WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 07:48 PM EDT

PDB ID	:	2B5J
Title	:	Crystal structure of HIV-1 reverse transcriptase (RT) in complex with JANSSEN-R165481
Authors	:	Himmel, D.H.; Das, K.; Clark Jr., A.D.; Hughes, S.H.; Benjahad, A.; Oumouch, S.; Guillemont, J.; Coupa, S.; Poncelet, A.; Csoka, I.; Meyer, C.; Andries, K.; Mguyen, C.H.; Grierson, D.S.; Arnold, E.
Deposited on	:	2005-09-28
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references ①) 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 2.90 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		0.293
Clashscore		45
Ramachandran outliers		7.6%
Sidechain outliers		10.2%
RSRZ outliers		3.2%

Worse ← → Better

▮ Percentile relative to all X-ray structures

◫ Percentile relative to X-ray structures of similar resolution
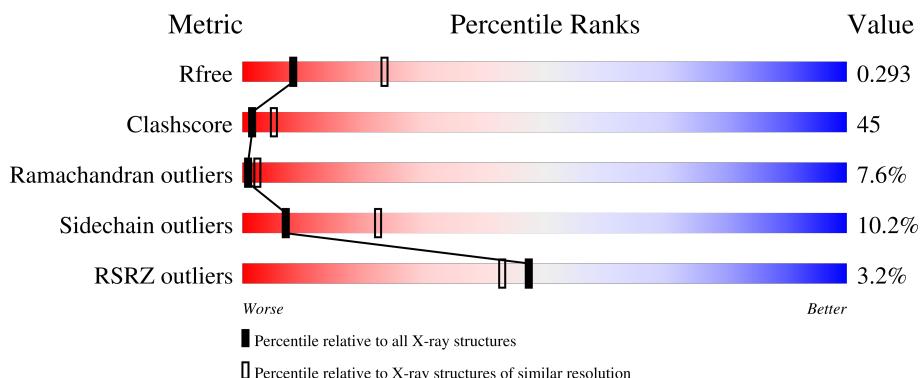
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	560	2% / 35% 52% 11% ••
2	B	430	5% / 34% 54% 11% •
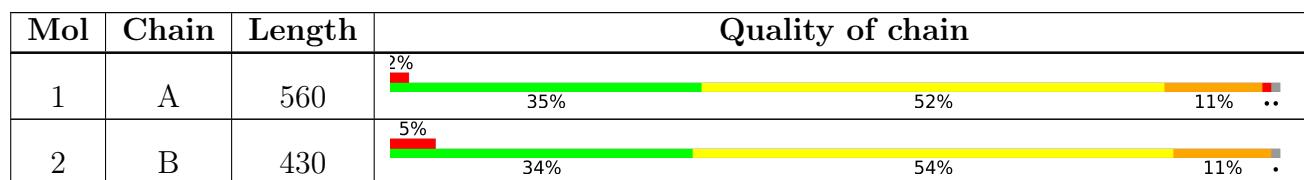
2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7924 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 P66 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4431	2864	733	827	7			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called Reverse transcriptase P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3469	2258	571	634	6			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is (2E)-3-{3-[(5-ETHYL-3-IODO-6-METHYL-2-OXO-1,2-DIHYDROP YRIDIN-4-YL)OXY]PHENYL}ACRYLONITRILE (three-letter code: 3AC) (formula: $C_{17}H_{15}IN_2O_2$).

3AC
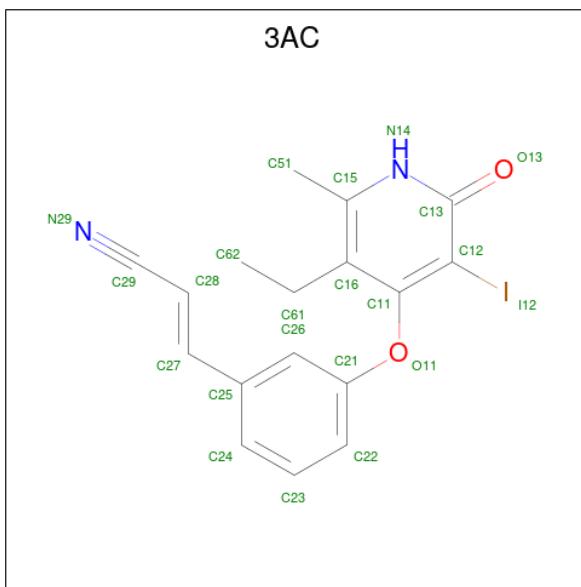
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	I	N	O	0	0
			22	17	1	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	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: Reverse transcriptase P66 SUBUNIT

Chain A:
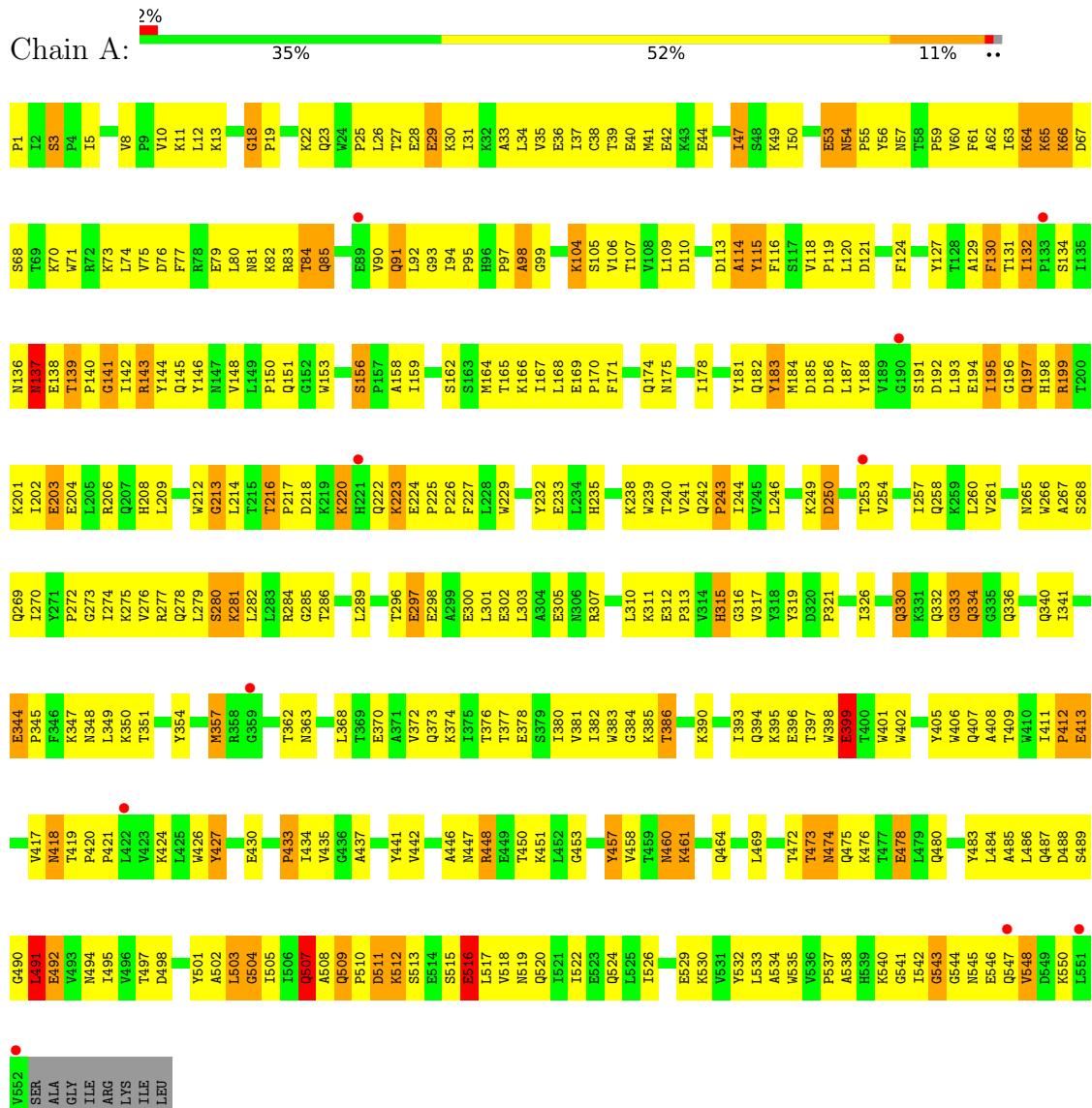
• Molecule 2: Reverse transcriptase P51 SUBUNIT

Chain B:
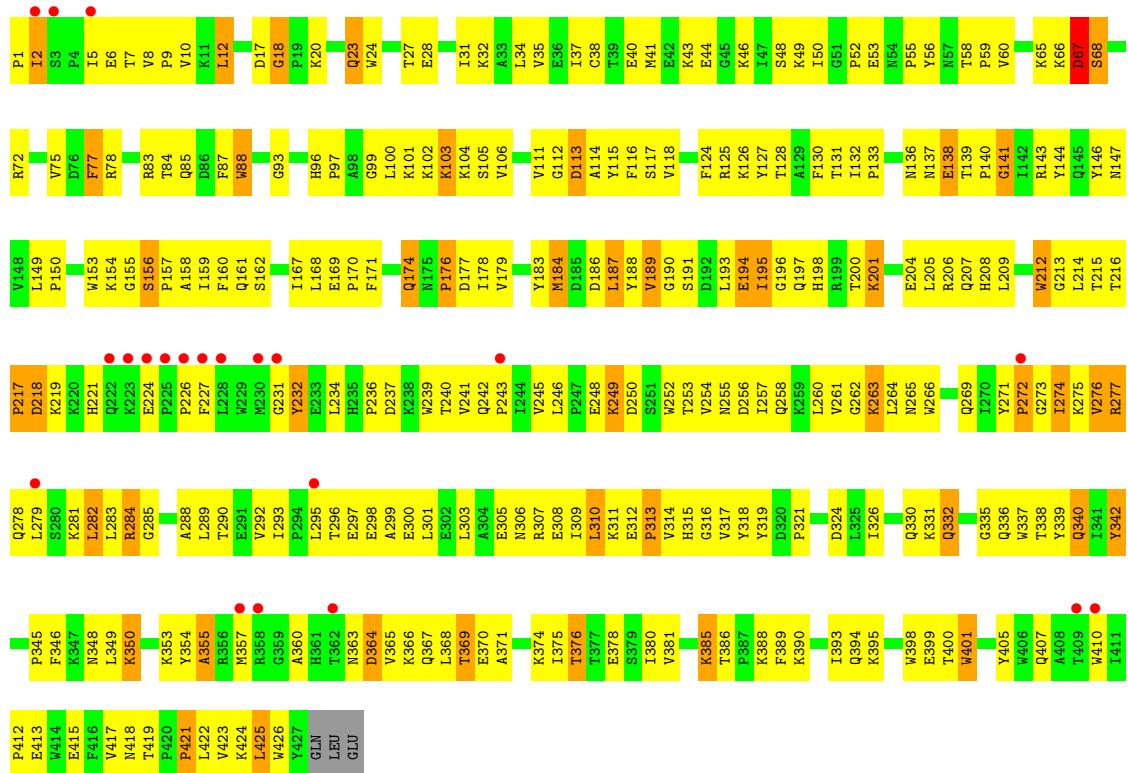
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	224.59Å 69.30Å 105.02Å 90.00° 106.47° 90.00°	Depositor
Resolution (Å)	19.92 – 2.90 32.76 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.8 (19.92-2.90) 93.6 (32.76-2.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.304 0.247 , 0.293	Depositor DCC
R_{free} test set	1609 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	79.6	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 69.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7924	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: MN, 3AC

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	0.43	0/4546	0.76	2/6185 (0.0%)
2	B	0.47	0/3570	0.77	2/4861 (0.0%)
All	All	0.45	0/8116	0.76	4/11046 (0.0%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	TRP	N-CA-C	5.27	125.22	111.00
1	A	67	ASP	N-CA-C	-5.12	97.16	111.00
1	A	139	THR	N-CA-C	5.09	124.76	111.00
2	B	88	TRP	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	318	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	4431	0	4413	434	0
2	B	3469	0	3462	306	0
3	A	1	0	0	0	0
4	A	22	0	15	4	0
5	A	1	0	0	0	0
All	All	7924	0	7890	718	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (718) 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:132:ILE:HG13	1:A:142:ILE:HB	1.20	1.14
1:A:55:PRO:HB3	1:A:143:ARG:HH12	1.13	1.12
1:A:362:THR:HG22	1:A:363:ASN:H	1.16	1.10
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.18	1.09
1:A:242:GLN:HB2	1:A:243:PRO:HD3	1.24	1.09
2:B:206:ARG:HH22	2:B:219:LYS:HG2	1.15	1.07
1:A:35:VAL:HG22	1:A:132:ILE:HD12	1.29	1.07
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.42	1.01
1:A:195:ILE:HD12	1:A:195:ILE:H	1.25	1.01
1:A:240:THR:HG22	1:A:241:VAL:H	1.25	1.01
1:A:542:ILE:HD11	1:A:546:GLU:HA	1.41	1.01
1:A:53:GLU:C	1:A:55:PRO:HD3	1.85	0.97
1:A:183:TYR:CD2	1:A:184:MET:HG2	2.00	0.96
2:B:118:VAL:HB	2:B:149:LEU:HD12	1.47	0.95
1:A:242:GLN:HB2	1:A:243:PRO:CD	1.99	0.92
1:A:65:LYS:HD3	1:A:66:LYS:HG3	1.55	0.87
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.10	0.87
1:A:478:GLU:HA	1:A:478:GLU:OE1	1.76	0.85
2:B:1:PRO:HD2	2:B:117:SER:HA	1.58	0.85
1:A:382:ILE:O	2:B:136:ASN:HB2	1.77	0.84
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.57	0.84
2:B:174:GLN:O	2:B:176:PRO:HD3	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:N	1:A:55:PRO:HD3	1.93	0.83
1:A:64:LYS:HG3	1:A:71:TRP:HA	1.61	0.82
2:B:275:LYS:HB2	2:B:277:ARG:HE	1.42	0.82
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.61	0.82
2:B:206:ARG:NH2	2:B:219:LYS:HG2	1.93	0.82
1:A:183:TYR:HD2	1:A:184:MET:HG2	1.41	0.81
1:A:362:THR:HG22	1:A:363:ASN:N	1.94	0.81
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.63	0.81
1:A:195:ILE:O	1:A:199:ARG:HB2	1.81	0.81
2:B:31:ILE:O	2:B:35:VAL:HG23	1.81	0.81
1:A:242:GLN:CB	1:A:243:PRO:HD3	2.09	0.80
2:B:149:LEU:HD21	2:B:159:ILE:HD12	1.63	0.80
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.45	0.80
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.17	0.80
1:A:368:LEU:O	1:A:372:VAL:HG23	1.82	0.79
1:A:434:ILE:HG21	1:A:492:GLU:HG2	1.63	0.79
1:A:537:PRO:HB2	1:A:541:GLY:HA3	1.63	0.79
1:A:376:THR:O	1:A:380:ILE:HG13	1.84	0.78
1:A:460:ASN:HD22	1:A:461:LYS:N	1.82	0.78
1:A:317:VAL:HG12	1:A:348:ASN:O	1.84	0.78
1:A:341:ILE:HG22	1:A:349:LEU:HD12	1.66	0.77
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.64	0.77
1:A:540:LYS:HE3	2:B:265:ASN:HD21	1.50	0.77
1:A:460:ASN:ND2	1:A:461:LYS:N	2.32	0.76
1:A:483:TYR:CE2	1:A:487:GLN:NE2	2.53	0.76
2:B:276:VAL:CG2	2:B:279:LEU:HB3	2.16	0.76
1:A:29:GLU:HG2	1:A:30:LYS:N	1.99	0.76
2:B:104:LYS:HG2	2:B:237:ASP:OD2	1.85	0.76
1:A:57:ASN:HD22	1:A:143:ARG:HH21	1.33	0.75
2:B:253:THR:HG22	2:B:292:VAL:HA	1.66	0.75
1:A:284:ARG:C	1:A:286:THR:H	1.88	0.75
1:A:376:THR:HG23	1:A:386:THR:HG22	1.69	0.75
1:A:23:GLN:OE1	1:A:60:VAL:N	2.20	0.74
1:A:509:GLN:N	1:A:510:PRO:HD3	2.02	0.74
1:A:195:ILE:H	1:A:195:ILE:CD1	1.98	0.74
1:A:518:VAL:O	1:A:522:ILE:HG13	1.85	0.74
2:B:65:LYS:HG3	2:B:72:ARG:HG3	1.68	0.74
2:B:149:LEU:HB3	2:B:156:SER:OG	1.87	0.74
1:A:138:GLU:O	1:A:140:PRO:HD3	1.87	0.74
1:A:376:THR:HG23	1:A:386:THR:CG2	2.18	0.74
1:A:508:ALA:O	1:A:509:GLN:HB2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:GLU:HG2	2:B:32:LYS:HE3	1.69	0.74
1:A:545:ASN:HA	1:A:548:VAL:HG23	1.70	0.73
1:A:186:ASP:HB3	1:A:188:TYR:CE2	2.23	0.73
2:B:277:ARG:HD3	2:B:277:ARG:N	2.03	0.73
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.24	0.73
2:B:241:VAL:HG12	2:B:242:GLN:N	2.04	0.73
1:A:132:ILE:CG1	1:A:142:ILE:HB	2.12	0.72
1:A:195:ILE:HD12	1:A:195:ILE:N	2.03	0.72
2:B:66:LYS:HZ1	2:B:218:ASP:HB2	1.55	0.72
1:A:238:LYS:HA	1:A:316:GLY:O	1.88	0.72
2:B:281:LYS:HG2	2:B:284:ARG:NH1	2.05	0.72
1:A:301:LEU:O	1:A:305:GLU:HG3	1.90	0.72
1:A:60:VAL:HG22	1:A:130:PHE:HB2	1.72	0.71
1:A:270:ILE:O	1:A:272:PRO:HD3	1.90	0.71
1:A:137:ASN:N	1:A:137:ASN:HD22	1.88	0.71
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.19	0.71
1:A:19:PRO:O	1:A:56:TYR:HB3	1.91	0.71
2:B:357:MET:SD	2:B:360:ALA:HB3	2.31	0.70
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.26	0.70
2:B:345:PRO:HB2	2:B:346:PHE:CD1	2.26	0.70
1:A:109:LEU:HD13	1:A:216:THR:HG21	1.74	0.70
1:A:60:VAL:C	1:A:61:PHE:HD1	1.95	0.70
1:A:8:VAL:CG2	1:A:159:ILE:HG23	2.21	0.69
1:A:63:ILE:HG22	1:A:64:LYS:N	2.07	0.69
1:A:426:TRP:O	1:A:526:ILE:HG12	1.93	0.69
1:A:494:ASN:HD22	2:B:289:LEU:HD12	1.58	0.69
2:B:157:PRO:HG2	2:B:158:ALA:H	1.56	0.69
1:A:315:HIS:H	1:A:315:HIS:CD2	2.11	0.69
1:A:55:PRO:HB3	1:A:143:ARG:NH1	1.98	0.69
2:B:206:ARG:HH22	2:B:219:LYS:CG	2.02	0.69
1:A:284:ARG:O	1:A:286:THR:N	2.25	0.69
2:B:274:ILE:HG12	2:B:309:ILE:HD12	1.74	0.68
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.74	0.68
1:A:64:LYS:HE3	1:A:71:TRP:CB	2.24	0.68
1:A:246:LEU:HD23	1:A:246:LEU:H	1.58	0.67
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.15	0.67
2:B:224:GLU:O	2:B:226:PRO:HD3	1.95	0.67
1:A:115:TYR:H	1:A:115:TYR:HD2	1.41	0.67
2:B:78:ARG:HD3	2:B:412:PRO:O	1.95	0.67
2:B:303:LEU:HD21	2:B:307:ARG:HH12	1.60	0.67
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:PRO:HB2	2:B:346:PHE:HD1	1.60	0.67
1:A:426:TRP:HB3	1:A:526:ILE:HD11	1.76	0.67
2:B:100:LEU:O	2:B:100:LEU:HD12	1.95	0.66
1:A:34:LEU:HD13	1:A:132:ILE:HG22	1.77	0.66
1:A:54:ASN:N	1:A:55:PRO:CD	2.58	0.66
2:B:66:LYS:C	2:B:68:SER:H	1.96	0.66
1:A:279:LEU:HD12	1:A:279:LEU:H	1.60	0.66
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	2.30	0.66
1:A:56:TYR:O	1:A:143:ARG:NH2	2.29	0.66
1:A:242:GLN:O	1:A:244:ILE:N	2.27	0.66
1:A:509:GLN:H	1:A:510:PRO:HD3	1.58	0.65
1:A:91:GLN:HE21	2:B:140:PRO:HA	1.61	0.65
2:B:20:LYS:NZ	2:B:55:PRO:HB2	2.11	0.65
1:A:132:ILE:HG13	1:A:142:ILE:CB	2.13	0.65
1:A:279:LEU:HD12	1:A:302:GLU:OE1	1.96	0.65
2:B:276:VAL:HG22	2:B:279:LEU:HB3	1.79	0.65
1:A:280:SER:C	1:A:282:LEU:H	1.99	0.65
1:A:170:PRO:HB2	1:A:174:GLN:HE21	1.61	0.65
2:B:101:LYS:O	2:B:236:PRO:HB2	1.96	0.64
1:A:413:GLU:HA	1:A:413:GLU:OE1	1.97	0.64
2:B:277:ARG:N	2:B:277:ARG:CD	2.59	0.64
1:A:41:MET:HB3	1:A:47:ILE:HD11	1.80	0.64
1:A:277:ARG:HH11	1:A:334:GLN:HB2	1.62	0.64
2:B:277:ARG:HD3	2:B:277:ARG:H	1.62	0.64
1:A:276:VAL:HG12	1:A:276:VAL:O	1.96	0.64
1:A:249:LYS:HG3	1:A:250:ASP:H	1.63	0.64
2:B:249:LYS:HG2	2:B:252:TRP:CE2	2.33	0.64
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.79	0.64
1:A:49:LYS:HA	1:A:143:ARG:O	1.99	0.63
2:B:10:VAL:HG13	2:B:88:TRP:CZ2	2.33	0.63
1:A:10:VAL:HG21	1:A:153:TRP:CH2	2.31	0.63
1:A:244:ILE:HD11	1:A:267:ALA:HB2	1.80	0.63
1:A:65:LYS:NZ	1:A:66:LYS:HG2	2.14	0.63
1:A:233:GLU:OE2	1:A:242:GLN:HG2	1.99	0.63
1:A:427:TYR:OH	1:A:509:GLN:HA	1.99	0.63
1:A:22:LYS:HD3	1:A:23:GLN:H	1.63	0.63
1:A:460:ASN:HD21	1:A:461:LYS:HG3	1.63	0.63
1:A:491:LEU:HD22	1:A:529:GLU:HB2	1.79	0.63
2:B:66:LYS:O	2:B:68:SER:N	2.31	0.63
2:B:277:ARG:O	2:B:281:LYS:HG3	1.98	0.63
2:B:315:HIS:O	2:B:317:VAL:N	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.34	0.63
2:B:345:PRO:C	2:B:346:PHE:HD1	2.02	0.63
1:A:511:ASP:OD1	1:A:512:LYS:HG2	1.99	0.63
1:A:11:LYS:O	1:A:85:GLN:HG2	1.99	0.62
1:A:53:GLU:CA	1:A:55:PRO:HD3	2.30	0.62
2:B:99:GLY:HA2	2:B:102:LYS:HD3	1.81	0.62
2:B:130:PHE:CE2	2:B:144:TYR:HB2	2.34	0.62
2:B:419:THR:O	2:B:421:PRO:HD3	1.99	0.62
2:B:130:PHE:CZ	2:B:144:TYR:CB	2.83	0.62
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.35	0.62
1:A:277:ARG:HH11	1:A:334:GLN:CB	2.13	0.62
1:A:540:LYS:HE3	2:B:265:ASN:ND2	2.15	0.61
2:B:65:LYS:CG	2:B:72:ARG:HG3	2.29	0.61
1:A:373:GLN:HG2	2:B:394:GLN:NE2	2.15	0.61
1:A:84:THR:HG23	1:A:124:PHE:HZ	1.66	0.61
1:A:164:MET:HB3	1:A:182:GLN:HE22	1.65	0.61
1:A:218:ASP:C	1:A:220:LYS:H	2.04	0.61
1:A:503:LEU:HG	1:A:507:GLN:HG3	1.83	0.61
2:B:66:LYS:NZ	2:B:218:ASP:HB2	2.14	0.61
2:B:194:GLU:O	2:B:196:GLY:N	2.34	0.61
1:A:183:TYR:CE2	1:A:184:MET:HG2	2.36	0.60
2:B:314:VAL:HG12	2:B:315:HIS:N	2.15	0.60
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.32	0.60
1:A:540:LYS:CE	2:B:265:ASN:HD21	2.14	0.60
1:A:450:THR:O	1:A:451:LYS:HG2	2.02	0.60
2:B:273:GLY:O	2:B:309:ILE:HD13	2.01	0.60
1:A:240:THR:HG22	1:A:241:VAL:N	2.07	0.60
2:B:366:LYS:O	2:B:370:GLU:HG3	2.01	0.60
2:B:115:TYR:O	2:B:117:SER:N	2.35	0.60
1:A:50:ILE:HD13	1:A:145:GLN:HB3	1.84	0.59
1:A:84:THR:HG23	1:A:124:PHE:CZ	2.37	0.59
2:B:257:ILE:O	2:B:261:VAL:HG23	2.01	0.59
1:A:59:PRO:HB2	1:A:61:PHE:CE1	2.37	0.59
1:A:406:TRP:CE3	1:A:407:GLN:HB2	2.37	0.59
2:B:278:GLN:HA	2:B:278:GLN:OE1	2.02	0.59
2:B:353:LYS:O	2:B:353:LYS:HG3	2.03	0.59
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.38	0.59
1:A:59:PRO:HB2	1:A:61:PHE:HE1	1.68	0.59
1:A:12:LEU:HD11	1:A:127:TYR:CE2	2.37	0.58
1:A:65:LYS:HD3	1:A:66:LYS:CG	2.30	0.58
1:A:5:ILE:HD11	1:A:167:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:HG21	1:A:159:ILE:HG23	1.85	0.58
1:A:362:THR:CG2	1:A:363:ASN:H	1.97	0.58
1:A:399:GLU:HG3	1:A:402:TRP:HE1	1.68	0.58
1:A:8:VAL:HG23	1:A:159:ILE:HG23	1.84	0.58
1:A:411:ILE:O	1:A:411:ILE:HG23	2.03	0.58
1:A:162:SER:HB2	2:B:52:PRO:HG3	1.85	0.58
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.68	0.58
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.86	0.58
2:B:306:ASN:HD22	2:B:309:ILE:HD12	1.67	0.58
1:A:503:LEU:HD22	1:A:535:TRP:CB	2.33	0.58
2:B:213:GLY:C	2:B:215:THR:H	2.05	0.58
1:A:223:LYS:C	1:A:225:PRO:HD3	2.23	0.58
1:A:434:ILE:HB	1:A:437:ALA:CB	2.34	0.58
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.84	0.58
1:A:277:ARG:NH1	1:A:334:GLN:HB2	2.19	0.57
1:A:233:GLU:HB2	1:A:242:GLN:HG3	1.84	0.57
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.39	0.57
1:A:486:LEU:CD2	1:A:495:ILE:HD11	2.34	0.57
1:A:148:VAL:O	1:A:150:PRO:HD3	2.05	0.57
2:B:100:LEU:HD11	2:B:106:VAL:HG13	1.86	0.57
2:B:339:TYR:C	2:B:340:GLN:OE1	2.43	0.57
2:B:241:VAL:HG12	2:B:242:GLN:H	1.70	0.57
1:A:188:TYR:CE2	4:A:562:3AC:H27	2.39	0.57
1:A:29:GLU:HG2	1:A:30:LYS:H	1.66	0.56
1:A:296:THR:CG2	1:A:297:GLU:N	2.68	0.56
1:A:284:ARG:C	1:A:286:THR:N	2.58	0.56
1:A:420:PRO:HA	1:A:421:PRO:C	2.25	0.56
1:A:298:GLU:N	1:A:298:GLU:CD	2.58	0.56
2:B:253:THR:O	2:B:257:ILE:HG22	2.04	0.56
1:A:244:ILE:HD13	1:A:310:LEU:HD21	1.87	0.56
2:B:336:GLN:HG2	2:B:355:ALA:HB2	1.88	0.56
2:B:388:LYS:CG	2:B:413:GLU:HB2	2.35	0.56
1:A:233:GLU:HG2	1:A:235:HIS:CD2	2.41	0.56
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.35	0.56
1:A:212:TRP:O	1:A:214:LEU:N	2.39	0.56
1:A:257:ILE:O	1:A:261:VAL:HG23	2.05	0.56
2:B:23:GLN:HG3	2:B:131:THR:O	2.05	0.56
2:B:49:LYS:HA	2:B:143:ARG:O	2.05	0.56
1:A:131:THR:OG1	1:A:143:ARG:NE	2.35	0.56
1:A:315:HIS:H	1:A:315:HIS:HD2	1.50	0.56
1:A:278:GLN:HB2	1:A:302:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:GLU:OE1	2:B:53:GLU:N	2.30	0.56
2:B:197:GLN:O	2:B:200:THR:HB	2.06	0.56
2:B:245:VAL:HG13	2:B:245:VAL:O	2.06	0.56
2:B:276:VAL:HG23	2:B:279:LEU:HB3	1.86	0.56
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.41	0.55
2:B:260:LEU:O	2:B:264:LEU:HB2	2.06	0.55
1:A:63:ILE:CG2	1:A:64:LYS:N	2.68	0.55
1:A:317:VAL:HG11	1:A:347:LYS:HB3	1.87	0.55
1:A:517:LEU:O	1:A:520:GLN:HB2	2.06	0.55
2:B:99:GLY:O	2:B:102:LYS:HB2	2.06	0.55
1:A:241:VAL:HG21	1:A:266:TRP:HE1	1.72	0.55
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.41	0.55
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.41	0.55
2:B:171:PHE:CE2	2:B:205:LEU:HA	2.42	0.55
2:B:183:TYR:OH	2:B:386:THR:HG23	2.06	0.55
1:A:65:LYS:HZ3	1:A:66:LYS:HG2	1.71	0.55
1:A:227:PHE:N	1:A:227:PHE:CD2	2.74	0.55
1:A:354:TYR:OH	1:A:370:GLU:HB3	2.06	0.55
1:A:206:ARG:HG3	1:A:216:THR:OG1	2.07	0.55
1:A:434:ILE:HG21	1:A:492:GLU:CG	2.35	0.55
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.35	0.55
1:A:193:LEU:HD22	1:A:197:GLN:OE1	2.07	0.55
2:B:241:VAL:CG1	2:B:242:GLN:N	2.70	0.55
2:B:209:LEU:HB3	2:B:215:THR:OG1	2.06	0.55
2:B:319:TYR:O	2:B:321:PRO:HD3	2.06	0.55
1:A:73:LYS:HE2	1:A:75:VAL:CG2	2.38	0.54
1:A:512:LYS:O	1:A:513:SER:HB2	2.08	0.54
2:B:340:GLN:OE1	2:B:340:GLN:N	2.40	0.54
1:A:203:GLU:HA	1:A:203:GLU:OE1	2.05	0.54
2:B:186:ASP:HB2	2:B:188:TYR:HE1	1.72	0.54
1:A:418:ASN:O	1:A:420:PRO:HD3	2.07	0.54
2:B:274:ILE:HG23	2:B:306:ASN:ND2	2.22	0.54
1:A:233:GLU:HG3	1:A:242:GLN:HE21	1.73	0.54
1:A:296:THR:HG22	1:A:298:GLU:H	1.72	0.54
2:B:371:ALA:O	2:B:375:ILE:HG13	2.07	0.54
2:B:376:THR:HG21	2:B:410:TRP:CH2	2.42	0.54
2:B:345:PRO:C	2:B:346:PHE:CD1	2.81	0.54
1:A:298:GLU:CD	1:A:298:GLU:H	2.11	0.54
2:B:340:GLN:HB3	2:B:348:ASN:HD22	1.73	0.54
2:B:363:ASN:N	2:B:367:GLN:HE21	2.05	0.54
1:A:195:ILE:CG2	1:A:199:ARG:HD3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.89	0.54
1:A:186:ASP:HB3	1:A:188:TYR:HE2	1.72	0.54
1:A:269:GLN:O	1:A:351:THR:N	2.32	0.54
1:A:265:ASN:O	1:A:268:SER:N	2.41	0.53
2:B:67:ASP:O	2:B:68:SER:O	2.26	0.53
1:A:34:LEU:CD1	1:A:132:ILE:HG22	2.39	0.53
1:A:280:SER:C	1:A:282:LEU:N	2.62	0.53
1:A:401:TRP:O	1:A:405:TYR:HB2	2.07	0.53
2:B:149:LEU:CD2	2:B:159:ILE:HD12	2.36	0.53
1:A:195:ILE:HG22	1:A:199:ARG:HD3	1.91	0.53
2:B:87:PHE:O	2:B:88:TRP:CD1	2.62	0.53
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.08	0.53
1:A:140:PRO:CD	1:A:141:GLY:H	2.20	0.53
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.90	0.53
1:A:473:THR:O	1:A:474:ASN:C	2.46	0.53
2:B:260:LEU:HG	2:B:264:LEU:HD12	1.91	0.53
1:A:486:LEU:HD21	1:A:495:ILE:HD11	1.90	0.53
1:A:116:PHE:HD2	1:A:148:VAL:HG21	1.73	0.53
1:A:277:ARG:HD2	1:A:334:GLN:HB2	1.90	0.53
2:B:346:PHE:CD1	2:B:346:PHE:N	2.77	0.53
1:A:297:GLU:HB2	1:A:298:GLU:OE2	2.08	0.53
1:A:303:LEU:O	1:A:307:ARG:HG3	2.08	0.53
1:A:33:ALA:O	1:A:36:GLU:HB3	2.08	0.52
1:A:244:ILE:O	1:A:244:ILE:HG23	2.08	0.52
2:B:331:LYS:HE3	2:B:364:ASP:OD1	2.09	0.52
1:A:150:PRO:HG2	1:A:153:TRP:HB2	1.91	0.52
1:A:183:TYR:CD2	1:A:184:MET:CG	2.84	0.52
2:B:40:GLU:O	2:B:43:LYS:HB3	2.08	0.52
2:B:7:THR:O	2:B:9:PRO:HD3	2.08	0.52
2:B:249:LYS:HB3	2:B:249:LYS:NZ	2.25	0.52
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.31	0.52
2:B:213:GLY:C	2:B:215:THR:N	2.63	0.52
1:A:254:VAL:O	1:A:258:GLN:HG3	2.10	0.52
2:B:281:LYS:C	2:B:283:LEU:H	2.13	0.52
2:B:307:ARG:HG3	2:B:307:ARG:HH11	1.75	0.52
2:B:366:LYS:HD2	2:B:405:TYR:CE2	2.44	0.52
1:A:167:ILE:O	1:A:208:HIS:HE1	1.92	0.52
2:B:193:LEU:N	2:B:193:LEU:HD23	2.24	0.52
1:A:130:PHE:CD1	1:A:130:PHE:N	2.78	0.52
2:B:363:ASN:H	2:B:367:GLN:HE21	1.58	0.52
1:A:90:VAL:O	1:A:92:LEU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:TYR:CE2	1:A:184:MET:CG	2.93	0.52
1:A:457:TYR:C	1:A:457:TYR:CD2	2.82	0.52
2:B:1:PRO:CD	2:B:117:SER:HA	2.33	0.52
2:B:18:GLY:HA3	2:B:56:TYR:CE1	2.45	0.52
1:A:426:TRP:O	1:A:427:TYR:HB3	2.10	0.51
2:B:305:GLU:O	2:B:309:ILE:HG13	2.10	0.51
2:B:314:VAL:HG12	2:B:315:HIS:H	1.75	0.51
2:B:331:LYS:HA	2:B:337:TRP:CE3	2.46	0.51
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.45	0.51
1:A:53:GLU:O	1:A:54:ASN:HB2	2.10	0.51
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.42	0.51
1:A:130:PHE:CE1	1:A:144:TYR:CB	2.90	0.51
1:A:278:GLN:HG3	1:A:298:GLU:HB3	1.93	0.51
2:B:83:ARG:O	2:B:84:THR:HG23	2.10	0.51
2:B:388:LYS:HG2	2:B:413:GLU:HB2	1.92	0.51
1:A:297:GLU:N	1:A:297:GLU:OE1	2.43	0.51
2:B:269:GLN:HB3	2:B:346:PHE:CD2	2.45	0.51
1:A:91:GLN:NE2	2:B:139:THR:O	2.44	0.51
1:A:170:PRO:HG2	1:A:171:PHE:H	1.75	0.51
1:A:434:ILE:HB	1:A:437:ALA:HB2	1.93	0.51
1:A:448:ARG:CZ	1:A:448:ARG:O	2.58	0.51
2:B:282:LEU:HG	2:B:293:ILE:CD1	2.40	0.51
1:A:28:GLU:H	1:A:28:GLU:CD	2.13	0.51
1:A:434:ILE:CG2	1:A:437:ALA:HB2	2.40	0.51
2:B:28:GLU:CG	2:B:32:LYS:HE3	2.39	0.51
2:B:350:LYS:HE3	2:B:378:GLU:OE1	2.10	0.51
1:A:113:ASP:O	1:A:114:ALA:C	2.48	0.51
1:A:115:TYR:N	1:A:115:TYR:CD2	2.79	0.51
1:A:116:PHE:HE2	1:A:146:TYR:HE1	1.56	0.51
1:A:393:ILE:HD13	1:A:398:TRP:HB2	1.92	0.51
1:A:181:TYR:CZ	2:B:138:GLU:HG2	2.46	0.50
2:B:205:LEU:O	2:B:208:HIS:HB3	2.11	0.50
2:B:337:TRP:O	2:B:353:LYS:HA	2.10	0.50
1:A:56:TYR:O	1:A:57:ASN:HB2	2.10	0.50
2:B:253:THR:H	2:B:256:ASP:HB2	1.75	0.50
1:A:63:ILE:CG2	1:A:64:LYS:H	2.24	0.50
1:A:460:ASN:HD22	1:A:460:ASN:C	2.14	0.50
1:A:63:ILE:HG22	1:A:64:LYS:H	1.77	0.50
1:A:130:PHE:N	1:A:130:PHE:HD1	2.09	0.50
1:A:340:GLN:CB	1:A:351:THR:HG22	2.41	0.50
2:B:419:THR:O	2:B:419:THR:HG23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:CD1	1:A:310:LEU:HD21	2.41	0.50
1:A:448:ARG:HG3	1:A:448:ARG:HH11	1.77	0.50
2:B:8:VAL:HG21	2:B:159:ILE:HG23	1.93	0.50
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.47	0.50
2:B:194:GLU:O	2:B:195:ILE:C	2.50	0.50
1:A:115:TYR:HD2	1:A:115:TYR:N	2.09	0.50
1:A:206:ARG:NH2	1:A:218:ASP:HA	2.27	0.50
1:A:424:LYS:HE2	1:A:426:TRP:CE2	2.47	0.50
2:B:104:LYS:HA	2:B:237:ASP:OD2	2.12	0.50
2:B:363:ASN:O	2:B:364:ASP:C	2.49	0.50
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.47	0.50
2:B:115:TYR:C	2:B:117:SER:H	2.15	0.50
1:A:460:ASN:ND2	1:A:461:LYS:HG3	2.25	0.49
1:A:193:LEU:HB3	1:A:197:GLN:HG3	1.94	0.49
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.93	0.49
1:A:326:ILE:HD12	1:A:326:ILE:N	2.27	0.49
2:B:209:LEU:HB3	2:B:215:THR:HG1	1.78	0.49
1:A:495:ILE:HB	1:A:533:LEU:HD12	1.94	0.49
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.27	0.49
1:A:434:ILE:HD13	1:A:492:GLU:HG3	1.95	0.49
1:A:509:GLN:N	1:A:510:PRO:CD	2.74	0.49
2:B:368:LEU:HD23	2:B:398:TRP:CZ3	2.46	0.49
1:A:62:ALA:O	1:A:63:ILE:HD13	2.12	0.49
1:A:378:GLU:O	1:A:382:ILE:HG13	2.13	0.49
1:A:120:LEU:HD12	1:A:121:ASP:H	1.78	0.49
1:A:433:PRO:HG3	2:B:255:ASN:ND2	2.27	0.49
1:A:469:LEU:CD1	1:A:480:GLN:HG2	2.43	0.49
2:B:156:SER:O	2:B:157:PRO:C	2.50	0.49
2:B:365:VAL:O	2:B:369:THR:HG22	2.13	0.49
1:A:233:GLU:O	1:A:239:TRP:HA	2.13	0.49
1:A:296:THR:HG22	1:A:298:GLU:N	2.28	0.49
1:A:18:GLY:HA3	1:A:127:TYR:HD2	1.78	0.48
1:A:201:LYS:O	1:A:204:GLU:HB2	2.13	0.48
1:A:332:GLN:HE21	1:A:336:GLN:HB3	1.78	0.48
1:A:542:ILE:HD11	1:A:546:GLU:CA	2.28	0.48
2:B:128:THR:OG1	2:B:146:TYR:HB2	2.13	0.48
2:B:303:LEU:HD21	2:B:307:ARG:NH1	2.26	0.48
2:B:308:GLU:C	2:B:310:LEU:H	2.17	0.48
1:A:61:PHE:HB2	1:A:74:LEU:HB3	1.93	0.48
1:A:93:GLY:C	1:A:94:ILE:HD12	2.33	0.48
1:A:301:LEU:O	1:A:301:LEU:HD12	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:LEU:HD23	2:B:12:LEU:N	2.29	0.48
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.48	0.48
1:A:384:GLY:O	2:B:27:THR:HG23	2.13	0.48
1:A:417:VAL:HG12	1:A:419:THR:H	1.78	0.48
1:A:424:LYS:HE2	1:A:426:TRP:CD2	2.48	0.48
1:A:426:TRP:HB3	1:A:526:ILE:CD1	2.42	0.48
1:A:473:THR:H	1:A:476:LYS:HB2	1.78	0.48
2:B:37:ILE:O	2:B:41:MET:HG3	2.13	0.48
1:A:1:PRO:O	1:A:213:GLY:HA3	2.13	0.48
2:B:326:ILE:HB	2:B:342:TYR:CE1	2.47	0.48
2:B:34:LEU:O	2:B:35:VAL:C	2.51	0.48
2:B:85:GLN:CB	2:B:154:LYS:HB2	2.43	0.48
1:A:469:LEU:HD13	1:A:480:GLN:HG2	1.94	0.48
2:B:85:GLN:O	2:B:85:GLN:HG2	2.13	0.48
1:A:3:SER:OG	1:A:212:TRP:C	2.52	0.48
2:B:283:LEU:O	2:B:285:GLY:N	2.47	0.48
2:B:417:VAL:HG12	2:B:418:ASN:N	2.27	0.48
1:A:407:GLN:CG	2:B:393:ILE:HA	2.43	0.48
1:A:434:ILE:H	1:A:494:ASN:HD21	1.61	0.48
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.49	0.48
1:A:115:TYR:CE1	1:A:156:SER:HB3	2.48	0.48
1:A:136:ASN:OD1	1:A:138:GLU:HG2	2.14	0.48
1:A:277:ARG:NH1	1:A:334:GLN:CB	2.77	0.48
1:A:363:ASN:ND2	1:A:509:GLN:O	2.47	0.48
2:B:357:MET:HG2	2:B:360:ALA:HB3	1.96	0.48
1:A:253:THR:O	1:A:254:VAL:C	2.51	0.48
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.34	0.48
1:A:107:THR:HB	1:A:202:ILE:HD11	1.96	0.47
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.14	0.47
2:B:201:LYS:O	2:B:204:GLU:HB3	2.14	0.47
2:B:249:LYS:HD2	2:B:252:TRP:CD2	2.49	0.47
2:B:332:GLN:NE2	2:B:332:GLN:HA	2.28	0.47
2:B:417:VAL:CG1	2:B:418:ASN:N	2.77	0.47
1:A:41:MET:CB	1:A:47:ILE:HD11	2.43	0.47
1:A:107:THR:HG21	1:A:202:ILE:HD12	1.97	0.47
1:A:478:GLU:OE1	1:A:478:GLU:CA	2.53	0.47
2:B:296:THR:HG22	2:B:298:GLU:N	2.29	0.47
2:B:314:VAL:HB	2:B:317:VAL:HG21	1.95	0.47
2:B:376:THR:HG22	2:B:380:ILE:HD11	1.94	0.47
1:A:224:GLU:O	1:A:226:PRO:O	2.32	0.47
1:A:487:GLN:HG2	1:A:524:GLN:HE22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:THR:HB	2:B:140:PRO:HD2	1.96	0.47
1:A:457:TYR:C	1:A:457:TYR:HD2	2.17	0.47
1:A:540:LYS:HG3	1:A:541:GLY:N	2.29	0.47
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.53	0.47
2:B:85:GLN:O	2:B:85:GLN:CG	2.62	0.47
2:B:103:LYS:HG3	2:B:190:GLY:C	2.35	0.47
1:A:81:ASN:O	1:A:83:ARG:N	2.48	0.47
1:A:188:TYR:CD2	4:A:562:3AC:H27	2.50	0.47
1:A:60:VAL:O	1:A:61:PHE:HD1	1.98	0.47
2:B:146:TYR:CG	2:B:150:PRO:HG3	2.49	0.47
2:B:160:PHE:O	2:B:162:SER:N	2.48	0.47
2:B:206:ARG:NH2	2:B:218:ASP:C	2.68	0.47
2:B:236:PRO:O	2:B:239:TRP:HB2	2.15	0.47
2:B:390:LYS:HB3	2:B:417:VAL:HG21	1.95	0.47
1:A:62:ALA:C	1:A:63:ILE:HG12	2.35	0.47
1:A:137:ASN:N	1:A:137:ASN:ND2	2.60	0.47
1:A:194:GLU:O	1:A:196:GLY:N	2.48	0.47
2:B:365:VAL:HG12	2:B:366:LYS:N	2.29	0.47
1:A:28:GLU:HA	1:A:31:ILE:CB	2.44	0.47
1:A:235:HIS:HB2	1:A:238:LYS:O	2.14	0.47
1:A:276:VAL:O	1:A:276:VAL:CG1	2.61	0.47
1:A:515:SER:O	1:A:516:GLU:C	2.52	0.47
2:B:354:TYR:CD1	2:B:355:ALA:N	2.82	0.47
1:A:487:GLN:CG	1:A:524:GLN:HE22	2.28	0.47
1:A:10:VAL:HG12	1:A:11:LYS:N	2.29	0.46
2:B:58:THR:HA	2:B:59:PRO:HD3	1.70	0.46
2:B:194:GLU:O	2:B:197:GLN:N	2.48	0.46
2:B:100:LEU:HD13	2:B:179:VAL:CG2	2.46	0.46
1:A:249:LYS:HG3	1:A:250:ASP:N	2.29	0.46
2:B:23:GLN:NE2	2:B:24:TRP:O	2.48	0.46
2:B:28:GLU:O	2:B:32:LYS:HG3	2.16	0.46
2:B:85:GLN:CD	2:B:154:LYS:HD2	2.35	0.46
2:B:241:VAL:CG1	2:B:242:GLN:H	2.26	0.46
1:A:109:LEU:HD22	1:A:217:PRO:HD2	1.97	0.46
1:A:278:GLN:OE1	1:A:298:GLU:HB2	2.15	0.46
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.98	0.46
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.51	0.46
2:B:115:TYR:N	2:B:115:TYR:CD2	2.80	0.46
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.51	0.46
2:B:308:GLU:OE2	2:B:311:LYS:HD2	2.14	0.46
1:A:12:LEU:O	1:A:13:LYS:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:CG	1:A:402:TRP:HE1	2.28	0.46
1:A:448:ARG:HG3	1:A:448:ARG:NH1	2.31	0.46
2:B:178:ILE:CG2	2:B:189:VAL:HG12	2.45	0.46
2:B:254:VAL:HG21	2:B:288:ALA:O	2.16	0.46
2:B:331:LYS:O	2:B:424:LYS:NZ	2.49	0.46
1:A:105:SER:HB2	1:A:198:HIS:CD2	2.51	0.46
1:A:277:ARG:O	1:A:281:LYS:HB2	2.16	0.46
1:A:435:VAL:HA	2:B:290:THR:OG1	2.15	0.46
2:B:271:TYR:HA	2:B:272:PRO:HD2	1.70	0.46
1:A:446:ALA:HA	1:A:453:GLY:HA2	1.96	0.46
1:A:490:GLY:O	1:A:492:GLU:N	2.48	0.46
1:A:511:ASP:CG	1:A:512:LYS:HG2	2.36	0.46
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.81	0.46
2:B:276:VAL:HG22	2:B:276:VAL:O	2.15	0.46
1:A:60:VAL:O	1:A:61:PHE:CD1	2.69	0.46
1:A:137:ASN:HD22	1:A:137:ASN:H	1.64	0.46
1:A:169:GLU:N	1:A:170:PRO:HD2	2.31	0.46
1:A:188:TYR:CD2	1:A:188:TYR:N	2.78	0.46
1:A:330:GLN:OE1	1:A:340:GLN:NE2	2.44	0.46
2:B:345:PRO:HB2	2:B:346:PHE:CE1	2.51	0.46
1:A:27:THR:O	1:A:30:LYS:HB2	2.15	0.46
1:A:38:CYS:O	1:A:41:MET:HB2	2.15	0.46
1:A:30:LYS:O	1:A:33:ALA:HB3	2.14	0.45
2:B:276:VAL:O	2:B:276:VAL:HG13	2.16	0.45
2:B:349:LEU:O	2:B:350:LYS:HB2	2.16	0.45
2:B:423:VAL:HG12	2:B:423:VAL:O	2.16	0.45
1:A:377:THR:O	1:A:381:VAL:HG23	2.16	0.45
2:B:66:LYS:C	2:B:68:SER:N	2.67	0.45
2:B:258:GLN:HG3	2:B:283:LEU:CD2	2.46	0.45
2:B:425:LEU:N	2:B:425:LEU:HD23	2.31	0.45
1:A:148:VAL:O	1:A:150:PRO:CD	2.64	0.45
1:A:159:ILE:HA	1:A:162:SER:HB3	1.98	0.45
1:A:448:ARG:NE	1:A:448:ARG:HA	2.32	0.45
2:B:243:PRO:O	2:B:245:VAL:HG12	2.16	0.45
1:A:25:PRO:O	1:A:26:LEU:HB2	2.16	0.45
1:A:118:VAL:HG13	1:A:119:PRO:HD2	1.99	0.45
1:A:394:GLN:O	1:A:396:GLU:N	2.50	0.45
2:B:167:ILE:O	2:B:170:PRO:HD2	2.17	0.45
1:A:399:GLU:HG3	1:A:402:TRP:NE1	2.31	0.45
1:A:41:MET:HB3	1:A:47:ILE:CD1	2.45	0.45
2:B:178:ILE:HG21	2:B:189:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PRO:HG2	1:A:153:TRP:CB	2.46	0.45
1:A:475:GLN:O	1:A:476:LYS:C	2.55	0.45
2:B:183:TYR:O	2:B:184:MET:HB2	2.16	0.45
2:B:262:GLY:O	2:B:265:ASN:N	2.49	0.45
1:A:485:ALA:O	1:A:489:SER:HB3	2.16	0.45
2:B:5:ILE:HG22	2:B:6:GLU:O	2.16	0.45
2:B:213:GLY:O	2:B:215:THR:N	2.50	0.45
2:B:279:LEU:HA	2:B:299:ALA:HB1	1.99	0.45
1:A:66:LYS:NZ	1:A:70:LYS:O	2.30	0.45
2:B:240:THR:O	2:B:241:VAL:HG23	2.17	0.45
1:A:134:SER:CB	1:A:136:ASN:O	2.65	0.45
2:B:157:PRO:O	2:B:160:PHE:N	2.50	0.45
2:B:262:GLY:O	2:B:263:LYS:C	2.55	0.45
1:A:233:GLU:CG	1:A:242:GLN:HE21	2.30	0.44
1:A:357:MET:H	1:A:357:MET:HG2	1.41	0.44
2:B:240:THR:HG22	2:B:241:VAL:N	2.32	0.44
2:B:312:GLU:HA	2:B:313:PRO:HD3	1.76	0.44
1:A:164:MET:CE	1:A:187:LEU:HD11	2.47	0.44
1:A:202:ILE:O	1:A:206:ARG:N	2.43	0.44
1:A:333:GLY:O	1:A:512:LYS:HE2	2.17	0.44
1:A:441:TYR:CE2	1:A:544:GLY:HA3	2.52	0.44
1:A:460:ASN:ND2	1:A:461:LYS:H	2.12	0.44
2:B:105:SER:HA	2:B:234:LEU:O	2.18	0.44
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.70	0.44
1:A:194:GLU:OE1	1:A:194:GLU:HA	2.17	0.44
2:B:48:SER:O	2:B:144:TYR:HA	2.17	0.44
2:B:65:LYS:O	2:B:407:GLN:NE2	2.51	0.44
2:B:111:VAL:O	2:B:113:ASP:N	2.50	0.44
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.99	0.44
2:B:421:PRO:HB2	2:B:422:LEU:H	1.61	0.44
2:B:85:GLN:HG3	2:B:154:LYS:HB2	1.96	0.44
1:A:279:LEU:HD12	1:A:279:LEU:N	2.31	0.44
2:B:198:HIS:C	2:B:200:THR:N	2.70	0.44
1:A:22:LYS:HD3	1:A:23:GLN:N	2.32	0.44
1:A:192:ASP:O	1:A:193:LEU:HG	2.18	0.44
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.82	0.44
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.99	0.44
2:B:308:GLU:C	2:B:310:LEU:N	2.71	0.44
1:A:79:GLU:HG3	1:A:83:ARG:HH12	1.83	0.44
1:A:98:ALA:HB2	1:A:350:LYS:HB2	2.00	0.44
1:A:165:THR:O	1:A:166:LYS:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:HH21	1:A:218:ASP:HA	1.82	0.44
1:A:332:GLN:NE2	1:A:336:GLN:HB3	2.32	0.44
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.99	0.44
4:A:562:3AC:H611	4:A:562:3AC:H511	1.81	0.44
1:A:53:GLU:O	1:A:54:ASN:CB	2.66	0.44
1:A:170:PRO:HB2	1:A:174:GLN:NE2	2.31	0.44
1:A:229:TRP:O	1:A:232:TYR:N	2.50	0.44
1:A:542:ILE:HG13	1:A:545:ASN:CB	2.47	0.44
2:B:128:THR:OG1	2:B:146:TYR:N	2.41	0.44
2:B:282:LEU:HG	2:B:293:ILE:HD12	2.00	0.44
2:B:125:ARG:O	2:B:127:TYR:N	2.51	0.43
2:B:131:THR:HG1	2:B:143:ARG:HH11	1.66	0.43
2:B:275:LYS:HB2	2:B:277:ARG:NE	2.21	0.43
2:B:306:ASN:ND2	2:B:309:ILE:HD12	2.32	0.43
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.49	0.43
1:A:450:THR:O	1:A:451:LYS:CG	2.64	0.43
2:B:388:LYS:NZ	2:B:415:GLU:OE1	2.49	0.43
2:B:395:LYS:HE3	2:B:399:GLU:OE1	2.18	0.43
1:A:498:ASP:HB3	1:A:545:ASN:HD21	1.81	0.43
2:B:258:GLN:HG3	2:B:283:LEU:HD21	2.00	0.43
1:A:34:LEU:HD21	1:A:62:ALA:HB2	2.00	0.43
1:A:183:TYR:CD2	1:A:183:TYR:C	2.92	0.43
1:A:472:THR:OG1	1:A:476:LYS:HB3	2.18	0.43
2:B:17:ASP:O	2:B:18:GLY:O	2.36	0.43
2:B:23:GLN:NE2	2:B:133:PRO:HG3	2.34	0.43
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.77	0.43
2:B:340:GLN:HG2	2:B:426:TRP:CZ2	2.53	0.43
1:A:503:LEU:O	1:A:504:GLY:C	2.56	0.43
1:A:136:ASN:O	1:A:138:GLU:N	2.51	0.43
1:A:277:ARG:CD	1:A:334:GLN:HB2	2.48	0.43
1:A:280:SER:O	1:A:282:LEU:N	2.52	0.43
2:B:206:ARG:HE	2:B:217:PRO:HB2	1.84	0.43
2:B:261:VAL:O	2:B:265:ASN:HB2	2.19	0.43
1:A:194:GLU:C	1:A:196:GLY:N	2.71	0.43
1:A:249:LYS:CG	1:A:250:ASP:H	2.27	0.43
1:A:532:TYR:CE1	1:A:534:ALA:HB2	2.54	0.43
2:B:374:LYS:O	2:B:375:ILE:C	2.56	0.43
1:A:209:LEU:HB3	1:A:214:LEU:HB2	2.01	0.43
1:A:218:ASP:C	1:A:220:LYS:N	2.72	0.43
1:A:275:LYS:HD3	1:A:336:GLN:HE22	1.84	0.43
1:A:408:ALA:HB3	2:B:393:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:PRO:O	2:B:141:GLY:C	2.57	0.43
2:B:295:LEU:O	2:B:296:THR:C	2.57	0.43
1:A:310:LEU:O	1:A:311:LYS:C	2.57	0.42
2:B:198:HIS:O	2:B:200:THR:N	2.52	0.42
2:B:357:MET:CG	2:B:360:ALA:HB3	2.48	0.42
2:B:385:LYS:O	2:B:385:LYS:HG3	2.18	0.42
1:A:273:GLY:O	1:A:274:ILE:C	2.55	0.42
2:B:84:THR:O	2:B:87:PHE:N	2.48	0.42
2:B:253:THR:HG22	2:B:292:VAL:CA	2.44	0.42
2:B:332:GLN:CB	2:B:336:GLN:O	2.67	0.42
2:B:376:THR:HG22	2:B:380:ILE:CD1	2.48	0.42
1:A:430:GLU:CD	1:A:530:LYS:HE3	2.40	0.42
1:A:515:SER:O	1:A:517:LEU:N	2.52	0.42
1:A:515:SER:OG	1:A:518:VAL:HG23	2.18	0.42
2:B:44:GLU:OE1	2:B:46:LYS:HE3	2.18	0.42
2:B:168:LEU:HD21	2:B:209:LEU:HD21	2.00	0.42
2:B:178:ILE:HD11	2:B:201:LYS:CG	2.49	0.42
2:B:299:ALA:O	2:B:301:LEU:N	2.53	0.42
1:A:40:GLU:O	1:A:44:GLU:HG3	2.19	0.42
1:A:94:ILE:HG13	1:A:183:TYR:HE1	1.84	0.42
1:A:136:ASN:OD1	1:A:136:ASN:O	2.38	0.42
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.18	0.42
1:A:542:ILE:HG23	1:A:542:ILE:O	2.18	0.42
1:A:60:VAL:C	1:A:61:PHE:CD1	2.84	0.42
1:A:90:VAL:O	1:A:91:GLN:C	2.58	0.42
1:A:181:TYR:CE2	2:B:138:GLU:HG2	2.55	0.42
1:A:233:GLU:CG	1:A:235:HIS:HE2	2.33	0.42
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.85	0.42
1:A:315:HIS:CD2	1:A:315:HIS:N	2.82	0.42
1:A:330:GLN:HE21	1:A:330:GLN:HB2	1.69	0.42
1:A:503:LEU:HD12	1:A:533:LEU:HD23	2.01	0.42
1:A:81:ASN:C	1:A:83:ARG:N	2.73	0.42
1:A:115:TYR:CD1	1:A:156:SER:HB3	2.55	0.42
1:A:203:GLU:OE1	1:A:203:GLU:CA	2.68	0.42
1:A:41:MET:O	1:A:42:GLU:C	2.57	0.42
1:A:132:ILE:HD11	1:A:142:ILE:HG21	2.02	0.42
1:A:183:TYR:HD2	1:A:183:TYR:C	2.23	0.42
1:A:242:GLN:O	1:A:244:ILE:HG22	2.19	0.42
1:A:420:PRO:HA	1:A:421:PRO:O	2.19	0.41
2:B:124:PHE:O	2:B:125:ARG:C	2.56	0.41
1:A:543:GLY:HA2	2:B:283:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLN:CG	2:B:154:LYS:HB2	2.50	0.41
2:B:153:TRP:O	2:B:156:SER:HB2	2.19	0.41
1:A:37:ILE:O	1:A:38:CYS:C	2.58	0.41
1:A:334:GLN:H	1:A:334:GLN:HG2	1.52	0.41
1:A:405:TYR:O	2:B:331:LYS:HD3	2.21	0.41
2:B:366:LYS:HB2	2:B:405:TYR:CE1	2.55	0.41
1:A:399:GLU:HA	1:A:402:TRP:HD1	1.79	0.41
2:B:266:TRP:HH2	2:B:426:TRP:CE3	2.39	0.41
2:B:354:TYR:CG	2:B:355:ALA:N	2.89	0.41
2:B:378:GLU:O	2:B:381:VAL:HB	2.19	0.41
1:A:77:PHE:O	1:A:80:LEU:N	2.48	0.41
1:A:265:ASN:O	1:A:266:TRP:C	2.59	0.41
2:B:75:VAL:CG1	2:B:77:PHE:CE2	3.01	0.41
1:A:484:LEU:HD12	1:A:484:LEU:HA	1.94	0.41
1:A:517:LEU:O	1:A:520:GLN:N	2.54	0.41
2:B:278:GLN:OE1	2:B:281:LYS:HD2	2.21	0.41
2:B:306:ASN:HD22	2:B:309:ILE:CD1	2.33	0.41
2:B:388:LYS:HA	2:B:413:GLU:O	2.20	0.41
2:B:389:PHE:CD1	2:B:389:PHE:N	2.88	0.41
1:A:64:LYS:CG	1:A:71:TRP:HA	2.40	0.41
1:A:77:PHE:O	1:A:80:LEU:HB3	2.21	0.41
1:A:241:VAL:O	1:A:241:VAL:HG13	2.21	0.41
1:A:340:GLN:HB2	1:A:351:THR:HG22	2.02	0.41
2:B:1:PRO:HB2	2:B:2:ILE:H	1.58	0.41
2:B:65:LYS:CD	2:B:72:ARG:HG3	2.51	0.41
2:B:283:LEU:C	2:B:285:GLY:H	2.22	0.41
2:B:314:VAL:CG1	2:B:315:HIS:N	2.82	0.41
2:B:332:GLN:HB3	2:B:336:GLN:O	2.21	0.41
2:B:395:LYS:HG2	2:B:399:GLU:OE1	2.20	0.41
2:B:422:LEU:HD12	2:B:425:LEU:CD1	2.51	0.41
1:A:183:TYR:HD2	1:A:184:MET:CG	2.23	0.41
1:A:233:GLU:CD	1:A:242:GLN:HE21	2.23	0.41
2:B:118:VAL:CB	2:B:149:LEU:HD12	2.34	0.41
2:B:226:PRO:O	2:B:227:PHE:CB	2.68	0.41
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.86	0.41
1:A:35:VAL:HG22	1:A:132:ILE:CD1	2.22	0.41
1:A:74:LEU:HD12	1:A:74:LEU:HA	1.78	0.41
1:A:164:MET:HG3	1:A:168:LEU:HD11	2.03	0.41
1:A:362:THR:CG2	1:A:363:ASN:N	2.64	0.41
1:A:488:ASP:N	1:A:488:ASP:OD1	2.54	0.41
1:A:540:LYS:CD	2:B:265:ASN:HD21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:VAL:HG12	2:B:88:TRP:HH2	1.86	0.41
2:B:274:ILE:HG23	2:B:306:ASN:OD1	2.19	0.41
2:B:331:LYS:NZ	2:B:364:ASP:OD2	2.49	0.41
2:B:376:THR:CG2	2:B:380:ILE:HD11	2.51	0.41
1:A:106:VAL:HG11	4:A:562:3AC:O11	2.20	0.41
1:A:233:GLU:OE2	1:A:242:GLN:CG	2.69	0.41
1:A:238:LYS:HB2	1:A:315:HIS:HB2	2.03	0.41
1:A:278:GLN:OE1	1:A:298:GLU:CB	2.69	0.41
1:A:307:ARG:O	1:A:311:LYS:HB2	2.21	0.41
1:A:319:TYR:CE2	1:A:321:PRO:HA	2.56	0.41
1:A:344:GLU:HA	1:A:345:PRO:HD3	1.87	0.41
1:A:411:ILE:O	1:A:412:PRO:O	2.38	0.41
1:A:473:THR:O	1:A:475:GLN:N	2.54	0.41
1:A:502:ALA:O	1:A:503:LEU:O	2.37	0.41
2:B:179:VAL:O	2:B:179:VAL:HG23	2.20	0.41
1:A:57:ASN:HA	1:A:129:ALA:O	2.21	0.40
2:B:201:LYS:HA	2:B:201:LYS:HD3	1.82	0.40
2:B:216:THR:HG22	2:B:217:PRO:O	2.21	0.40
2:B:400:THR:HB	2:B:401:TRP:CD1	2.56	0.40
1:A:178:ILE:HD12	1:A:191:SER:HB3	2.04	0.40
1:A:184:MET:HB2	1:A:185:ASP:H	1.56	0.40
2:B:10:VAL:HG13	2:B:88:TRP:CE2	2.55	0.40
2:B:335:GLY:O	2:B:355:ALA:HA	2.21	0.40
1:A:116:PHE:HD2	1:A:148:VAL:CG2	2.33	0.40
1:A:201:LYS:O	1:A:202:ILE:C	2.59	0.40
1:A:201:LYS:HD3	1:A:201:LYS:HA	1.83	0.40
1:A:209:LEU:HD22	1:A:214:LEU:HD12	2.03	0.40
2:B:269:GLN:HB3	2:B:346:PHE:CE2	2.56	0.40
2:B:274:ILE:HG12	2:B:309:ILE:CD1	2.46	0.40
2:B:422:LEU:O	2:B:422:LEU:HG	2.21	0.40
1:A:39:THR:C	1:A:41:MET:N	2.75	0.40
1:A:277:ARG:HH11	1:A:334:GLN:HE21	1.69	0.40
1:A:510:PRO:O	1:A:522:ILE:HD13	2.21	0.40
2:B:103:LYS:HD2	2:B:191:SER:C	2.42	0.40
2:B:326:ILE:HB	2:B:342:TYR:CD1	2.56	0.40
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.45	0.40
1:A:97:PRO:O	1:A:99:GLY:N	2.55	0.40
1:A:473:THR:O	1:A:476:LYS:N	2.55	0.40
2:B:240:THR:O	2:B:241:VAL:CG2	2.69	0.40
2:B:366:LYS:HD2	2:B:405:TYR:CD2	2.57	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	550/560 (98%)	413 (75%)	98 (18%)	39 (7%)	1	3
2	B	425/430 (99%)	298 (70%)	92 (22%)	35 (8%)	1	2
All	All	975/990 (98%)	711 (73%)	190 (20%)	74 (8%)	1	2

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	114	ALA
1	A	137	ASN
1	A	151	GLN
1	A	509	GLN
2	B	68	SER
2	B	116	PHE
2	B	138	GLU
2	B	195	ILE
1	A	18	GLY
1	A	82	LYS
1	A	91	GLN
1	A	98	ALA
1	A	141	GLY
1	A	158	ALA
1	A	213	GLY
1	A	222	GLN
1	A	250	ASP
1	A	285	GLY
1	A	412	PRO
1	A	491	LEU
1	A	503	LEU
1	A	504	GLY
1	A	516	GLU
1	A	538	ALA

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W O R L D W I D E
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PROTEIN DATA BANK

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Mol	Chain	Res	Type
1	A	543	GLY
2	B	18	GLY
2	B	67	ASP
2	B	93	GLY
2	B	103	LYS
2	B	161	GLN
2	B	174	GLN
2	B	232	TYR
2	B	284	ARG
2	B	300	GLU
2	B	421	PRO
1	A	104	LYS
1	A	220	LYS
1	A	289	LEU
1	A	395	LYS
1	A	550	LYS
2	B	77	PHE
2	B	126	LYS
2	B	212	TRP
2	B	282	LEU
2	B	316	GLY
2	B	376	THR
1	A	139	THR
1	A	195	ILE
1	A	243	PRO
1	A	281	LYS
1	A	399	GLU
1	A	474	ASN
1	A	507	GLN
2	B	2	ILE
2	B	141	GLY
2	B	184	MET
2	B	217	PRO
2	B	355	ALA
1	A	95	PRO
1	A	427	TYR
1	A	461	LYS
2	B	112	GLY
2	B	231	GLY
2	B	313	PRO
2	B	350	LYS
2	B	214	LEU

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Mol	Chain	Res	Type
2	B	263	LYS
2	B	364	ASP
2	B	274	ILE
1	A	333	GLY
2	B	272	PRO
1	A	433	PRO
2	B	276	VAL

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	477/500 (95%)	424 (89%)	53 (11%)	6	19
2	B	376/392 (96%)	342 (91%)	34 (9%)	9	29
All	All	853/892 (96%)	766 (90%)	87 (10%)	7	22

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	29	GLU
1	A	47	ILE
1	A	53	GLU
1	A	64	LYS
1	A	65	LYS
1	A	66	LYS
1	A	68	SER
1	A	76	ASP
1	A	84	THR
1	A	85	GLN
1	A	110	ASP
1	A	115	TYR
1	A	130	PHE
1	A	132	ILE
1	A	137	ASN

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Mol	Chain	Res	Type
1	A	143	ARG
1	A	156	SER
1	A	175	ASN
1	A	183	TYR
1	A	197	GLN
1	A	199	ARG
1	A	203	GLU
1	A	216	THR
1	A	223	LYS
1	A	280	SER
1	A	297	GLU
1	A	300	GLU
1	A	315	HIS
1	A	330	GLN
1	A	334	GLN
1	A	344	GLU
1	A	357	MET
1	A	386	THR
1	A	397	THR
1	A	399	GLU
1	A	409	THR
1	A	413	GLU
1	A	418	ASN
1	A	448	ARG
1	A	457	TYR
1	A	460	ASN
1	A	473	THR
1	A	478	GLU
1	A	491	LEU
1	A	492	GLU
1	A	497	THR
1	A	507	GLN
1	A	511	ASP
1	A	512	LYS
1	A	516	GLU
1	A	547	GLN
1	A	548	VAL
2	B	12	LEU
2	B	23	GLN
2	B	50	ILE
2	B	67	ASP
2	B	113	ASP

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Mol	Chain	Res	Type
2	B	137	ASN
2	B	156	SER
2	B	169	GLU
2	B	176	PRO
2	B	177	ASP
2	B	187	LEU
2	B	189	VAL
2	B	194	GLU
2	B	201	LYS
2	B	207	GLN
2	B	212	TRP
2	B	218	ASP
2	B	221	HIS
2	B	232	TYR
2	B	248	GLU
2	B	249	LYS
2	B	250	ASP
2	B	277	ARG
2	B	297	GLU
2	B	310	LEU
2	B	324	ASP
2	B	330	GLN
2	B	332	GLN
2	B	338	THR
2	B	340	GLN
2	B	342	TYR
2	B	369	THR
2	B	385	LYS
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	137	ASN
1	A	151	GLN
1	A	174	GLN
1	A	182	GLN
1	A	208	HIS
1	A	242	GLN
1	A	315	HIS

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Mol	Chain	Res	Type
1	A	330	GLN
1	A	332	GLN
1	A	334	GLN
1	A	340	GLN
1	A	418	ASN
1	A	428	GLN
1	A	460	ASN
1	A	494	ASN
1	A	507	GLN
1	A	519	ASN
1	A	524	GLN
1	A	545	ASN
1	A	547	GLN
2	B	91	GLN
2	B	136	ASN
2	B	161	GLN
2	B	207	GLN
2	B	306	ASN
2	B	394	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	3AC	A	562	-	22,23,23	2.39	10 (45%)	24,31,31	1.39	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3AC	A	562	-	-	3/9/10/10	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	562	3AC	O13-C13	6.01	1.39	1.24
4	A	562	3AC	C12-I12	-4.34	2.03	2.10
4	A	562	3AC	C11-C16	2.97	1.44	1.39
4	A	562	3AC	C28-C27	2.95	1.49	1.30
4	A	562	3AC	C22-C21	2.86	1.44	1.38
4	A	562	3AC	C16-C15	2.51	1.43	1.39
4	A	562	3AC	C23-C24	2.17	1.43	1.38
4	A	562	3AC	C24-C25	2.12	1.43	1.39
4	A	562	3AC	C26-C21	2.07	1.42	1.38
4	A	562	3AC	C25-C27	2.02	1.53	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	562	3AC	C15-N14-C13	3.72	122.58	117.92
4	A	562	3AC	C25-C27-C28	-2.43	112.59	125.50
4	A	562	3AC	C21-O11-C11	2.26	122.12	118.48
4	A	562	3AC	C61-C16-C11	2.16	121.70	119.44

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	562	3AC	C25-C27-C28-C29

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| Mol	Chain	Res	Type	Atoms
4	A	562	3AC	C26-C25-C27-C28
4	A	562	3AC	C24-C25-C27-C28

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	562	3AC	4	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 3AC A 562

Bond lengths

Bond angles

Torsions

Rings
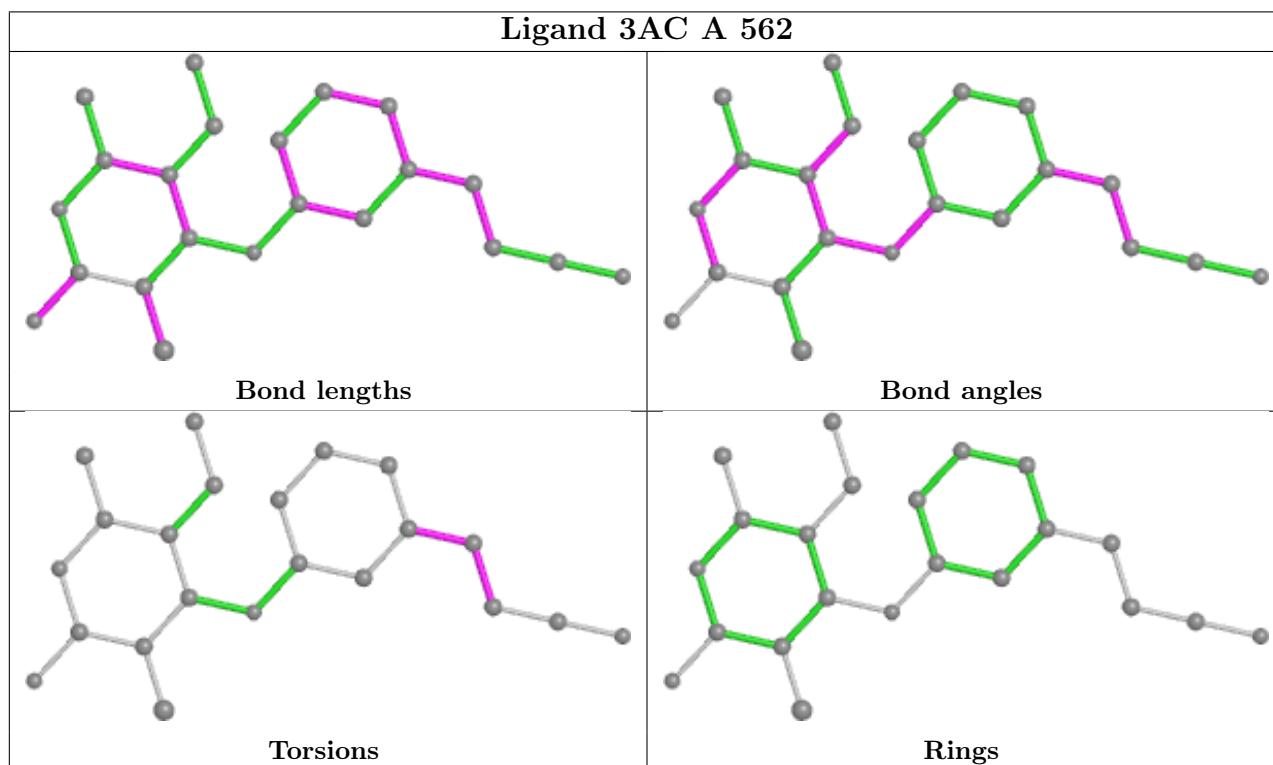
5.7 Other polymers ⓘ

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	552/560 (98%)	-0.05	10 (1%)	68	67	40, 88, 114, 127	0
2	B	427/430 (99%)	0.08	21 (4%)	29	26	31, 77, 118, 128	0
All	All	979/990 (98%)	0.01	31 (3%)	47	43	31, 84, 116, 128	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	231	GLY	6.5
2	B	2	ILE	5.4
1	A	133	PRO	5.4
2	B	295	LEU	4.8
2	B	227	PHE	4.5
2	B	225	PRO	4.2
1	A	547	GLN	4.0
1	A	551	LEU	4.0
2	B	230	MET	4.0
2	B	222	GLN	3.8
2	B	223	LYS	3.6
2	B	224	GLU	3.3
1	A	221	HIS	3.3
2	B	228	LEU	3.0
2	B	357	MET	2.7
1	A	359	GLY	2.6
2	B	3	SER	2.6
2	B	226	PRO	2.6
2	B	5	ILE	2.6
1	A	253	THR	2.6
1	A	552	VAL	2.5
2	B	410	TRP	2.4
1	A	422	LEU	2.4
2	B	272	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	358	ARG	2.4
2	B	362	THR	2.3
1	A	190	GLY	2.3
2	B	243	PRO	2.2
2	B	409	THR	2.2
1	A	89	GLU	2.1
2	B	279	LEU	2.1

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	MN	A	561	1/1	0.87	0.12	93,93,93,93	0
4	3AC	A	562	22/22	0.97	0.22	74,84,99,101	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 3AC A 562:

$2mF_o$-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.