
1	A	520	GLN
1	A	527	LYS
1	A	530	LYS
1	A	540	LYS

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Mol	Chain	Res	Type
1	A	547	GLN
1	A	548	VAL
1	A	550	LYS
1	A	557	ARG
2	B	8	VAL
2	B	10	VAL
2	B	11	LYS
2	B	12	LEU
2	B	13	LYS
2	B	17	ASP
2	B	22	LYS
2	B	29	GLU
2	B	32	LYS
2	B	39	THR
2	B	40	GLU
2	B	46	LYS
2	B	64	LYS
2	B	66	LYS
2	B	67	ASP
2	B	69	THR
2	B	72	ARG
2	B	80	LEU
2	B	89	GLU
2	B	90	VAL
2	B	91	GLN
2	B	111	VAL
2	B	120	LEU
2	B	122	GLU
2	B	126	LYS
2	B	138	GLU
2	B	166	LYS
2	B	173	LYS
2	B	195	ILE
2	B	205	LEU
2	B	209	LEU
2	B	215	THR
2	B	232	TYR
2	B	234	LEU
2	B	241	VAL
2	B	248	GLU
2	B	249	LYS
2	B	253	THR

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Mol	Chain	Res	Type
2	B	256	ASP
2	B	257	ILE
2	B	260	LEU
2	B	261	VAL
2	B	268	SER
2	B	269	GLN
2	B	270	ILE
2	B	275	LYS
2	B	276	VAL
2	B	277	ARG
2	B	278	GLN
2	B	280	CYS
2	B	281	LYS
2	B	282	LEU
2	B	286	THR
2	B	287	LYS
2	B	293	ILE
2	B	295	LEU
2	B	297	GLU
2	B	298	GLU
2	B	301	LEU
2	B	303	LEU
2	B	305	GLU
2	B	308	GLU
2	B	310	LEU
2	B	311	LYS
2	B	314	VAL
2	B	336	GLN
2	B	349	LEU
2	B	353	LYS
2	B	362	THR
2	B	385	LYS
2	B	400	THR
2	B	403	THR
2	B	407	GLN
2	B	413	GLU
2	B	414	TRP
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	147	ASN
1	A	161	GLN
1	A	175	ASN
1	A	198	HIS
1	A	222	GLN
1	A	235	HIS
1	A	258	GLN
1	A	278	GLN
1	A	330	GLN
1	A	332	GLN
1	A	373	GLN
1	A	394	GLN
1	A	407	GLN
1	A	464	GLN
1	A	480	GLN
1	A	500	GLN
1	A	524	GLN
1	A	547	GLN
2	B	137	ASN
2	B	161	GLN
2	B	175	ASN
2	B	208	HIS
2	B	235	HIS
2	B	255	ASN
2	B	278	GLN
2	B	306	ASN
2	B	330	GLN
2	B	332	GLN
2	B	336	GLN
2	B	340	GLN
2	B	361	HIS
2	B	373	GLN
2	B	407	GLN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	M22	A	561	-	29,31,31	1.29	3 (10%)	35,43,43	1.50	3 (8%)

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	M22	A	561	-	-	5/9/11/11	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	M22	C13-C14	-3.08	1.47	1.50
3	A	561	M22	C18-C17	-2.12	1.38	1.41
3	A	561	M22	C19-C18	2.07	1.41	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	561	M22	C13-O12-C4	4.98	129.95	117.65
3	A	561	M22	C14-N-N15	-2.48	102.18	106.98
3	A	561	M22	C21-C16-C17	2.43	121.39	118.17

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	561	M22	C14-C13-O12-C4
3	A	561	M22	C5-C4-O12-C13
3	A	561	M22	C3-C4-O12-C13
3	A	561	M22	C1-C-O-C7
3	A	561	M22	N24-C23-C9-C8

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	M22	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand M22 A 561

Bond lengths

Bond angles

Torsions

Rings
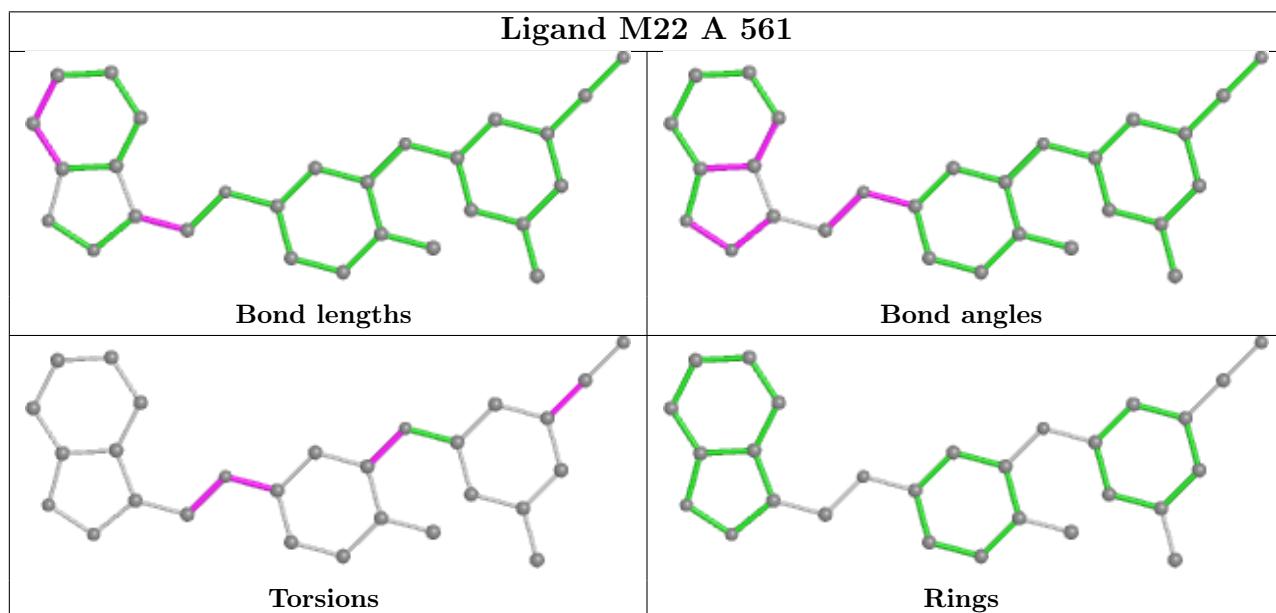
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	558/563 (99%)	-0.11	22 (3%)	39	38	23, 49, 77, 109	0
2	B	404/443 (91%)	-0.09	23 (5%)	23	22	24, 46, 90, 108	0
All	All	962/1006 (95%)	-0.10	45 (4%)	31	30	23, 48, 86, 109	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	67	ASP	7.3
1	A	286	THR	5.0
2	B	240	THR	4.3
2	B	361	HIS	3.9
2	B	251	SER	3.8
1	A	357	MET	3.8
2	B	66	LYS	3.7
1	A	284	ARG	3.7
2	B	90	VAL	3.6
2	B	14	PRO	3.5
1	A	358	ARG	3.5
2	B	69	THR	3.4
2	B	311	LYS	3.3
2	B	297	GLU	3.3
1	A	67	ASP	3.2
2	B	362	THR	3.1
1	A	359	GLY	3.1
2	B	231	GLY	3.0
1	A	15	GLY	2.8
1	A	285	GLY	2.8
1	A	68	SER	2.8
2	B	70	LYS	2.8
1	A	24	TRP	2.8
2	B	68	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	66	LYS	2.7
2	B	248	GLU	2.7
1	A	140	PRO	2.6
1	A	65	LYS	2.6
2	B	15	GLY	2.6
1	A	137	ASN	2.5
1	A	221	HIS	2.5
1	A	557	ARG	2.5
1	A	360	ALA	2.5
1	A	220	LYS	2.5
2	B	6	GLU	2.4
1	A	356	ARG	2.2
1	A	52	PRO	2.2
1	A	554	ALA	2.2
2	B	13	LYS	2.2
2	B	241	VAL	2.1
2	B	250	ASP	2.1
2	B	269	GLN	2.1
2	B	237	ASP	2.1
2	B	24	TRP	2.0
1	A	70	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	M22	A	561	28/28	0.96	0.14	37,45,50,51	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 M22 A 561:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
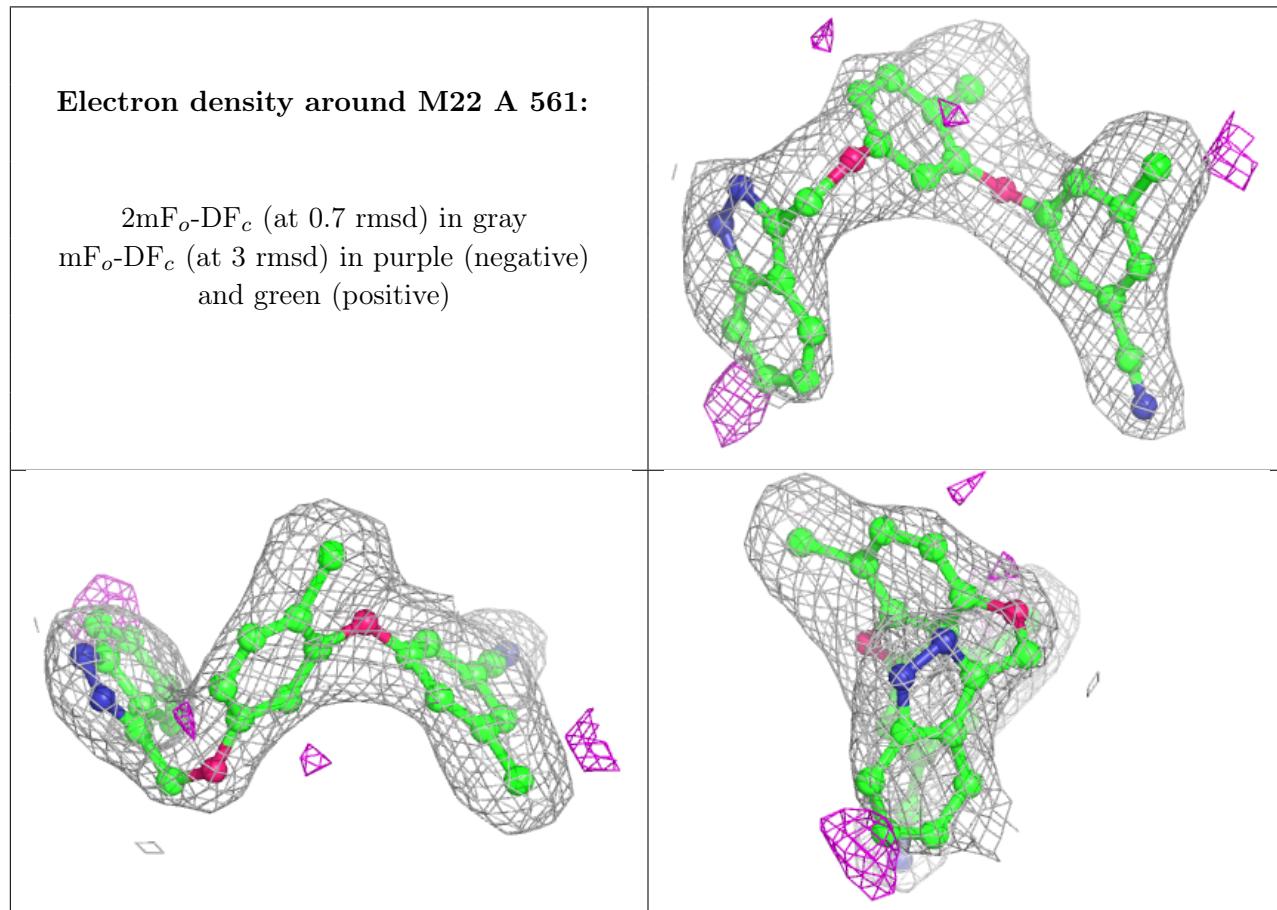
6.5 Other polymers (i)

There are no such residues in this entry.