WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2024 – 05:08 PM EST

PDB ID	:	1HNV
Title	:	STRUCTURE OF HIV-1 RT(SLASH)TIBO R 86183 COMPLEX REVEALS SIMILARITY IN THE BINDING OF DIVERSE NONNUCLEOSIDE IN-HIBITORS
Authors	:	Das, K.; Ding, J.; Arnold, E.
Deposited on	:	1995-03-30
Resolution	:	3.00 Å(reported)

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

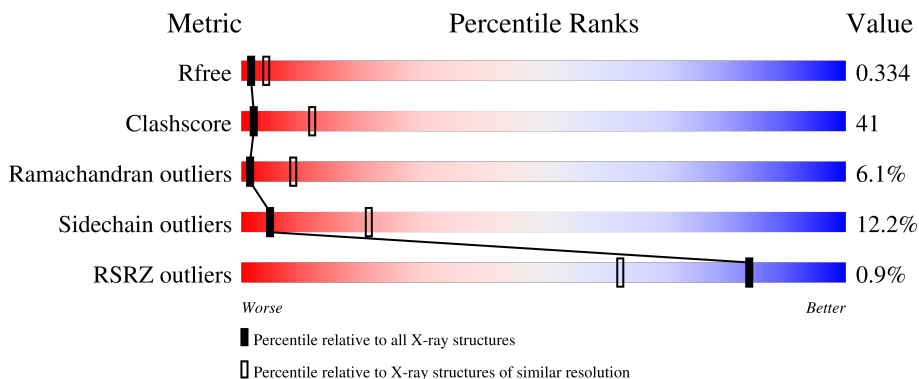|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.334
Clashscore		41
Ramachandran outliers		6.1%
Sidechain outliers		12.2%
RSRZ outliers		0.9%

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	558	38% 53% 8%
2	B	427	35% 49% 14%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7833 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4370	2827	725	812	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	conflict	UNP P03366

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3442	2240	567	630	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	conflict	UNP P03366

- Molecule 3 is 5-CHLORO-8-METHYL-7-(3-METHYL-BUT-2-ENYL)-6,7,8,9-TETRAHYDRO-2H-2,7,9A-TRIAZA-BENZO[CD]AZULENE-1-THIONE (three-letter code: TBO) (formula: $C_{16}H_{20}ClN_3S$).

TBO

C16

C14

C15

C13

CL8

Cl

C12

C7

C8

N6(R)

N

C9

C11

C7A

C5(S)

C3A

C10

C4

N

C1A

N3

C2

N

C2

H

N1

S

S2

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	S	0	0
			21	16	1	3	1		

3 Residue-property plots ⓘ

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

● Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)
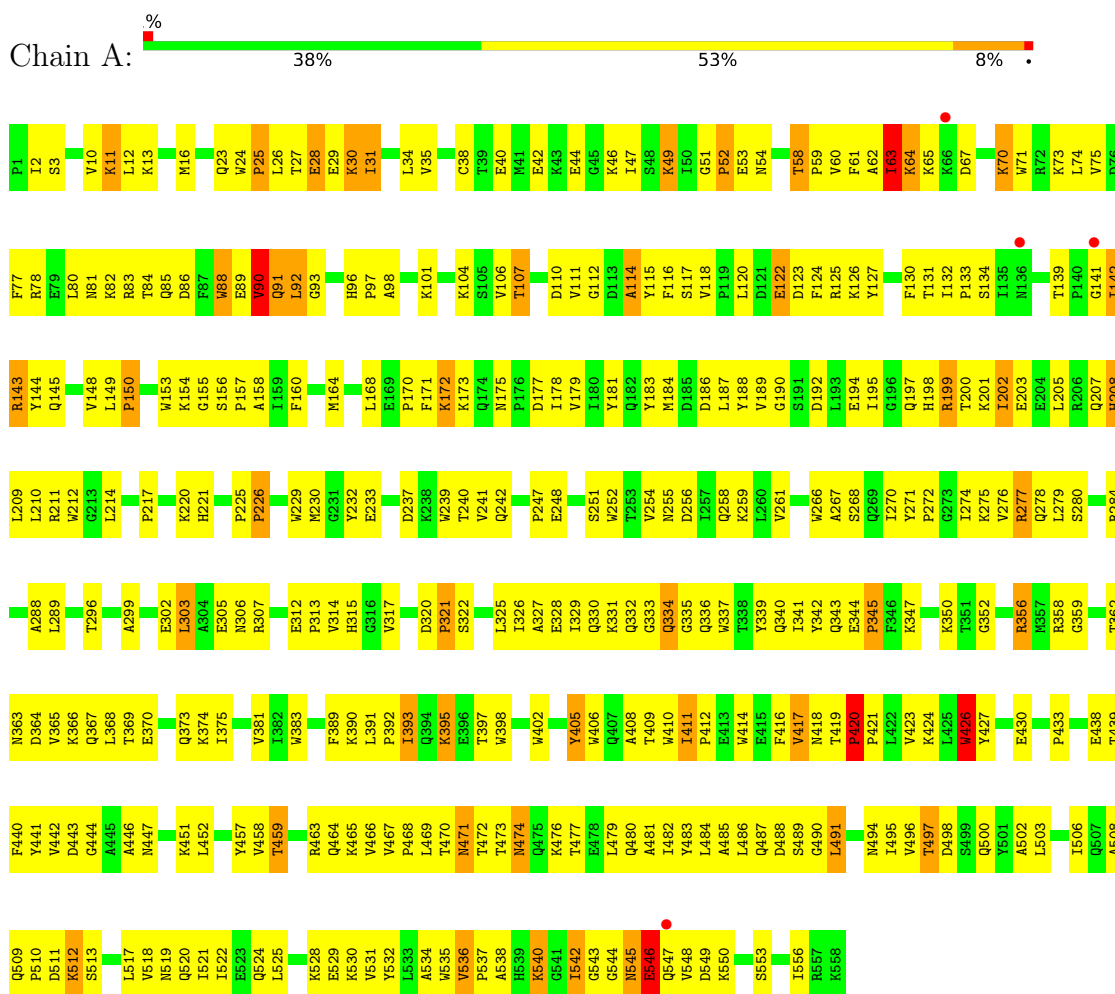
● Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)
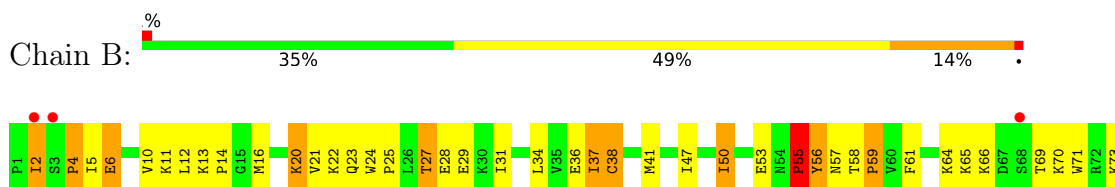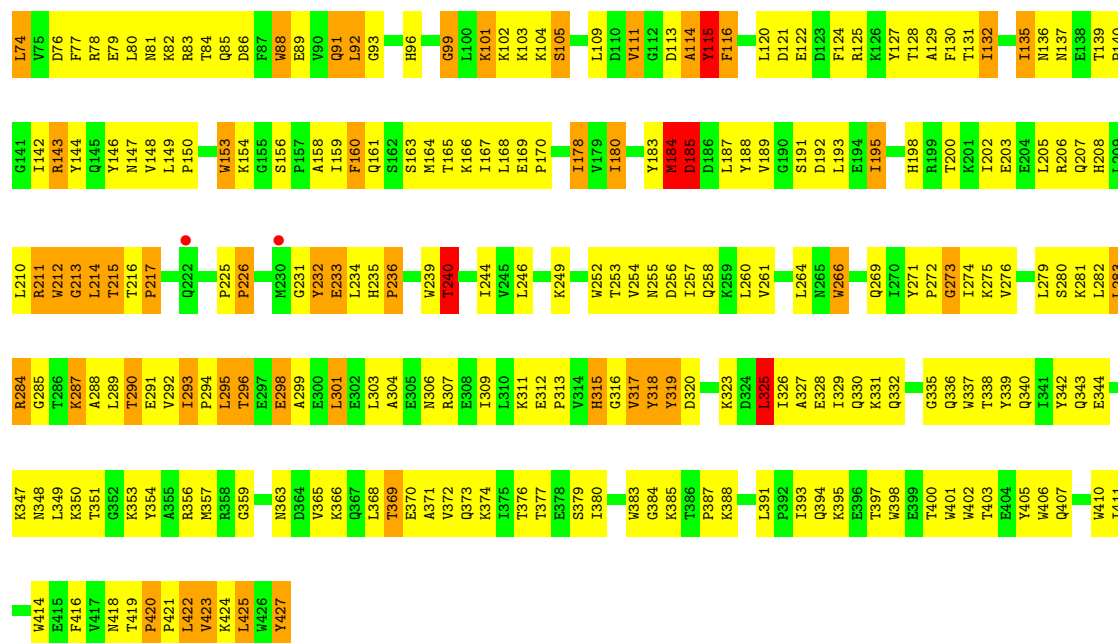
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	227.20Å 70.20Å 105.70Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 14.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.2 (10.00-3.00) 81.1 (14.97-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.249 , 0.356 0.248 , 0.334	Depositor DCC
R_{free} test set	1594 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å²)	55.2	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.19 , 62.6	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7833	wwPDB-VP
Average B, all atoms (Å²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.64	0/4484	0.85	4/6113 (0.1%)
2	B	0.72	1/3541 (0.0%)	0.91	7/4822 (0.1%)
All	All	0.68	1/8025 (0.0%)	0.88	11/10935 (0.1%)

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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	153	TRP	CB-CG	-6.62	1.38	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	SER	N-CA-C	6.52	128.60	111.00
2	B	184	MET	CG-SD-CE	6.40	110.45	100.20
2	B	215	THR	N-CA-C	-5.80	95.35	111.00
1	A	288	ALA	N-CA-C	-5.74	95.50	111.00
2	B	225	PRO	N-CA-CB	5.67	110.11	103.30
2	B	226	PRO	N-CA-CB	5.51	109.91	103.30
1	A	420	PRO	N-CA-C	5.32	125.92	112.10
2	B	2	ILE	N-CA-C	5.28	125.24	111.00
2	B	325	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	92	LEU	CA-CB-CG	5.12	127.08	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	295	LEU	N-CA-C	5.08	124.73	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	56	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4370	0	4265	368	0
2	B	3442	0	3405	298	0
3	A	21	0	20	7	0
All	All	7833	0	7690	632	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 41.

All (632) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD11	2:B:22:LYS:NZ	1.25	1.47
1:A:13:LYS:HB2	1:A:16:MET:HG3	1.29	1.10
1:A:92:LEU:CD1	2:B:22:LYS:NZ	2.16	1.08
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.36	1.08
1:A:92:LEU:CD1	2:B:22:LYS:HZ3	1.68	1.07
1:A:542:ILE:HG23	1:A:545:ASN:HB2	1.35	1.03
2:B:86:ASP:O	2:B:89:GLU:HG2	1.68	0.93
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.04	0.92
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.04	0.92
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.53	0.90
1:A:419:THR:HB	1:A:420:PRO:HD2	1.53	0.90
1:A:183:TYR:CA	1:A:184:MET:N	2.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.52	0.89
2:B:292:VAL:HG12	2:B:294:PRO:HD3	1.53	0.89
1:A:479:LEU:HA	1:A:482:ILE:HD12	1.53	0.89
1:A:92:LEU:HD11	2:B:22:LYS:HZ1	1.34	0.89
1:A:540:LYS:HE3	1:A:540:LYS:HA	1.54	0.88
1:A:46:LYS:HE2	1:A:116:PHE:HB3	1.56	0.87
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.41	0.86
1:A:543:GLY:HA3	2:B:284:ARG:O	1.76	0.85
1:A:525:LEU:HD23	1:A:531:VAL:HG21	1.59	0.85
1:A:107:THR:HG21	1:A:202:ILE:HG13	1.57	0.85
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.12	0.85
1:A:420:PRO:HB2	1:A:421:PRO:HD3	1.59	0.84
1:A:240:THR:HG23	1:A:270:ILE:HG21	1.59	0.84
2:B:330:GLN:HE21	2:B:340:GLN:HE22	1.27	0.83
2:B:330:GLN:NE2	2:B:340:GLN:HE22	1.76	0.83
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.60	0.82
1:A:328:GLU:HA	1:A:390:LYS:HB2	1.62	0.82
1:A:111:VAL:HG12	1:A:114:ALA:HB2	1.60	0.82
2:B:323:LYS:HB2	2:B:343:GLN:OE1	1.81	0.80
2:B:306:ASN:O	2:B:309:ILE:HG22	1.81	0.80
1:A:397:THR:HG21	1:A:424:LYS:HA	1.64	0.79
1:A:479:LEU:HB2	1:A:517:LEU:HD21	1.64	0.79
2:B:28:GLU:HA	2:B:31:ILE:HD12	1.64	0.78
1:A:543:GLY:H	2:B:284:ARG:HA	1.48	0.78
1:A:88:TRP:NE1	2:B:143:ARG:HD2	1.98	0.78
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.20	0.76
2:B:326:ILE:HD12	2:B:388:LYS:HE2	1.66	0.76
1:A:47:ILE:HG21	1:A:144:TYR:HB3	1.68	0.75
2:B:128:THR:CB	2:B:146:TYR:HB2	2.16	0.75
2:B:253:THR:HG22	2:B:289:LEU:O	1.85	0.75
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.68	0.74
2:B:257:ILE:O	2:B:261:VAL:HG23	1.87	0.74
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.68	0.74
2:B:328:GLU:O	2:B:339:TYR:HA	1.88	0.74
1:A:47:ILE:CG2	1:A:144:TYR:HB3	2.18	0.74
2:B:285:GLY:HA3	2:B:287:LYS:HD2	1.69	0.74
2:B:325:LEU:HD21	2:B:385:LYS:HG3	1.70	0.73
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.69	0.73
2:B:292:VAL:HG12	2:B:294:PRO:CD	2.18	0.73
1:A:439:THR:OG1	2:B:288:ALA:HA	1.89	0.73
2:B:128:THR:HB	2:B:146:TYR:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:THR:HG22	2:B:140:PRO:CD	2.18	0.72
2:B:158:ALA:O	2:B:161:GLN:HB2	1.89	0.72
1:A:123:ASP:O	1:A:126:LYS:HG2	1.90	0.72
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.72	0.72
2:B:253:THR:CG2	2:B:290:THR:HA	2.19	0.72
1:A:255:ASN:HA	1:A:258:GLN:OE1	1.89	0.72
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.70	0.72
1:A:333:GLY:O	1:A:334:GLN:HG2	1.90	0.71
1:A:398:TRP:CZ2	1:A:411:ILE:HG12	2.25	0.71
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.73	0.71
1:A:474:ASN:HD22	1:A:474:ASN:H	1.36	0.71
2:B:319:TYR:CE2	2:B:383:TRP:HD1	2.09	0.70
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.26	0.70
1:A:426:TRP:CE3	1:A:426:TRP:HA	2.27	0.70
2:B:195:ILE:HD12	2:B:195:ILE:H	1.55	0.70
2:B:193:LEU:HD12	2:B:198:HIS:HA	1.74	0.69
2:B:69:THR:HG22	2:B:70:LYS:H	1.58	0.69
1:A:540:LYS:HA	1:A:540:LYS:CE	2.16	0.69
1:A:92:LEU:CD1	2:B:22:LYS:HZ1	1.94	0.69
1:A:326:ILE:O	1:A:341:ILE:HA	1.91	0.69
2:B:132:ILE:CG2	2:B:142:ILE:HB	2.22	0.69
2:B:366:LYS:O	2:B:369:THR:HG22	1.92	0.69
2:B:99:GLY:HA2	2:B:102:LYS:HD2	1.75	0.69
2:B:320:ASP:CG	2:B:323:LYS:HG2	2.12	0.69
2:B:325:LEU:H	2:B:325:LEU:HD23	1.56	0.69
2:B:203:GLU:HA	2:B:206:ARG:HG3	1.74	0.69
1:A:317:VAL:HG11	1:A:347:LYS:HE3	1.75	0.68
1:A:61:PHE:HB3	1:A:74:LEU:HD23	1.73	0.68
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.76	0.68
1:A:132:ILE:O	1:A:142:ILE:HG12	1.94	0.68
2:B:2:ILE:O	2:B:4:PRO:HD3	1.94	0.68
2:B:280:SER:HA	2:B:283:LEU:HD23	1.76	0.68
1:A:486:LEU:HA	1:A:489:SER:HG	1.59	0.67
2:B:65:LYS:HG3	2:B:66:LYS:N	2.07	0.67
1:A:509:GLN:N	1:A:510:PRO:HD3	2.09	0.67
2:B:330:GLN:HE21	2:B:340:GLN:NE2	1.91	0.67
2:B:163:SER:O	2:B:167:ILE:HG12	1.94	0.67
1:A:73:LYS:HG2	1:A:74:LEU:N	2.10	0.67
1:A:277:ARG:HD3	1:A:278:GLN:NE2	2.10	0.67
2:B:57:ASN:OD1	2:B:58:THR:N	2.28	0.66
1:A:96:HIS:CD2	1:A:98:ALA:HB3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ALA:O	2:B:116:PHE:N	2.29	0.66
2:B:115:TYR:HD1	2:B:115:TYR:H	1.42	0.66
1:A:373:GLN:NE2	2:B:397:THR:HA	2.09	0.66
1:A:474:ASN:H	1:A:474:ASN:ND2	1.92	0.66
1:A:26:LEU:HG	1:A:27:THR:N	2.11	0.66
1:A:420:PRO:HB2	1:A:421:PRO:CD	2.26	0.65
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.26	0.65
2:B:304:ALA:O	2:B:307:ARG:HB3	1.96	0.65
2:B:92:LEU:HB3	2:B:158:ALA:HB1	1.77	0.65
1:A:23:GLN:HG2	1:A:24:TRP:N	2.11	0.65
2:B:61:PHE:HE1	2:B:76:ASP:HB2	1.62	0.65
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.32	0.65
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.79	0.65
1:A:398:TRP:HZ2	1:A:411:ILE:HG12	1.61	0.64
1:A:441:TYR:O	1:A:548:VAL:HG11	1.98	0.64
2:B:139:THR:CG2	2:B:140:PRO:HD2	2.20	0.64
1:A:106:VAL:HG12	1:A:107:THR:N	2.12	0.64
1:A:328:GLU:CA	1:A:390:LYS:HB2	2.28	0.64
1:A:430:GLU:HG3	1:A:530:LYS:HG2	1.80	0.64
2:B:5:ILE:HG22	2:B:6:GLU:N	2.12	0.64
2:B:344:GLU:O	2:B:347:LYS:HB2	1.98	0.64
1:A:363:ASN:OD1	1:A:365:VAL:N	2.30	0.64
2:B:253:THR:HG23	2:B:291:GLU:H	1.62	0.64
2:B:253:THR:HG21	2:B:290:THR:HA	1.79	0.64
1:A:473:THR:H	1:A:476:LYS:HD2	1.63	0.64
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.79	0.64
1:A:369:THR:OG1	1:A:398:TRP:CZ3	2.50	0.63
1:A:438:GLU:O	1:A:440:PHE:HD1	1.80	0.63
1:A:240:THR:HG22	1:A:241:VAL:N	2.14	0.63
1:A:438:GLU:HG2	1:A:459:THR:HB	1.81	0.63
2:B:77:PHE:O	2:B:81:ASN:HB2	1.98	0.63
1:A:118:VAL:O	1:A:148:VAL:HA	1.99	0.63
2:B:143:ARG:HH11	2:B:143:ARG:CG	2.11	0.63
1:A:418:ASN:O	1:A:419:THR:HG23	1.98	0.63
1:A:229:TRP:CZ3	3:A:559:TBO:H151	2.34	0.62
2:B:79:GLU:O	2:B:83:ARG:HG3	1.99	0.62
2:B:115:TYR:HD2	2:B:156:SER:HB3	1.64	0.62
1:A:10:VAL:HG12	1:A:124:PHE:CE1	2.34	0.62
1:A:202:ILE:HG21	1:A:221:HIS:CB	2.29	0.62
1:A:91:GLN:OE1	1:A:91:GLN:HA	1.92	0.62
1:A:410:TRP:NE1	2:B:401:TRP:CZ3	2.67	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:HIS:O	1:A:211:ARG:HB2	2.00	0.62
1:A:518:VAL:O	1:A:522:ILE:HG13	1.99	0.62
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.30	0.62
1:A:433:PRO:HG2	2:B:255:ASN:HB2	1.81	0.62
2:B:5:ILE:HG22	2:B:6:GLU:H	1.64	0.62
1:A:46:LYS:HG2	1:A:148:VAL:HG21	1.80	0.61
2:B:78:ARG:O	2:B:82:LYS:HG3	2.00	0.61
2:B:160:PHE:HE2	2:B:164:MET:HE3	1.65	0.61
1:A:63:ILE:HG12	1:A:64:LYS:H	1.64	0.61
2:B:160:PHE:CE2	2:B:164:MET:HB2	2.35	0.61
2:B:266:TRP:HA	2:B:266:TRP:CE3	2.35	0.61
2:B:27:THR:O	2:B:31:ILE:HG13	2.01	0.61
1:A:447:ASN:O	1:A:451:LYS:N	2.34	0.61
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.36	0.61
1:A:341:ILE:HD13	1:A:350:LYS:HB3	1.83	0.61
1:A:465:LYS:HD3	1:A:488:ASP:OD2	2.01	0.61
1:A:479:LEU:HB3	1:A:521:ILE:HD11	1.82	0.61
1:A:101:LYS:HD3	1:A:321:PRO:CD	2.31	0.61
2:B:65:LYS:HG3	2:B:66:LYS:H	1.66	0.60
2:B:315:HIS:O	2:B:317:VAL:N	2.34	0.60
2:B:350:LYS:HG2	2:B:351:THR:H	1.66	0.60
1:A:521:ILE:O	1:A:525:LEU:HD12	2.01	0.60
2:B:132:ILE:HG23	2:B:142:ILE:HB	1.83	0.60
2:B:269:GLN:OE1	2:B:269:GLN:HA	2.00	0.60
2:B:249:LYS:HB2	2:B:252:TRP:CE3	2.37	0.60
1:A:104:LYS:HG3	1:A:192:ASP:HA	1.84	0.60
1:A:325:LEU:HD11	1:A:383:TRP:CB	2.31	0.60
2:B:340:GLN:HA	2:B:351:THR:HG22	1.84	0.60
2:B:10:VAL:HG22	2:B:88:TRP:CH2	2.37	0.60
2:B:79:GLU:HG3	2:B:83:ARG:HD2	1.84	0.60
2:B:125:ARG:HE	2:B:147:ASN:HA	1.66	0.60
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.83	0.59
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.98	0.59
1:A:508:ALA:HB3	1:A:510:PRO:HG3	1.83	0.59
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.37	0.59
1:A:433:PRO:HG2	2:B:255:ASN:CB	2.32	0.59
1:A:317:VAL:CG1	1:A:347:LYS:HE3	2.32	0.59
1:A:433:PRO:HG2	2:B:255:ASN:CG	2.23	0.59
1:A:267:ALA:HB1	1:A:271:TYR:HD2	1.66	0.59
1:A:412:PRO:O	1:A:414:TRP:HD1	1.86	0.59
2:B:183:TYR:HB3	2:B:188:TYR:HE2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:THR:HB	2:B:299:ALA:CB	2.33	0.59
1:A:23:GLN:HG2	1:A:24:TRP:H	1.67	0.58
1:A:153:TRP:CH2	1:A:155:GLY:HA3	2.38	0.58
2:B:292:VAL:CG1	2:B:294:PRO:HD3	2.31	0.58
1:A:30:LYS:HZ3	1:A:71:TRP:CB	2.17	0.58
1:A:77:PHE:CZ	1:A:150:PRO:HB3	2.38	0.58
1:A:47:ILE:HD13	1:A:130:PHE:HZ	1.69	0.58
1:A:85:GLN:NE2	2:B:53:GLU:O	2.37	0.58
2:B:254:VAL:HB	2:B:289:LEU:O	2.03	0.58
1:A:465:LYS:O	1:A:466:VAL:HG23	2.04	0.58
1:A:466:VAL:HG12	1:A:467:VAL:N	2.18	0.57
2:B:180:ILE:HG23	2:B:189:VAL:HG22	1.85	0.57
1:A:199:ARG:HB2	1:A:199:ARG:CZ	2.34	0.57
2:B:343:GLN:HG3	2:B:349:LEU:HD11	1.87	0.57
1:A:92:LEU:HD11	2:B:22:LYS:CE	2.26	0.57
2:B:423:VAL:HG12	2:B:427:TYR:HE1	1.68	0.57
2:B:296:THR:HB	2:B:299:ALA:HB3	1.85	0.57
1:A:164:MET:SD	1:A:168:LEU:HD21	2.45	0.57
2:B:193:LEU:HB2	2:B:198:HIS:HB2	1.86	0.57
1:A:375:ILE:HG21	1:A:389:PHE:HE1	1.69	0.56
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.33	0.56
2:B:210:LEU:HD12	2:B:214:LEU:HA	1.88	0.56
2:B:393:ILE:HG21	2:B:398:TRP:HB2	1.87	0.56
2:B:253:THR:HG23	2:B:291:GLU:N	2.20	0.56
1:A:199:ARG:HD3	1:A:220:LYS:O	2.05	0.56
1:A:439:THR:HG23	2:B:289:LEU:HG	1.88	0.56
1:A:277:ARG:HD2	1:A:334:GLN:OE1	2.06	0.56
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.40	0.56
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.88	0.56
2:B:391:LEU:O	2:B:416:PHE:HA	2.05	0.56
1:A:278:GLN:HB2	1:A:299:ALA:HA	1.86	0.56
1:A:375:ILE:HG21	1:A:389:PHE:CE1	2.40	0.56
1:A:393:ILE:HB	1:A:423:VAL:HB	1.87	0.56
2:B:232:TYR:O	2:B:234:LEU:HG	2.05	0.56
2:B:252:TRP:O	2:B:292:VAL:HG13	2.05	0.56
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.41	0.56
2:B:239:TRP:O	2:B:240:THR:HG23	2.06	0.55
1:A:111:VAL:HG12	1:A:111:VAL:O	2.06	0.55
1:A:194:GLU:O	1:A:198:HIS:N	2.39	0.55
1:A:486:LEU:HA	1:A:489:SER:OG	2.07	0.55
1:A:517:LEU:O	1:A:521:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:CYS:HB3	2:B:144:TYR:CE2	2.41	0.55
2:B:266:TRP:HA	2:B:266:TRP:HE3	1.70	0.55
1:A:276:VAL:HG12	1:A:276:VAL:O	2.06	0.55
1:A:303:LEU:HD11	1:A:307:ARG:HH21	1.72	0.55
1:A:356:ARG:CB	1:A:367:GLN:NE2	2.69	0.55
2:B:160:PHE:HE2	2:B:164:MET:CE	2.20	0.55
2:B:320:ASP:H	2:B:343:GLN:HE22	1.55	0.55
1:A:416:PHE:CD1	1:A:417:VAL:N	2.74	0.55
2:B:320:ASP:N	2:B:343:GLN:HE22	2.05	0.55
2:B:282:LEU:HD11	2:B:293:ILE:O	2.07	0.55
2:B:365:VAL:HG22	2:B:393:ILE:HD11	1.89	0.55
1:A:458:VAL:HG12	1:A:458:VAL:O	2.06	0.55
2:B:91:GLN:C	2:B:93:GLY:H	2.10	0.55
2:B:292:VAL:O	2:B:293:ILE:HD13	2.07	0.55
2:B:81:ASN:OD1	2:B:154:LYS:N	2.37	0.55
2:B:5:ILE:CG2	2:B:6:GLU:H	2.21	0.54
1:A:106:VAL:CG1	1:A:107:THR:N	2.70	0.54
1:A:188:TYR:CE2	3:A:559:TBO:H163	2.42	0.54
1:A:325:LEU:HD11	1:A:383:TRP:CG	2.42	0.54
1:A:92:LEU:HD11	2:B:22:LYS:HZ3	0.73	0.54
1:A:512:LYS:NZ	1:A:512:LYS:HB2	2.22	0.54
2:B:377:THR:O	2:B:380:ILE:HB	2.07	0.54
1:A:482:ILE:HG21	1:A:506:ILE:HD11	1.88	0.54
2:B:311:LYS:O	2:B:313:PRO:HD3	2.07	0.54
1:A:90:VAL:O	1:A:91:GLN:NE2	2.40	0.54
1:A:466:VAL:CG1	1:A:467:VAL:N	2.70	0.54
2:B:231:GLY:C	2:B:233:GLU:H	2.11	0.54
2:B:398:TRP:O	2:B:400:THR:N	2.41	0.54
1:A:101:LYS:HD3	1:A:321:PRO:HD3	1.89	0.54
2:B:132:ILE:HG22	2:B:142:ILE:O	2.08	0.54
2:B:309:ILE:HG12	2:B:309:ILE:O	2.07	0.54
1:A:369:THR:HG1	1:A:398:TRP:HZ3	1.51	0.53
2:B:10:VAL:HG11	2:B:153:TRP:CH2	2.42	0.53
2:B:38:CYS:O	2:B:41:MET:HB2	2.07	0.53
2:B:376:THR:O	2:B:377:THR:C	2.46	0.53
2:B:165:THR:HG22	2:B:166:LYS:N	2.22	0.53
1:A:411:ILE:HG22	1:A:414:TRP:CD1	2.43	0.53
2:B:38:CYS:HB3	2:B:144:TYR:HE2	1.73	0.53
2:B:402:TRP:CG	2:B:403:THR:N	2.76	0.53
2:B:130:PHE:CE2	2:B:144:TYR:HD2	2.26	0.53
1:A:74:LEU:O	1:A:75:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LYS:CB	1:A:336:GLN:HE22	2.22	0.53
2:B:400:THR:HG22	2:B:401:TRP:CD1	2.43	0.53
1:A:410:TRP:CD1	2:B:401:TRP:CE3	2.96	0.53
2:B:10:VAL:HG11	2:B:153:TRP:HH2	1.74	0.53
1:A:150:PRO:HB2	1:A:153:TRP:HB3	1.91	0.53
1:A:479:LEU:HB3	1:A:521:ILE:CD1	2.39	0.53
1:A:542:ILE:HG12	1:A:544:GLY:N	2.24	0.53
2:B:206:ARG:HH21	2:B:217:PRO:C	2.12	0.52
1:A:208:HIS:HE1	1:A:212:TRP:HE1	1.56	0.52
2:B:373:GLN:NE2	2:B:406:TRP:CD2	2.78	0.52
1:A:51:GLY:N	1:A:52:PRO:CD	2.72	0.52
1:A:540:LYS:HE3	1:A:540:LYS:CA	2.33	0.52
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.92	0.52
1:A:92:LEU:HD21	2:B:22:LYS:HE2	1.91	0.52
1:A:511:ASP:OD2	1:A:512:LYS:HG3	2.10	0.52
1:A:479:LEU:O	1:A:482:ILE:N	2.42	0.52
2:B:28:GLU:O	2:B:31:ILE:N	2.42	0.52
2:B:78:ARG:HD3	2:B:411:ILE:HG22	1.92	0.52
2:B:198:HIS:O	2:B:202:ILE:HG12	2.09	0.52
2:B:239:TRP:HE3	2:B:350:LYS:HE3	1.74	0.52
1:A:88:TRP:HE3	1:A:88:TRP:HA	1.75	0.52
1:A:116:PHE:O	1:A:148:VAL:HB	2.10	0.52
1:A:303:LEU:HD12	1:A:303:LEU:C	2.30	0.52
1:A:410:TRP:CD1	2:B:401:TRP:CZ3	2.97	0.52
1:A:427:TYR:OH	1:A:510:PRO:HD2	2.10	0.52
1:A:531:VAL:HG12	1:A:532:TYR:H	1.75	0.52
2:B:260:LEU:HD21	2:B:303:LEU:HD13	1.92	0.52
1:A:252:TRP:CZ3	1:A:256:ASP:HB3	2.44	0.51
1:A:397:THR:CG2	1:A:424:LYS:HA	2.38	0.51
1:A:63:ILE:HG12	1:A:64:LYS:N	2.25	0.51
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.44	0.51
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.46	0.51
2:B:160:PHE:CG	2:B:160:PHE:O	2.63	0.51
1:A:420:PRO:O	1:A:421:PRO:C	2.45	0.51
2:B:128:THR:OG1	2:B:146:TYR:HB2	2.10	0.51
2:B:213:GLY:C	2:B:215:THR:N	2.63	0.51
2:B:329:ILE:HA	2:B:338:THR:O	2.09	0.51
1:A:531:VAL:HG12	1:A:532:TYR:N	2.25	0.51
2:B:167:ILE:O	2:B:208:HIS:NE2	2.39	0.51
1:A:519:ASN:HA	1:A:522:ILE:HD12	1.91	0.51
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TRP:HD1	2:B:401:TRP:CD2	2.28	0.51
2:B:109:LEU:HD12	2:B:187:LEU:HD23	1.91	0.51
2:B:115:TYR:OH	2:B:185:ASP:HA	2.11	0.51
2:B:336:GLN:HB3	2:B:353:LYS:HE2	1.92	0.51
1:A:139:THR:C	1:A:141:GLY:H	2.14	0.51
1:A:40:GLU:O	1:A:44:GLU:HG2	2.11	0.51
2:B:31:ILE:CD1	2:B:135:ILE:HG13	2.41	0.51
2:B:73:LYS:NZ	2:B:130:PHE:CZ	2.79	0.51
2:B:206:ARG:HE	2:B:217:PRO:HB2	1.76	0.51
1:A:544:GLY:O	1:A:548:VAL:HG22	2.11	0.51
2:B:203:GLU:HG3	2:B:206:ARG:HD3	1.92	0.50
2:B:232:TYR:O	2:B:234:LEU:N	2.43	0.50
2:B:350:LYS:HG2	2:B:351:THR:N	2.26	0.50
1:A:23:GLN:HG3	1:A:59:PRO:CB	2.41	0.50
1:A:171:PHE:CB	1:A:208:HIS:CD2	2.89	0.50
1:A:254:VAL:HB	1:A:289:LEU:HA	1.93	0.50
1:A:498:ASP:HB2	1:A:538:ALA:CB	2.41	0.50
2:B:34:LEU:O	2:B:38:CYS:HB2	2.10	0.50
2:B:120:LEU:HD12	2:B:121:ASP:H	1.77	0.50
1:A:443:ASP:HB3	1:A:548:VAL:HB	1.93	0.50
2:B:330:GLN:NE2	2:B:340:GLN:NE2	2.51	0.50
1:A:143:ARG:HG3	1:A:143:ARG:HH11	1.77	0.50
1:A:512:LYS:HB2	1:A:512:LYS:HZ3	1.77	0.50
2:B:47:ILE:HD12	2:B:130:PHE:HZ	1.76	0.50
2:B:50:ILE:HD11	2:B:144:TYR:O	2.11	0.50
1:A:81:ASN:OD1	1:A:154:LYS:N	2.44	0.50
1:A:270:ILE:O	1:A:272:PRO:HD3	2.11	0.50
1:A:70:LYS:HD3	1:A:70:LYS:N	2.27	0.50
2:B:5:ILE:CG2	2:B:6:GLU:N	2.75	0.50
2:B:20:LYS:HE2	2:B:56:TYR:CD1	2.46	0.50
1:A:207:GLN:HB3	1:A:211:ARG:HH12	1.77	0.50
2:B:80:LEU:O	2:B:81:ASN:C	2.50	0.50
2:B:370:GLU:O	2:B:373:GLN:N	2.44	0.50
1:A:96:HIS:HD2	1:A:98:ALA:HB3	1.75	0.49
1:A:178:ILE:HD11	1:A:201:LYS:HG3	1.95	0.49
2:B:303:LEU:HD21	2:B:307:ARG:NH2	2.26	0.49
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.93	0.49
2:B:125:ARG:HG2	2:B:146:TYR:O	2.12	0.49
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.47	0.49
1:A:459:THR:HG21	1:A:463:ARG:HD2	1.94	0.49
1:A:11:LYS:HE3	1:A:11:LYS:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:LEU:HB3	2:B:274:ILE:HD11	1.94	0.49
1:A:3:SER:N	1:A:117:SER:O	2.45	0.49
1:A:420:PRO:CB	1:A:421:PRO:HD3	2.37	0.49
2:B:423:VAL:CG1	2:B:427:TYR:HE1	2.25	0.49
1:A:26:LEU:HD21	1:A:30:LYS:HB2	1.95	0.49
1:A:479:LEU:O	1:A:482:ILE:HB	2.12	0.49
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.42	0.49
2:B:213:GLY:O	2:B:215:THR:N	2.46	0.49
2:B:369:THR:CG2	2:B:370:GLU:N	2.76	0.49
1:A:34:LEU:HD13	1:A:60:VAL:HG11	1.94	0.48
1:A:484:LEU:O	1:A:486:LEU:N	2.45	0.48
2:B:427:TYR:OXT	2:B:427:TYR:CD1	2.66	0.48
1:A:181:TYR:HB3	3:A:559:TBO:H121	1.94	0.48
1:A:199:ARG:HB2	1:A:199:ARG:NH1	2.27	0.48
1:A:241:VAL:HG11	1:A:266:TRP:CD1	2.48	0.48
1:A:452:LEU:HD23	1:A:470:THR:HA	1.94	0.48
1:A:482:ILE:HD13	1:A:506:ILE:HD11	1.95	0.48
1:A:27:THR:HG23	1:A:30:LYS:H	1.77	0.48
1:A:47:ILE:HG22	1:A:144:TYR:HB3	1.96	0.48
1:A:124:PHE:O	1:A:127:TYR:N	2.47	0.48
1:A:233:GLU:HB3	1:A:240:THR:O	2.13	0.48
1:A:271:TYR:HE1	1:A:314:VAL:H	1.60	0.48
1:A:143:ARG:HG3	1:A:143:ARG:NH1	2.27	0.48
1:A:542:ILE:HG12	1:A:544:GLY:H	1.78	0.48
1:A:546:GLU:O	1:A:549:ASP:HB2	2.14	0.48
2:B:57:ASN:HA	2:B:129:ALA:O	2.12	0.48
1:A:35:VAL:O	1:A:38:CYS:N	2.47	0.48
1:A:77:PHE:O	1:A:80:LEU:N	2.46	0.48
1:A:203:GLU:HA	1:A:203:GLU:OE1	2.13	0.48
1:A:484:LEU:O	1:A:487:GLN:N	2.45	0.48
2:B:12:LEU:HD23	2:B:84:THR:HG23	1.95	0.48
2:B:253:THR:H	2:B:256:ASP:HB2	1.78	0.48
2:B:255:ASN:O	2:B:258:GLN:HB2	2.13	0.48
1:A:419:THR:HB	1:A:420:PRO:CD	2.34	0.48
2:B:319:TYR:CZ	2:B:383:TRP:CD1	3.02	0.48
1:A:239:TRP:O	1:A:240:THR:OG1	2.32	0.48
1:A:254:VAL:HG12	1:A:258:GLN:NE2	2.29	0.48
2:B:131:THR:OG1	2:B:143:ARG:NH1	2.47	0.48
1:A:443:ASP:CG	1:A:444:GLY:H	2.16	0.47
1:A:518:VAL:HG12	1:A:522:ILE:HD11	1.96	0.47
2:B:260:LEU:HD21	2:B:303:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:GLN:HE21	2:B:349:LEU:HD11	1.78	0.47
1:A:255:ASN:C	1:A:259:LYS:HE3	2.35	0.47
2:B:64:LYS:CE	2:B:71:TRP:CZ2	2.97	0.47
2:B:159:ILE:C	2:B:161:GLN:H	2.17	0.47
2:B:401:TRP:CD1	2:B:401:TRP:N	2.82	0.47
1:A:240:THR:CG2	1:A:241:VAL:N	2.77	0.47
1:A:277:ARG:HD2	1:A:334:GLN:CD	2.35	0.47
2:B:136:ASN:CG	2:B:136:ASN:O	2.52	0.47
2:B:154:LYS:HE2	2:B:184:MET:SD	2.55	0.47
2:B:281:LYS:C	2:B:283:LEU:H	2.17	0.47
1:A:329:ILE:O	1:A:392:PRO:HD3	2.14	0.47
1:A:439:THR:HA	1:A:494:ASN:HB2	1.95	0.47
2:B:136:ASN:O	2:B:137:ASN:C	2.52	0.47
1:A:2:ILE:HG22	1:A:3:SER:N	2.29	0.47
2:B:354:TYR:HE1	2:B:374:LYS:HZ2	1.60	0.47
1:A:120:LEU:HD13	1:A:149:LEU:HD23	1.96	0.47
1:A:276:VAL:O	1:A:280:SER:HB2	2.15	0.47
1:A:320:ASP:C	1:A:322:SER:H	2.18	0.47
1:A:369:THR:OG1	1:A:398:TRP:HZ3	1.95	0.47
1:A:410:TRP:HA	1:A:410:TRP:CE3	2.50	0.47
1:A:441:TYR:HD2	1:A:544:GLY:HA3	1.80	0.47
2:B:419:THR:HA	2:B:420:PRO:HD2	1.62	0.47
2:B:203:GLU:HA	2:B:206:ARG:CG	2.43	0.47
1:A:110:ASP:O	1:A:217:PRO:HD2	2.14	0.47
1:A:395:LYS:HA	1:A:414:TRP:HH2	1.80	0.47
1:A:483:TYR:HE1	1:A:524:GLN:HE21	1.63	0.47
1:A:491:LEU:HB3	1:A:529:GLU:OE1	2.15	0.47
2:B:178:ILE:O	2:B:178:ILE:HG22	2.14	0.47
1:A:240:THR:HG22	1:A:241:VAL:O	2.15	0.47
2:B:61:PHE:CE1	2:B:76:ASP:HB2	2.48	0.47
1:A:230:MET:O	1:A:232:TYR:CD1	2.68	0.46
1:A:230:MET:O	1:A:232:TYR:HD1	1.99	0.46
1:A:275:LYS:HG2	1:A:332:GLN:NE2	2.30	0.46
1:A:442:VAL:HG12	1:A:443:ASP:N	2.30	0.46
2:B:103:LYS:HD3	2:B:192:ASP:OD1	2.15	0.46
1:A:77:PHE:CE1	1:A:150:PRO:HB3	2.50	0.46
1:A:229:TRP:CE3	3:A:559:TBO:H151	2.51	0.46
2:B:111:VAL:O	2:B:111:VAL:CG1	2.63	0.46
1:A:237:ASP:OD1	1:A:237:ASP:N	2.48	0.46
1:A:320:ASP:O	1:A:343:GLN:NE2	2.48	0.46
1:A:440:PHE:CE2	1:A:457:TYR:CE1	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLU:CD	1:A:92:LEU:HB2	2.36	0.46
2:B:12:LEU:HD23	2:B:84:THR:CG2	2.45	0.46
2:B:111:VAL:HG12	2:B:115:TYR:HE1	1.79	0.46
2:B:298:GLU:O	2:B:301:LEU:HB2	2.15	0.46
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.98	0.46
1:A:81:ASN:OD1	1:A:153:TRP:HA	2.16	0.46
2:B:327:ALA:HB2	2:B:387:PRO:HB2	1.98	0.46
1:A:189:VAL:HG21	1:A:205:LEU:CD2	2.46	0.46
1:A:482:ILE:CD1	1:A:502:ALA:HB1	2.46	0.46
1:A:252:TRP:HZ3	1:A:256:ASP:HB3	1.81	0.46
1:A:509:GLN:N	1:A:510:PRO:CD	2.78	0.46
1:A:543:GLY:N	2:B:284:ARG:HA	2.24	0.46
2:B:210:LEU:HD12	2:B:210:LEU:HA	1.69	0.46
1:A:92:LEU:HD21	2:B:22:LYS:CE	2.46	0.45
1:A:363:ASN:OD1	1:A:364:ASP:N	2.49	0.45
1:A:472:THR:OG1	1:A:477:THR:HG23	2.16	0.45
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.52	0.45
1:A:34:LEU:HD12	1:A:132:ILE:HG23	1.97	0.45
1:A:86:ASP:O	2:B:55:PRO:HG3	2.16	0.45
1:A:179:VAL:HG12	3:A:559:TBO:H112	1.97	0.45
2:B:246:LEU:HD13	2:B:264:LEU:HD21	1.98	0.45
2:B:342:TYR:CB	2:B:348:ASN:HA	2.46	0.45
2:B:421:PRO:HG2	2:B:424:LYS:HB2	1.98	0.45
1:A:54:ASN:HD21	1:A:126:LYS:HA	1.81	0.45
1:A:267:ALA:HB1	1:A:271:TYR:CD2	2.47	0.45
1:A:467:VAL:HG13	1:A:468:PRO:HD2	1.98	0.45
2:B:214:LEU:HG	2:B:214:LEU:O	2.17	0.45
2:B:202:ILE:O	2:B:205:LEU:N	2.49	0.45
1:A:133:PRO:HB3	1:A:139:THR:CB	2.47	0.45
2:B:36:GLU:O	2:B:37:ILE:C	2.55	0.45
2:B:96:HIS:CD2	2:B:384:GLY:HA3	2.51	0.45
1:A:171:PHE:CE2	1:A:205:LEU:HA	2.51	0.45
1:A:482:ILE:HD11	1:A:502:ALA:HB1	1.99	0.45
2:B:422:LEU:C	2:B:424:LYS:H	2.20	0.45
2:B:266:TRP:CE3	2:B:269:GLN:HB2	2.52	0.45
2:B:279:LEU:HD12	2:B:279:LEU:HA	1.84	0.45
1:A:398:TRP:NE1	1:A:402:TRP:CD1	2.85	0.45
1:A:31:ILE:O	1:A:35:VAL:HG23	2.17	0.44
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.99	0.44
1:A:459:THR:CG2	1:A:463:ARG:HD2	2.47	0.44
2:B:160:PHE:CD2	2:B:164:MET:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ILE:O	2:B:416:PHE:HB3	2.17	0.44
2:B:422:LEU:O	2:B:424:LYS:N	2.50	0.44
1:A:194:GLU:HB2	1:A:197:GLN:HB3	1.97	0.44
1:A:320:ASP:O	1:A:322:SER:N	2.50	0.44
2:B:319:TYR:CD2	2:B:383:TRP:HD1	2.35	0.44
1:A:82:LYS:HA	1:A:82:LYS:HD3	1.76	0.44
1:A:275:LYS:HB3	1:A:336:GLN:HE22	1.82	0.44
1:A:302:GLU:O	1:A:305:GLU:HB3	2.17	0.44
2:B:105:SER:HA	2:B:234:LEU:O	2.18	0.44
2:B:210:LEU:HD13	2:B:215:THR:O	2.17	0.44
2:B:253:THR:HB	2:B:256:ASP:OD1	2.16	0.44
2:B:380:ILE:O	2:B:384:GLY:HA2	2.17	0.44
2:B:206:ARG:HB3	2:B:206:ARG:NH1	2.33	0.44
2:B:394:GLN:HG2	2:B:397:THR:H	1.83	0.44
1:A:106:VAL:CG1	1:A:107:THR:H	2.30	0.44
1:A:477:THR:O	1:A:481:ALA:N	2.50	0.44
2:B:56:TYR:CE2	2:B:127:TYR:CE1	3.06	0.44
2:B:164:MET:O	2:B:164:MET:SD	2.75	0.44
2:B:325:LEU:HD11	2:B:383:TRP:CE3	2.53	0.44
2:B:398:TRP:C	2:B:400:THR:N	2.70	0.44
1:A:368:LEU:CD2	1:A:393:ILE:HG21	2.47	0.44
1:A:426:TRP:HA	1:A:426:TRP:HE3	1.80	0.44
1:A:490:GLY:O	1:A:528:LYS:CE	2.65	0.44
2:B:81:ASN:ND2	2:B:154:LYS:HG3	2.32	0.44
2:B:104:LYS:O	2:B:235:HIS:HA	2.17	0.44
1:A:106:VAL:HA	1:A:190:GLY:HA2	2.00	0.43
1:A:172:LYS:HA	1:A:175:ASN:O	2.18	0.43
1:A:446:ALA:CB	1:A:472:THR:O	2.66	0.43
2:B:368:LEU:O	2:B:372:VAL:HG23	2.18	0.43
1:A:365:VAL:O	1:A:366:LYS:C	2.56	0.43
1:A:381:VAL:HG22	2:B:25:PRO:HG3	1.99	0.43
2:B:149:LEU:HD23	2:B:149:LEU:HA	1.83	0.43
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.53	0.43
2:B:338:THR:HG22	2:B:339:TYR:N	2.33	0.43
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.59	0.43
1:A:122:GLU:HA	1:A:125:ARG:NE	2.33	0.43
1:A:178:ILE:HG22	1:A:189:VAL:HG13	2.01	0.43
2:B:13:LYS:HA	2:B:14:PRO:HD2	1.83	0.43
1:A:326:ILE:HG21	1:A:342:TYR:CE1	2.53	0.43
1:A:327:ALA:O	1:A:389:PHE:HA	2.18	0.43
1:A:328:GLU:HA	1:A:390:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:THR:CB	1:A:420:PRO:HD2	2.35	0.43
1:A:500:GLN:OE1	1:A:500:GLN:HA	2.18	0.43
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.99	0.43
2:B:318:TYR:O	2:B:320:ASP:N	2.52	0.43
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.01	0.43
1:A:274:ILE:HA	1:A:306:ASN:OD1	2.18	0.43
2:B:160:PHE:O	2:B:160:PHE:CD2	2.72	0.43
2:B:253:THR:O	2:B:256:ASP:HB2	2.19	0.43
1:A:97:PRO:HG2	1:A:232:TYR:CG	2.53	0.43
1:A:442:VAL:HG13	1:A:481:ALA:HB1	2.01	0.43
1:A:495:ILE:HG22	1:A:496:VAL:N	2.34	0.43
2:B:10:VAL:HG13	2:B:88:TRP:CE2	2.54	0.43
1:A:334:GLN:CG	1:A:335:GLY:H	2.31	0.43
1:A:418:ASN:OD1	1:A:419:THR:N	2.51	0.43
1:A:484:LEU:O	1:A:485:ALA:C	2.56	0.43
2:B:23:GLN:NE2	2:B:24:TRP:O	2.52	0.43
1:A:255:ASN:O	1:A:259:LYS:HE3	2.18	0.43
1:A:279:LEU:HD11	1:A:303:LEU:HB2	2.00	0.43
1:A:545:ASN:O	1:A:546:GLU:C	2.56	0.43
2:B:391:LEU:HD23	2:B:391:LEU:HA	1.79	0.43
1:A:325:LEU:HD11	1:A:383:TRP:HB2	2.00	0.43
2:B:28:GLU:O	2:B:29:GLU:C	2.56	0.43
2:B:101:LYS:O	2:B:236:PRO:HB2	2.17	0.43
2:B:271:TYR:O	2:B:273:GLY:N	2.52	0.43
2:B:354:TYR:CD2	2:B:371:ALA:HB2	2.54	0.43
1:A:490:GLY:O	1:A:528:LYS:HE2	2.18	0.42
1:A:497:THR:HG22	1:A:498:ASP:H	1.83	0.42
2:B:211:ARG:HB2	2:B:212:TRP:H	1.66	0.42
2:B:164:MET:O	2:B:168:LEU:HD12	2.19	0.42
2:B:339:TYR:O	2:B:340:GLN:HG3	2.19	0.42
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.48	0.42
1:A:90:VAL:HG13	1:A:158:ALA:HA	2.00	0.42
1:A:122:GLU:O	1:A:122:GLU:HG3	2.19	0.42
2:B:266:TRP:HZ3	2:B:269:GLN:NE2	2.18	0.42
2:B:330:GLN:CG	2:B:340:GLN:HE22	2.31	0.42
1:A:124:PHE:O	1:A:125:ARG:C	2.57	0.42
1:A:312:GLU:HA	1:A:313:PRO:HD2	1.74	0.42
1:A:410:TRP:HA	1:A:410:TRP:HE3	1.83	0.42
1:A:170:PRO:O	1:A:173:LYS:HB3	2.20	0.42
1:A:480:GLN:HA	1:A:517:LEU:HD11	2.01	0.42
1:A:547:GLN:O	1:A:550:LYS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:TRP:CH2	3:A:559:TBO:H151	2.55	0.42
1:A:373:GLN:O	1:A:374:LYS:C	2.57	0.42
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.83	0.42
2:B:213:GLY:C	2:B:215:THR:H	2.22	0.42
2:B:335:GLY:HA3	2:B:357:MET:HA	2.02	0.42
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.76	0.42
2:B:319:TYR:CE2	2:B:383:TRP:CD1	2.98	0.42
2:B:363:ASN:O	2:B:366:LYS:HB3	2.19	0.42
1:A:317:VAL:HG11	1:A:347:LYS:HB3	2.01	0.42
1:A:550:LYS:HA	1:A:550:LYS:HD3	1.82	0.42
2:B:79:GLU:HG3	2:B:83:ARG:HH11	1.85	0.42
2:B:207:GLN:O	2:B:208:HIS:C	2.57	0.42
1:A:24:TRP:HA	1:A:25:PRO:HD2	1.72	0.42
1:A:225:PRO:N	1:A:226:PRO:HD2	2.35	0.42
1:A:362:THR:HG22	1:A:363:ASN:N	2.35	0.42
1:A:369:THR:O	1:A:370:GLU:C	2.57	0.42
1:A:440:PHE:CE2	1:A:459:THR:HG22	2.55	0.42
2:B:10:VAL:HG12	2:B:11:LYS:N	2.35	0.42
2:B:84:THR:HG21	2:B:124:PHE:CE1	2.55	0.42
2:B:274:ILE:CG1	2:B:275:LYS:N	2.82	0.42
2:B:276:VAL:HG22	2:B:276:VAL:O	2.20	0.42
2:B:312:GLU:H	2:B:312:GLU:HG3	1.67	0.42
1:A:320:ASP:C	1:A:322:SER:N	2.73	0.42
1:A:329:ILE:HD11	1:A:375:ILE:CD1	2.46	0.42
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.55	0.42
1:A:486:LEU:CA	1:A:489:SER:HG	2.28	0.42
1:A:197:GLN:O	1:A:200:THR:HB	2.20	0.41
1:A:277:ARG:CD	1:A:334:GLN:OE1	2.67	0.41
2:B:77:PHE:CD1	2:B:80:LEU:HD23	2.55	0.41
2:B:216:THR:HA	2:B:217:PRO:HD3	1.65	0.41
2:B:393:ILE:CG2	2:B:398:TRP:HB2	2.49	0.41
2:B:143:ARG:CG	2:B:143:ARG:NH1	2.75	0.41
2:B:315:HIS:O	2:B:315:HIS:CD2	2.74	0.41
2:B:325:LEU:CD1	2:B:383:TRP:CE3	3.03	0.41
1:A:42:GLU:OE2	1:A:49:LYS:HG2	2.21	0.41
1:A:49:LYS:HA	1:A:144:TYR:HA	2.01	0.41
1:A:111:VAL:CG1	1:A:114:ALA:HB2	2.41	0.41
1:A:170:PRO:HG2	1:A:171:PHE:H	1.86	0.41
1:A:247:PRO:O	1:A:252:TRP:CH2	2.74	0.41
1:A:439:THR:CG2	2:B:289:LEU:HG	2.50	0.41
1:A:91:GLN:C	1:A:93:GLY:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:CD1	1:A:156:SER:HB3	2.55	0.41
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.55	0.41
1:A:248:GLU:HG3	1:A:248:GLU:O	2.21	0.41
1:A:314:VAL:HG12	1:A:315:HIS:N	2.34	0.41
1:A:410:TRP:CE3	1:A:411:ILE:N	2.86	0.41
1:A:469:LEU:HD13	1:A:477:THR:HG22	2.03	0.41
2:B:113:ASP:O	2:B:116:PHE:HB2	2.20	0.41
1:A:47:ILE:HG23	1:A:145:GLN:O	2.21	0.41
1:A:208:HIS:CE1	1:A:212:TRP:NE1	2.88	0.41
1:A:503:LEU:HD22	1:A:535:TRP:CD1	2.55	0.41
1:A:12:LEU:HD22	1:A:83:ARG:O	2.20	0.41
1:A:23:GLN:HG3	1:A:59:PRO:HB2	2.02	0.41
1:A:111:VAL:O	1:A:114:ALA:HB2	2.21	0.41
1:A:189:VAL:HG21	1:A:205:LEU:HD22	2.03	0.41
1:A:408:ALA:HB3	2:B:393:ILE:CG1	2.43	0.41
1:A:470:THR:O	1:A:471:ASN:HB2	2.21	0.41
2:B:159:ILE:O	2:B:161:GLN:N	2.53	0.41
2:B:281:LYS:C	2:B:283:LEU:N	2.74	0.41
1:A:329:ILE:HD12	1:A:391:LEU:HD21	2.00	0.41
2:B:74:LEU:HD21	2:B:411:ILE:HD12	2.03	0.41
1:A:28:GLU:O	1:A:31:ILE:HB	2.21	0.40
1:A:148:VAL:O	1:A:150:PRO:HD3	2.21	0.40
1:A:433:PRO:CG	2:B:255:ASN:CG	2.89	0.40
1:A:536:VAL:HA	1:A:537:PRO:HD2	1.91	0.40
2:B:206:ARG:HB3	2:B:206:ARG:CZ	2.51	0.40
2:B:330:GLN:CD	2:B:340:GLN:HE22	2.25	0.40
1:A:331:LYS:HE3	1:A:334:GLN:O	2.20	0.40
1:A:443:ASP:CG	1:A:444:GLY:N	2.74	0.40
2:B:335:GLY:O	2:B:337:TRP:HD1	2.04	0.40
1:A:84:THR:HG22	1:A:85:GLN:N	2.36	0.40
2:B:13:LYS:O	2:B:16:MET:HB2	2.20	0.40
2:B:91:GLN:C	2:B:93:GLY:N	2.74	0.40
2:B:191:SER:HB2	2:B:193:LEU:HG	2.03	0.40
1:A:188:TYR:CD2	3:A:559:TBO:H163	2.57	0.40
1:A:226:PRO:O	1:A:226:PRO:HG2	2.21	0.40
1:A:405:TYR:O	2:B:331:LYS:HD3	2.22	0.40
2:B:77:PHE:CE2	2:B:150:PRO:HB2	2.57	0.40
2:B:109:LEU:HD12	2:B:187:LEU:CD2	2.51	0.40
2:B:165:THR:O	2:B:168:LEU:N	2.47	0.40
2:B:169:GLU:HB3	2:B:170:PRO:CD	2.51	0.40
1:A:89:GLU:O	1:A:90:VAL:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:CG1	1:A:347:LYS:HB3	2.51	0.40
1:A:329:ILE:HG22	1:A:330:GLN:N	2.37	0.40
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.71	0.40
2:B:114:ALA:C	2:B:116:PHE:N	2.75	0.40
2:B:349:LEU:H	2:B:349:LEU:HG	1.60	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	554/558 (99%)	426 (77%)	104 (19%)	24 (4%)	2	15
2	B	425/427 (100%)	322 (76%)	67 (16%)	36 (8%)	1	4
All	All	979/985 (99%)	748 (76%)	171 (18%)	60 (6%)	1	8

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	A	90	VAL
1	A	345	PRO
1	A	358	ARG
1	A	420	PRO
2	B	115	TYR
2	B	226	PRO
2	B	295	LEU
2	B	316	GLY
2	B	317	VAL
1	A	25	PRO
1	A	112	GLY
1	A	284	ARG

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Mol	Chain	Res	Type
1	A	556	ILE
2	B	296	THR
2	B	423	VAL
2	B	425	LEU
1	A	122	GLU
1	A	242	GLN
1	A	251	SER
1	A	277	ARG
1	A	356	ARG
2	B	59	PRO
2	B	160	PHE
2	B	211	ARG
2	B	212	TRP
2	B	214	LEU
2	B	233	GLU
2	B	395	LYS
1	A	114	ALA
1	A	426	TRP
1	A	546	GLU
2	B	114	ALA
2	B	116	PHE
2	B	319	TYR
2	B	4	PRO
2	B	148	VAL
2	B	185	ASP
2	B	240	THR
1	A	29	GLU
1	A	195	ILE
1	A	459	THR
2	B	195	ILE
2	B	232	TYR
2	B	244	ILE
2	B	272	PRO
2	B	273	GLY
1	A	63	ILE
1	A	226	PRO
2	B	37	ILE
2	B	420	PRO
2	B	213	GLY
2	B	359	GLY
1	A	321	PRO
1	A	359	GLY

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Mol	Chain	Res	Type
2	B	55	PRO
2	B	99	GLY
2	B	217	PRO
2	B	236	PRO
2	B	135	ILE

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	454/498 (91%)	398 (88%)	56 (12%)	4	21
2	B	367/389 (94%)	323 (88%)	44 (12%)	5	22
All	All	821/887 (93%)	721 (88%)	100 (12%)	5	21

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	28	GLU
1	A	30	LYS
1	A	31	ILE
1	A	49	LYS
1	A	53	GLU
1	A	58	THR
1	A	63	ILE
1	A	64	LYS
1	A	65	LYS
1	A	67	ASP
1	A	70	LYS
1	A	78	ARG
1	A	88	TRP
1	A	90	VAL
1	A	91	GLN
1	A	107	THR
1	A	131	THR

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Mol	Chain	Res	Type
1	A	142	ILE
1	A	143	ARG
1	A	150	PRO
1	A	172	LYS
1	A	177	ASP
1	A	186	ASP
1	A	187	LEU
1	A	199	ARG
1	A	202	ILE
1	A	208	HIS
1	A	210	LEU
1	A	268	SER
1	A	296	THR
1	A	303	LEU
1	A	334	GLN
1	A	340	GLN
1	A	344	GLU
1	A	345	PRO
1	A	393	ILE
1	A	395	LYS
1	A	405	TYR
1	A	409	THR
1	A	411	ILE
1	A	417	VAL
1	A	426	TRP
1	A	471	ASN
1	A	474	ASN
1	A	491	LEU
1	A	497	THR
1	A	512	LYS
1	A	513	SER
1	A	520	GLN
1	A	536	VAL
1	A	540	LYS
1	A	542	ILE
1	A	545	ASN
1	A	546	GLU
1	A	553	SER
2	B	6	GLU
2	B	20	LYS
2	B	27	THR
2	B	38	CYS

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Mol	Chain	Res	Type
2	B	50	ILE
2	B	55	PRO
2	B	74	LEU
2	B	88	TRP
2	B	91	GLN
2	B	92	LEU
2	B	101	LYS
2	B	105	SER
2	B	111	VAL
2	B	115	TYR
2	B	122	GLU
2	B	132	ILE
2	B	143	ARG
2	B	178	ILE
2	B	180	ILE
2	B	184	MET
2	B	185	ASP
2	B	200	THR
2	B	240	THR
2	B	266	TRP
2	B	283	LEU
2	B	284	ARG
2	B	287	LYS
2	B	290	THR
2	B	293	ILE
2	B	298	GLU
2	B	301	LEU
2	B	315	HIS
2	B	318	TYR
2	B	325	LEU
2	B	332	GLN
2	B	356	ARG
2	B	369	THR
2	B	379	SER
2	B	407	GLN
2	B	410	TRP
2	B	414	TRP
2	B	422	LEU
2	B	425	LEU
2	B	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	208	HIS
1	A	235	HIS
1	A	265	ASN
1	A	269	GLN
1	A	332	GLN
1	A	367	GLN
1	A	373	GLN
1	A	407	GLN
1	A	474	ASN
1	A	524	GLN
2	B	145	GLN
2	B	147	ASN
2	B	207	GLN
2	B	255	ASN
2	B	315	HIS
2	B	330	GLN
2	B	340	GLN
2	B	343	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 monosaccharides 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	TBO	A	559	-	18,23,23	2.87	5 (27%)	17,34,34	2.61	5 (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	TBO	A	559	-	-	1/4/17/17	0/2/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	559	TBO	C4-N3	-9.07	1.42	1.49
3	A	559	TBO	C10-C9	4.39	1.45	1.36
3	A	559	TBO	C12-N6	3.30	1.52	1.47
3	A	559	TBO	C7-N6	-2.97	1.43	1.47
3	A	559	TBO	C1A-N1	2.09	1.45	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	559	TBO	C16-C14-C15	7.48	131.13	114.60
3	A	559	TBO	C15-C14-C13	-5.32	107.28	122.65
3	A	559	TBO	C9-C8-C7A	-2.87	118.77	122.50
3	A	559	TBO	C4-C5-N6	2.49	116.17	111.83
3	A	559	TBO	C12-C13-C14	2.00	130.84	127.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
3	A	559	TBO	C13-C12-N6-C7

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	559	TBO	7	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 TBO A 559

Bond lengths

Bond angles

Torsions

Rings
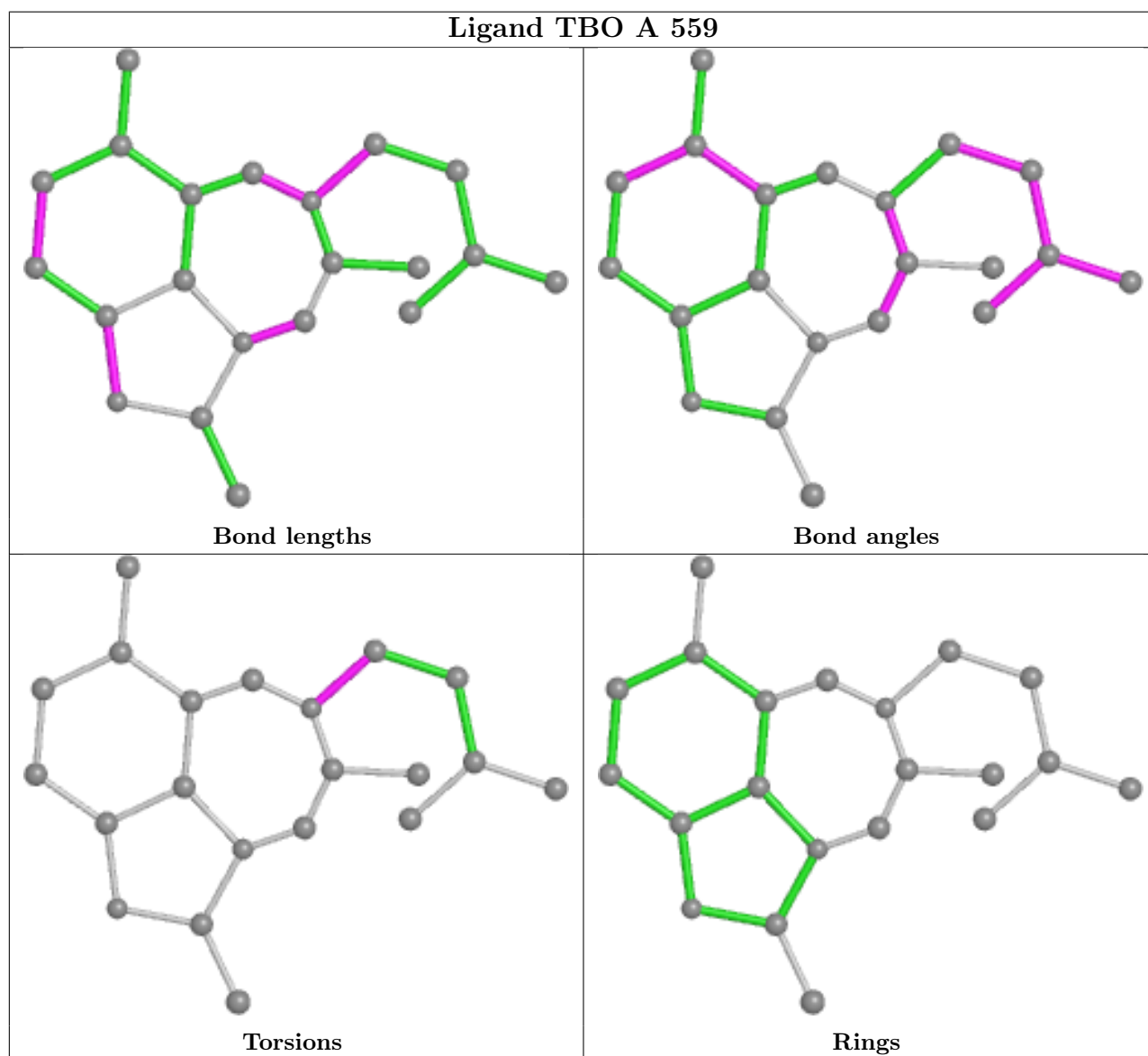
5.7 Other polymers ⓘ

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	558/558 (100%)	-0.56	4 (0%)	87	69	10, 43, 60, 67	0
2	B	427/427 (100%)	-0.59	5 (1%)	79	54	10, 35, 61, 69	0
All	All	985/985 (100%)	-0.57	9 (0%)	84	63	10, 41, 60, 69	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	LYS	3.4
2	B	3	SER	3.4
2	B	222	GLN	3.1
2	B	2	ILE	3.0
1	A	141	GLY	2.9
1	A	136	ASN	2.8
1	A	547	GLN	2.7
2	B	68	SER	2.1
2	B	230	MET	2.0

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

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

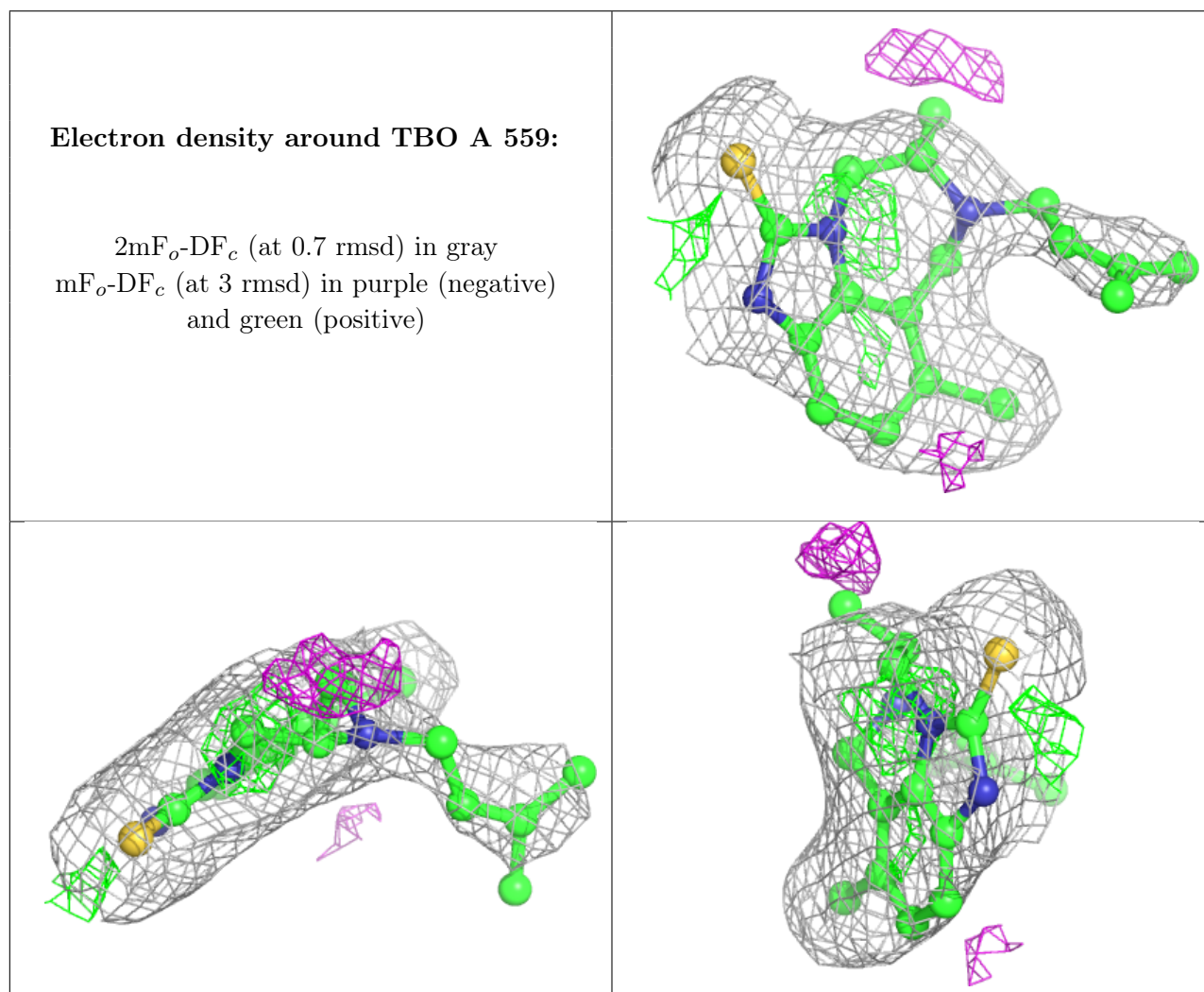## 6.3 Carbohydrates ⓘ

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	TBO	A	559	21/21	0.93	0.24	45,45,45,45	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 TBO A 559:

$2mF_o$-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 ⓘ

There are no such residues in this entry.