



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:07 AM EDT

PDB ID : 1SV5 / pdb_00001sv5
Title : CRYSTAL STRUCTURE OF K103N MUTANT HIV-1 REVERSE TRANSCRIPTASE (RT) IN COMPLEX WITH JANSSEN-R165335
Authors : Das, K.; Arnold, E.
Deposited on : 2004-03-27
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

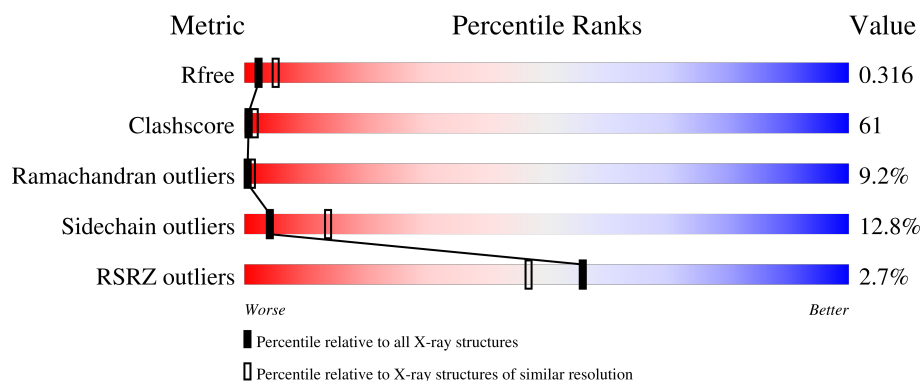
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

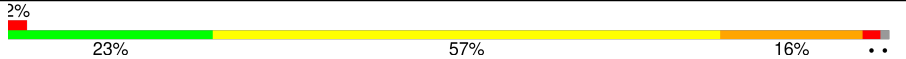
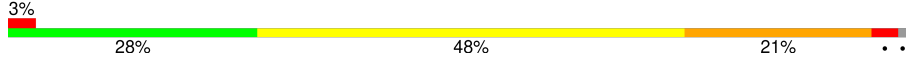
The reported resolution of this entry is 2.90 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	430	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	65B	A	600	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7905 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Reverse Transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4435	2873	739	816	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

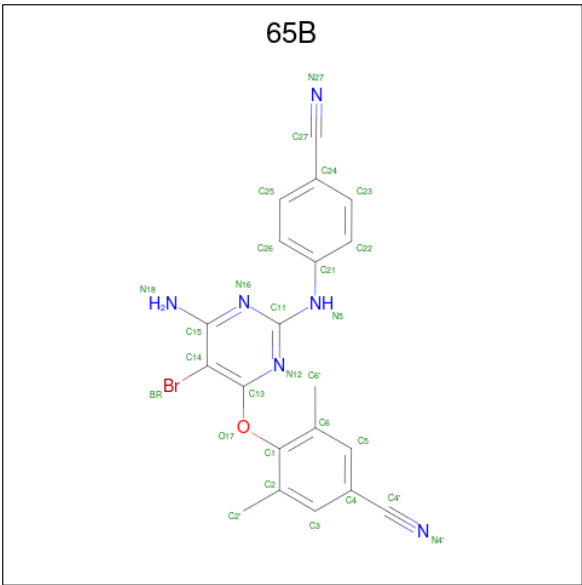
- Molecule 2 is a protein called Reverse Transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3442	2238	570	628	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	103	ASN	LYS	engineered mutation	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-({6-AMINO-5-BROMO-2-[(4-CYANOPHENYL)AMINO]PYRIMIDIN-4-YL}OXY)-3,5-DIMETHYLBENZONITRILE (CCD ID: 65B) (formula: C₂₀H₁₅BrN₆O).

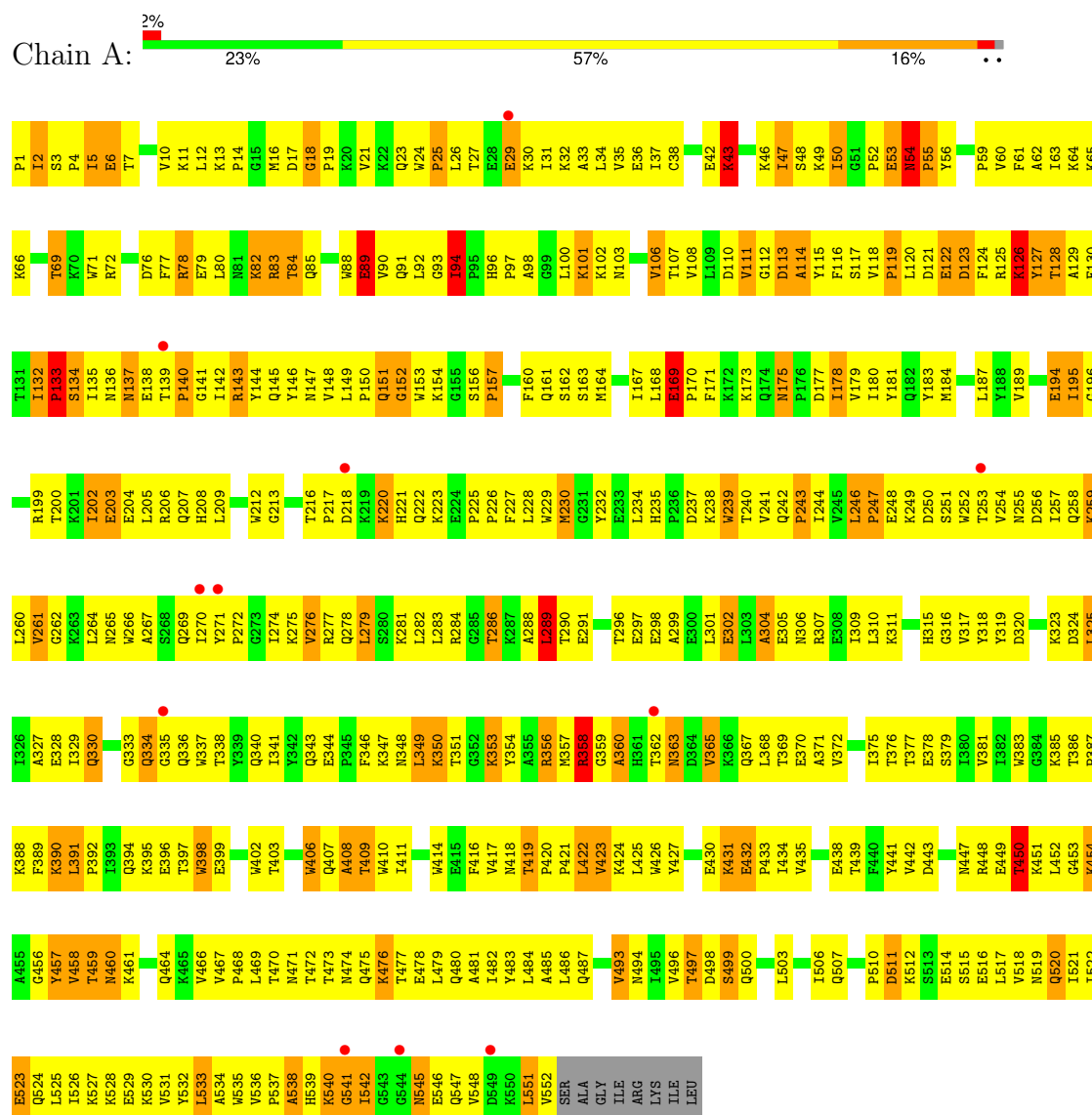


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
3	A	1	28	1	20	6	1	0	0

3 Residue-property plots

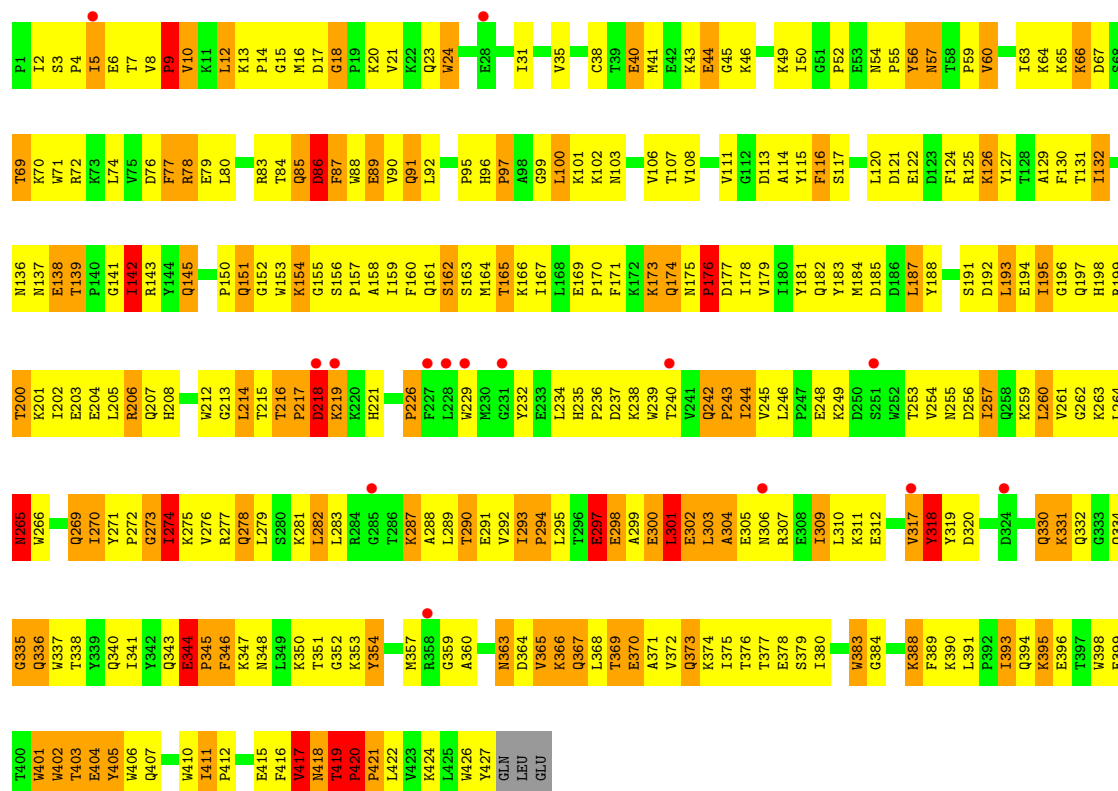
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: Reverse Transcriptase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	222.51Å 67.74Å 103.29Å 90.00° 107.47° 90.00°	Depositor
Resolution (Å)	19.95 – 2.90 19.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.4 (19.95-2.90) 95.0 (19.95-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.326 0.249 , 0.316	Depositor DCC
R_{free} test set	1624 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7905	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 65B

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	0.72	1/4553 (0.0%)	1.25	50/6196 (0.8%)
2	B	0.81	1/3542 (0.0%)	1.48	71/4826 (1.5%)
All	All	0.76	2/8095 (0.0%)	1.36	121/11022 (1.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	ILE	CA-CB	-6.83	1.47	1.54
2	B	60	VAL	CA-CB	-5.64	1.48	1.55

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	219	LYS	N-CA-C	-14.60	93.76	113.18
2	B	218	ASP	N-CA-C	14.43	132.03	108.52
2	B	89	GLU	N-CA-C	-12.69	97.89	113.50
1	A	132	ILE	CA-C-N	11.64	134.39	119.84
1	A	132	ILE	C-N-CA	11.64	134.39	119.84
2	B	242	GLN	CA-C-N	11.13	133.76	119.84
2	B	242	GLN	C-N-CA	11.13	133.76	119.84
2	B	419	THR	CA-C-N	-11.10	108.94	120.38
2	B	419	THR	C-N-CA	-11.10	108.94	120.38
2	B	298	GLU	N-CA-C	-10.80	98.61	112.23
2	B	96	HIS	CA-C-N	10.28	132.69	119.84
2	B	96	HIS	C-N-CA	10.28	132.69	119.84
2	B	295	LEU	N-CA-C	9.72	125.27	113.41
1	A	89	GLU	N-CA-C	9.56	124.30	110.24
2	B	87	PHE	N-CA-C	-9.48	102.32	112.93
1	A	347	LYS	N-CA-C	-9.37	95.00	109.52
2	B	278	GLN	OE1-CD-NE2	-9.29	113.31	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	417	VAL	N-CA-C	9.23	122.40	109.29
2	B	297	GLU	N-CA-C	9.19	123.11	109.24
1	A	349	LEU	N-CA-C	-9.09	101.75	113.12
1	A	319	TYR	N-CA-C	9.01	124.08	109.40
1	A	92	LEU	N-CA-C	-9.00	102.07	113.23
2	B	331	LYS	CB-CA-C	8.76	124.11	109.84
2	B	242	GLN	N-CA-C	8.73	123.82	109.58
1	A	141	GLY	N-CA-C	-8.47	93.11	113.18
1	A	493	VAL	N-CA-C	7.91	117.35	107.70
2	B	232	TYR	N-CA-C	7.88	121.86	107.99
1	A	542	ILE	N-CA-C	7.79	114.55	106.21
2	B	269	GLN	N-CA-C	-7.64	101.82	113.89
2	B	56	TYR	N-CA-C	7.57	121.17	110.50
1	A	6	GLU	N-CA-C	-7.56	100.55	110.53
2	B	411	ILE	CA-C-N	-7.47	110.50	119.84
2	B	411	ILE	C-N-CA	-7.47	110.50	119.84
1	A	106	VAL	N-CA-C	7.42	119.29	108.53
1	A	54	ASN	N-CA-C	-7.33	96.97	110.02
2	B	86	ASP	N-CA-C	-7.25	103.41	111.82
2	B	301	LEU	N-CA-C	-7.22	104.20	112.87
2	B	213	GLY	N-CA-C	7.17	123.40	114.37
2	B	293	ILE	CA-C-N	7.13	128.76	119.84
2	B	293	ILE	C-N-CA	7.13	128.76	119.84
2	B	200	THR	N-CA-C	-7.13	104.56	113.55
2	B	214	LEU	N-CA-C	7.13	121.31	108.69
2	B	303	LEU	N-CA-C	-7.02	103.22	112.34
2	B	278	GLN	CG-CD-NE2	7.01	126.91	116.40
1	A	500	GLN	N-CA-C	-6.89	103.78	111.71
2	B	44	GLU	N-CA-C	-6.88	104.88	113.20
2	B	401	TRP	N-CA-C	6.87	122.20	113.55
2	B	344	GLU	CA-C-N	6.86	128.41	119.84
2	B	344	GLU	C-N-CA	6.86	128.41	119.84
1	A	220	LYS	N-CA-C	-6.84	99.65	109.29
2	B	226	PRO	N-CA-CB	6.73	110.31	103.25
2	B	142	ILE	N-CA-C	-6.71	98.92	108.58
1	A	118	VAL	CA-C-N	6.61	128.10	119.84
1	A	118	VAL	C-N-CA	6.61	128.10	119.84
2	B	204	GLU	N-CA-C	-6.57	103.73	111.03
2	B	331	LYS	N-CA-C	-6.50	99.43	109.76
2	B	216	THR	CA-C-N	6.42	127.86	119.84
2	B	216	THR	C-N-CA	6.42	127.86	119.84
1	A	143	ARG	N-CA-C	6.41	118.97	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	274	ILE	CA-C-N	6.29	131.26	121.76
2	B	274	ILE	C-N-CA	6.29	131.26	121.76
2	B	179	VAL	CB-CA-C	-6.20	102.72	111.21
1	A	82	LYS	N-CA-C	-6.17	105.91	113.50
1	A	203	GLU	N-CA-C	-6.15	104.58	111.28
1	A	216	THR	CA-C-N	5.96	127.29	119.84
1	A	216	THR	C-N-CA	5.96	127.29	119.84
1	A	29	GLU	N-CA-C	-5.95	104.73	112.23
1	A	53	GLU	N-CA-C	5.94	119.91	110.70
2	B	237	ASP	N-CA-C	5.82	119.20	111.75
1	A	134	SER	N-CA-C	5.81	123.17	110.80
2	B	318	TYR	N-CA-CB	-5.80	101.67	110.77
1	A	43	LYS	N-CA-C	-5.78	105.48	112.54
1	A	261	VAL	N-CA-C	-5.78	104.29	110.36
2	B	132	ILE	N-CA-C	-5.78	101.30	107.77
2	B	10	VAL	N-CA-C	-5.73	100.18	108.89
2	B	249	LYS	N-CA-C	5.68	117.25	109.18
1	A	26	LEU	N-CA-C	5.65	116.03	108.23
1	A	88	TRP	N-CA-C	-5.64	99.93	108.67
2	B	265	ASN	N-CA-C	-5.61	105.08	111.14
1	A	246	LEU	CA-C-N	5.60	126.84	119.84
1	A	246	LEU	C-N-CA	5.60	126.84	119.84
2	B	389	PHE	N-CA-C	5.59	119.35	109.96
2	B	263	LYS	N-CA-C	-5.56	104.85	111.69
1	A	239	TRP	N-CA-C	-5.56	99.61	109.06
2	B	420	PRO	CA-C-N	5.52	126.73	119.84
2	B	420	PRO	C-N-CA	5.52	126.73	119.84
1	A	94	ILE	CA-C-N	-5.50	114.58	120.03
1	A	94	ILE	C-N-CA	-5.50	114.58	120.03
2	B	343	GLN	N-CA-C	-5.47	106.53	113.43
1	A	50	ILE	N-CA-C	5.44	117.02	109.29
1	A	499	SER	N-CA-C	5.41	117.81	107.75
2	B	240	THR	N-CA-C	5.34	122.18	110.80
1	A	390	LYS	N-CA-C	-5.34	100.03	108.73
2	B	391	LEU	N-CA-C	5.33	116.37	109.65
1	A	69	THR	N-CA-C	5.30	116.86	111.14
2	B	235	HIS	N-CA-C	5.30	117.76	108.75
1	A	514	GLU	N-CA-C	-5.29	105.68	111.82
2	B	160	PHE	N-CA-C	5.29	118.83	112.38
2	B	294	PRO	CA-N-CD	-5.22	104.69	112.00
2	B	96	HIS	N-CA-C	5.21	119.99	108.73
1	A	459	THR	N-CA-C	5.21	117.78	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	GLU	N-CA-C	-5.18	105.33	110.97
1	A	515	SER	N-CA-C	5.17	117.73	108.17
2	B	312	GLU	CA-C-N	5.14	126.27	119.84
2	B	312	GLU	C-N-CA	5.14	126.27	119.84
1	A	511	ASP	N-CA-C	-5.14	107.67	114.04
2	B	218	ASP	CA-C-O	5.12	125.95	120.32
1	A	33	ALA	N-CA-C	-5.11	105.35	111.03
1	A	4	PRO	N-CA-C	-5.11	108.84	114.92
1	A	202	ILE	N-CA-C	-5.09	105.88	110.82
2	B	318	TYR	N-CA-C	5.09	116.69	108.34
2	B	194	GLU	N-CA-C	-5.08	103.23	110.59
2	B	370	GLU	N-CA-C	-5.06	104.75	112.04
1	A	18	GLY	CA-C-N	5.06	124.99	119.78
1	A	18	GLY	C-N-CA	5.06	124.99	119.78
1	A	432	GLU	CA-C-N	5.05	126.15	119.84
1	A	432	GLU	C-N-CA	5.05	126.15	119.84
2	B	192	ASP	N-CA-C	-5.01	107.21	113.38
2	B	24	TRP	CA-C-N	-5.01	114.19	120.51
2	B	24	TRP	C-N-CA	-5.01	114.19	120.51
2	B	275	LYS	N-CA-C	-5.01	98.90	107.61

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4435	0	4426	581	0
2	B	3442	0	3399	399	0
3	A	28	0	15	9	0
All	All	7905	0	7840	967	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 61.

All (967) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:ILE:HG12	2:B:306:ASN:HB3	1.21	1.15
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.27	1.09
2:B:13:LYS:HG2	2:B:87:PHE:HB2	1.37	1.06
2:B:85:GLN:HG3	2:B:154:LYS:HG2	1.31	1.06
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.33	1.06
1:A:246:LEU:HD11	1:A:260:LEU:HD12	1.42	1.00
1:A:240:THR:HG22	1:A:241:VAL:H	1.26	1.00
2:B:274:ILE:HG12	2:B:306:ASN:CB	1.92	0.99
1:A:249:LYS:HG3	1:A:251:SER:H	1.25	0.98
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.28	0.98
1:A:517:LEU:O	1:A:520:GLN:HB2	1.63	0.97
2:B:357:MET:HG2	2:B:360:ALA:HB2	1.46	0.97
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.41	0.97
1:A:406:TRP:CZ2	2:B:419:THR:HG22	2.01	0.96
2:B:90:VAL:HG23	2:B:91:GLN:H	1.28	0.96
1:A:170:PRO:O	1:A:173:LYS:HG2	1.65	0.95
1:A:140:PRO:HB3	1:A:142:ILE:HG13	1.47	0.95
1:A:101:LYS:C	3:A:600:65B:H181	1.75	0.94
1:A:356:ARG:NH2	1:A:359:GLY:HA3	1.81	0.94
2:B:242:GLN:HG3	2:B:243:PRO:HD2	1.48	0.93
1:A:96:HIS:HD2	1:A:98:ALA:H	1.10	0.92
1:A:102:LYS:N	3:A:600:65B:H181	1.66	0.92
1:A:84:THR:HG22	1:A:154:LYS:HE2	1.50	0.92
1:A:235:HIS:CD2	1:A:238:LYS:HE3	2.05	0.91
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.54	0.90
1:A:278:GLN:HE21	1:A:298:GLU:HB3	1.35	0.90
1:A:281:LYS:HA	1:A:358:ARG:HH22	1.38	0.89
2:B:66:LYS:HG3	2:B:218:ASP:OD2	1.71	0.89
1:A:473:THR:HG22	1:A:475:GLN:H	1.37	0.89
1:A:498:ASP:HB2	1:A:538:ALA:HA	1.53	0.89
1:A:460:ASN:HD21	1:A:461:LYS:HG3	1.36	0.88
1:A:320:ASP:OD2	1:A:323:LYS:HE3	1.73	0.88
1:A:90:VAL:HG21	1:A:157:PRO:HB2	1.56	0.87
1:A:394:GLN:HG3	1:A:397:THR:OG1	1.73	0.87
1:A:126:LYS:H	1:A:126:LYS:HD2	1.39	0.87
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.56	0.87
2:B:2:ILE:HG21	2:B:9:PRO:HD2	1.56	0.87
2:B:85:GLN:HG3	2:B:154:LYS:CG	2.04	0.87
2:B:332:GLN:HB3	2:B:336:GLN:HG2	1.57	0.86
1:A:1:PRO:HD2	1:A:213:GLY:HA2	1.55	0.86
1:A:48:SER:HB2	1:A:147:ASN:HD21	1.41	0.85
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:CG1	1:A:266:TRP:HE1	1.89	0.85
1:A:448:ARG:HH12	1:A:473:THR:HG23	1.40	0.85
1:A:356:ARG:HH22	1:A:359:GLY:HA3	1.41	0.85
1:A:452:LEU:HD23	1:A:470:THR:HA	1.59	0.85
1:A:371:ALA:O	1:A:375:ILE:HD12	1.75	0.84
2:B:418:ASN:CG	2:B:419:THR:H	1.83	0.84
1:A:96:HIS:CD2	1:A:98:ALA:H	1.95	0.84
2:B:174:GLN:O	2:B:176:PRO:HD3	1.76	0.84
2:B:332:GLN:HB3	2:B:336:GLN:CG	2.07	0.84
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.12	0.84
2:B:66:LYS:CG	2:B:218:ASP:OD2	2.26	0.84
1:A:3:SER:OG	1:A:5:ILE:HG13	1.77	0.84
1:A:334:GLN:HG2	1:A:336:GLN:HG3	1.56	0.84
2:B:305:GLU:O	2:B:309:ILE:HG22	1.78	0.84
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.60	0.83
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	2.13	0.83
1:A:10:VAL:HG12	1:A:11:LYS:N	1.91	0.83
1:A:3:SER:HB3	1:A:119:PRO:HD3	1.60	0.83
1:A:10:VAL:HG12	1:A:11:LYS:H	1.44	0.82
1:A:30:LYS:HG2	1:A:71:TRP:CZ3	2.13	0.82
2:B:131:THR:OG1	2:B:143:ARG:HD2	1.78	0.82
1:A:246:LEU:HD11	1:A:260:LEU:CD1	2.09	0.82
1:A:317:VAL:HG12	1:A:348:ASN:O	1.78	0.82
1:A:163:SER:O	1:A:167:ILE:HD13	1.80	0.82
1:A:435:VAL:HG23	2:B:290:THR:HG21	1.62	0.82
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.62	0.81
1:A:442:VAL:HG22	1:A:481:ALA:HB1	1.62	0.81
1:A:47:ILE:HD11	1:A:130:PHE:HE1	1.45	0.81
2:B:366:LYS:HB2	2:B:405:TYR:CE2	2.15	0.81
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.45	0.80
2:B:332:GLN:HG2	2:B:336:GLN:HE21	1.45	0.80
1:A:458:VAL:HB	1:A:548:VAL:HG22	1.63	0.80
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.17	0.80
2:B:76:ASP:OD1	2:B:78:ARG:HD3	1.81	0.80
2:B:246:LEU:CD1	2:B:264:LEU:HD21	2.12	0.80
1:A:520:GLN:HE21	1:A:520:GLN:HA	1.47	0.79
2:B:31:ILE:O	2:B:35:VAL:HG23	1.82	0.79
1:A:356:ARG:CZ	1:A:359:GLY:HA3	2.13	0.79
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.63	0.79
1:A:64:LYS:HE3	1:A:69:THR:O	1.81	0.79
1:A:406:TRP:CE3	1:A:407:GLN:HB2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:HG22	1:A:241:VAL:N	1.96	0.78
1:A:97:PRO:HA	1:A:100:LEU:CD1	2.14	0.78
1:A:164:MET:O	1:A:167:ILE:HB	1.83	0.78
1:A:460:ASN:ND2	1:A:461:LYS:N	2.32	0.77
1:A:167:ILE:O	1:A:170:PRO:HD2	1.84	0.77
2:B:357:MET:HG2	2:B:360:ALA:CB	2.15	0.77
1:A:239:TRP:HB3	1:A:318:TYR:HE2	1.50	0.76
2:B:368:LEU:O	2:B:372:VAL:HG23	1.86	0.76
1:A:138:GLU:C	1:A:140:PRO:HD3	2.10	0.76
2:B:287:LYS:HD3	2:B:291:GLU:OE2	1.85	0.76
1:A:441:TYR:HB2	1:A:458:VAL:HG12	1.67	0.76
2:B:218:ASP:OD1	2:B:218:ASP:N	2.18	0.75
1:A:281:LYS:O	1:A:284:ARG:HG3	1.86	0.75
1:A:31:ILE:O	1:A:35:VAL:HG23	1.85	0.75
1:A:111:VAL:HG11	1:A:164:MET:HE1	1.69	0.75
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.52	0.75
2:B:97:PRO:HG3	2:B:181:TYR:HB2	1.69	0.75
1:A:84:THR:CG2	1:A:154:LYS:HE2	2.15	0.75
1:A:460:ASN:ND2	1:A:461:LYS:HG3	2.00	0.75
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.69	0.74
2:B:303:LEU:HA	2:B:306:ASN:OD1	1.87	0.74
1:A:239:TRP:HB3	1:A:318:TYR:CE2	2.22	0.74
2:B:20:LYS:HE2	2:B:55:PRO:HB2	1.69	0.74
2:B:163:SER:O	2:B:167:ILE:HG12	1.87	0.74
2:B:257:ILE:O	2:B:261:VAL:HG23	1.88	0.74
1:A:96:HIS:HD2	1:A:98:ALA:N	1.84	0.74
1:A:284:ARG:C	1:A:286:THR:H	1.95	0.73
1:A:333:GLY:O	1:A:335:GLY:N	2.20	0.73
1:A:448:ARG:HH22	1:A:473:THR:HG23	1.52	0.73
1:A:30:LYS:HG2	1:A:71:TRP:HZ3	1.51	0.73
2:B:8:VAL:O	2:B:9:PRO:C	2.32	0.73
2:B:279:LEU:HA	2:B:299:ALA:HB1	1.71	0.73
1:A:460:ASN:HD22	1:A:461:LYS:N	1.87	0.73
1:A:392:PRO:O	1:A:423:VAL:HG23	1.88	0.73
2:B:257:ILE:HG12	2:B:283:LEU:HD11	1.71	0.73
1:A:253:THR:O	1:A:256:ASP:HB2	1.88	0.73
2:B:85:GLN:CG	2:B:154:LYS:HG2	2.17	0.72
1:A:286:THR:O	1:A:286:THR:HG22	1.88	0.72
1:A:470:THR:HG23	1:A:471:ASN:ND2	2.04	0.72
2:B:7:THR:HB	2:B:121:ASP:HA	1.72	0.72
1:A:416:PHE:CD2	1:A:417:VAL:N	2.58	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:NH1	1:A:473:THR:HG23	2.04	0.72
2:B:353:LYS:HZ3	2:B:427:TYR:HB2	1.55	0.72
2:B:395:LYS:O	2:B:399:GLU:HG3	1.89	0.72
1:A:350:LYS:HE3	1:A:378:GLU:OE2	1.89	0.71
2:B:297:GLU:HB3	2:B:300:GLU:H	1.54	0.71
1:A:125:ARG:O	1:A:126:LYS:C	2.33	0.71
2:B:306:ASN:HA	2:B:309:ILE:CG2	2.20	0.71
1:A:254:VAL:O	1:A:258:GLN:HG3	1.90	0.71
1:A:539:HIS:CG	1:A:540:LYS:H	2.06	0.71
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.24	0.71
1:A:254:VAL:CG1	1:A:286:THR:HG23	2.20	0.71
1:A:356:ARG:NH1	1:A:359:GLY:HA3	2.05	0.71
1:A:540:LYS:O	1:A:542:ILE:N	2.23	0.71
2:B:202:ILE:HG21	2:B:219:LYS:HD2	1.73	0.71
2:B:257:ILE:CG1	2:B:283:LEU:HD11	2.20	0.71
1:A:167:ILE:HG22	1:A:168:LEU:N	2.03	0.71
2:B:352:GLY:O	2:B:353:LYS:HG3	1.91	0.71
1:A:450:THR:O	1:A:451:LYS:HG2	1.90	0.71
2:B:107:THR:HG21	2:B:219:LYS:HD2	1.72	0.71
1:A:324:ASP:O	1:A:343:GLN:HG2	1.91	0.70
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.73	0.70
2:B:419:THR:O	2:B:420:PRO:C	2.28	0.70
2:B:346:PHE:N	2:B:346:PHE:HD1	1.89	0.70
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.26	0.70
1:A:3:SER:HB2	1:A:117:SER:O	1.91	0.70
2:B:46:LYS:HD3	2:B:116:PHE:CD2	2.27	0.70
2:B:238:LYS:HG3	2:B:239:TRP:N	2.05	0.70
2:B:10:VAL:HA	2:B:88:TRP:HZ2	1.55	0.70
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.26	0.69
1:A:394:GLN:CG	1:A:397:THR:OG1	2.40	0.69
1:A:473:THR:C	1:A:475:GLN:N	2.48	0.69
1:A:2:ILE:O	1:A:213:GLY:HA3	1.92	0.69
1:A:484:LEU:O	1:A:487:GLN:HB2	1.92	0.69
1:A:240:THR:CG2	1:A:241:VAL:H	2.03	0.69
1:A:53:GLU:C	1:A:55:PRO:HD3	2.17	0.69
1:A:124:PHE:CE2	1:A:153:TRP:CZ2	2.79	0.69
1:A:102:LYS:N	3:A:600:65B:N18	2.40	0.69
1:A:284:ARG:C	1:A:286:THR:N	2.49	0.69
2:B:100:LEU:O	2:B:100:LEU:HD12	1.92	0.69
2:B:281:LYS:C	2:B:283:LEU:H	2.01	0.69
2:B:171:PHE:HB2	2:B:208:HIS:HD2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:CG	2:B:336:GLN:HE21	2.06	0.68
1:A:101:LYS:CA	3:A:600:65B:H181	2.05	0.68
2:B:299:ALA:O	2:B:302:GLU:HB2	1.93	0.68
2:B:346:PHE:N	2:B:346:PHE:CD1	2.62	0.68
1:A:97:PRO:HA	1:A:100:LEU:HD12	1.76	0.68
2:B:371:ALA:O	2:B:375:ILE:HG13	1.94	0.68
2:B:239:TRP:HD1	2:B:239:TRP:O	1.76	0.68
1:A:411:ILE:O	1:A:411:ILE:HG23	1.94	0.68
2:B:417:VAL:HG12	2:B:418:ASN:H	1.58	0.68
1:A:406:TRP:CE2	2:B:419:THR:HG22	2.29	0.67
1:A:126:LYS:HD2	1:A:126:LYS:N	2.08	0.67
1:A:473:THR:C	1:A:475:GLN:H	2.01	0.67
2:B:301:LEU:HG	2:B:302:GLU:OE2	1.93	0.67
2:B:365:VAL:HG12	2:B:366:LYS:N	2.09	0.67
1:A:47:ILE:HD11	1:A:130:PHE:CE1	2.29	0.67
1:A:460:ASN:HD22	1:A:460:ASN:C	2.03	0.66
2:B:137:ASN:C	2:B:139:THR:H	2.04	0.66
1:A:327:ALA:HB2	1:A:341:ILE:HG12	1.76	0.66
1:A:416:PHE:HD2	1:A:417:VAL:H	1.44	0.66
1:A:96:HIS:H	2:B:136:ASN:HD21	1.41	0.66
1:A:356:ARG:HH11	1:A:356:ARG:CG	2.08	0.66
1:A:474:ASN:O	1:A:478:GLU:HG3	1.96	0.66
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.25	0.66
1:A:458:VAL:HG23	1:A:464:GLN:HG2	1.77	0.66
2:B:90:VAL:O	2:B:91:GLN:C	2.39	0.66
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.60	0.66
1:A:64:LYS:HD2	1:A:71:TRP:CE2	2.31	0.66
2:B:76:ASP:OD2	2:B:78:ARG:NH1	2.28	0.66
1:A:12:LEU:HD11	1:A:127:TYR:CE2	2.31	0.65
1:A:90:VAL:CG2	1:A:157:PRO:HB2	2.25	0.65
2:B:330:GLN:HG2	2:B:338:THR:OG1	1.96	0.65
2:B:302:GLU:O	2:B:306:ASN:CG	2.39	0.65
2:B:332:GLN:NE2	2:B:424:LYS:O	2.26	0.65
1:A:32:LYS:O	1:A:36:GLU:HG3	1.96	0.65
1:A:112:GLY:C	1:A:114:ALA:H	2.04	0.65
1:A:255:ASN:OD1	1:A:259:LYS:HE3	1.97	0.65
1:A:101:LYS:N	3:A:600:65B:N18	2.45	0.65
2:B:380:ILE:O	2:B:384:GLY:HA2	1.96	0.65
1:A:64:LYS:HB2	1:A:71:TRP:CD2	2.32	0.65
1:A:235:HIS:NE2	1:A:238:LYS:HE3	2.11	0.65
1:A:447:ASN:CG	1:A:450:THR:HG23	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:ASP:OD1	2:B:78:ARG:CD	2.45	0.65
2:B:90:VAL:HG23	2:B:91:GLN:N	2.07	0.65
2:B:317:VAL:HG13	2:B:347:LYS:HB3	1.77	0.65
1:A:96:HIS:N	2:B:136:ASN:HD21	1.94	0.65
2:B:3:SER:OG	2:B:4:PRO:HD2	1.97	0.65
1:A:246:LEU:CD1	1:A:260:LEU:HD12	2.23	0.64
1:A:125:ARG:HG2	1:A:146:TYR:O	1.97	0.64
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.78	0.64
1:A:238:LYS:HB2	1:A:315:HIS:HB2	1.79	0.64
1:A:448:ARG:NH2	1:A:473:THR:HG23	2.12	0.64
1:A:542:ILE:HG12	1:A:546:GLU:HA	1.79	0.64
2:B:273:GLY:C	2:B:274:ILE:HG13	2.21	0.64
1:A:17:ASP:CG	1:A:18:GLY:N	2.55	0.64
1:A:179:VAL:HG21	3:A:600:65B:BR	2.53	0.64
1:A:442:VAL:CG2	1:A:481:ALA:HB1	2.27	0.64
2:B:303:LEU:HD12	2:B:303:LEU:O	1.97	0.64
2:B:57:ASN:HB2	2:B:143:ARG:HH12	1.62	0.64
2:B:21:VAL:O	2:B:57:ASN:ND2	2.30	0.64
1:A:475:GLN:O	1:A:477:THR:N	2.31	0.64
2:B:3:SER:OG	2:B:4:PRO:CD	2.46	0.63
2:B:238:LYS:HG3	2:B:239:TRP:H	1.62	0.63
1:A:7:THR:HG22	1:A:119:PRO:CB	2.28	0.63
2:B:84:THR:HG21	2:B:124:PHE:CZ	2.34	0.63
2:B:173:LYS:O	2:B:174:GLN:C	2.42	0.63
2:B:239:TRP:O	2:B:239:TRP:CD1	2.51	0.63
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.34	0.63
1:A:148:VAL:O	1:A:150:PRO:HD3	1.99	0.63
2:B:217:PRO:HB2	2:B:218:ASP:OD1	1.98	0.63
2:B:418:ASN:CG	2:B:419:THR:N	2.56	0.63
2:B:421:PRO:HG2	2:B:422:LEU:H	1.63	0.63
1:A:249:LYS:HD2	1:A:250:ASP:H	1.62	0.63
1:A:10:VAL:CG1	1:A:11:LYS:N	2.62	0.63
2:B:243:PRO:HB2	2:B:353:LYS:HZ1	1.62	0.63
1:A:153:TRP:CD1	1:A:154:LYS:H	2.16	0.62
2:B:84:THR:O	2:B:86:ASP:N	2.32	0.62
1:A:350:LYS:HB2	1:A:350:LYS:HZ3	1.65	0.62
1:A:518:VAL:O	1:A:522:ILE:HG12	1.99	0.62
1:A:23:GLN:HG2	1:A:133:PRO:HD3	1.81	0.62
2:B:354:TYR:HD2	2:B:374:LYS:HG3	1.65	0.62
2:B:243:PRO:HB2	2:B:353:LYS:NZ	2.14	0.62
1:A:43:LYS:HD2	1:A:43:LYS:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.81	0.62
2:B:13:LYS:HB3	2:B:14:PRO:HD2	1.81	0.62
2:B:84:THR:HG21	2:B:124:PHE:HZ	1.65	0.62
1:A:89:GLU:OE1	1:A:89:GLU:HA	2.00	0.62
2:B:301:LEU:O	2:B:304:ALA:HB3	2.00	0.62
1:A:10:VAL:CG1	1:A:11:LYS:H	2.12	0.61
1:A:63:ILE:HG13	1:A:63:ILE:O	1.99	0.61
2:B:282:LEU:HD13	2:B:297:GLU:OE2	2.00	0.61
1:A:477:THR:HA	1:A:480:GLN:HB2	1.83	0.61
2:B:153:TRP:C	2:B:155:GLY:H	2.08	0.61
1:A:94:ILE:HG13	1:A:229:TRP:CZ2	2.35	0.61
1:A:526:ILE:HG22	1:A:527:LYS:N	2.16	0.61
1:A:542:ILE:HG12	1:A:546:GLU:CB	2.31	0.61
1:A:416:PHE:HD2	1:A:417:VAL:N	1.97	0.61
2:B:2:ILE:O	2:B:3:SER:C	2.44	0.61
2:B:376:THR:O	2:B:380:ILE:HG13	2.00	0.61
1:A:194:GLU:HG2	1:A:196:GLY:H	1.66	0.61
1:A:418:ASN:O	1:A:420:PRO:HD3	2.00	0.61
2:B:152:GLY:O	2:B:184:MET:HE1	2.00	0.61
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.36	0.61
1:A:406:TRP:HZ2	2:B:419:THR:HG22	1.60	0.61
2:B:254:VAL:HG21	2:B:288:ALA:O	2.01	0.61
1:A:523:GLU:O	1:A:526:ILE:HB	2.00	0.60
2:B:115:TYR:O	2:B:117:SER:N	2.34	0.60
1:A:257:ILE:O	1:A:260:LEU:HB3	2.00	0.60
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.31	0.60
1:A:325:LEU:HD11	1:A:383:TRP:CG	2.36	0.60
2:B:10:VAL:HA	2:B:88:TRP:CZ2	2.37	0.60
2:B:302:GLU:C	2:B:304:ALA:N	2.57	0.60
2:B:50:ILE:HG23	2:B:145:GLN:HB3	1.84	0.60
1:A:78:ARG:O	1:A:82:LYS:HG3	2.01	0.60
1:A:458:VAL:CG2	1:A:464:GLN:HG2	2.30	0.60
1:A:494:ASN:OD1	1:A:532:TYR:HB3	2.02	0.60
2:B:419:THR:O	2:B:421:PRO:N	2.34	0.60
1:A:84:THR:HG22	1:A:154:LYS:CE	2.28	0.60
2:B:318:TYR:HD1	2:B:318:TYR:O	1.83	0.60
1:A:261:VAL:HG12	1:A:265:ASN:ND2	2.17	0.60
1:A:49:LYS:HG3	1:A:144:TYR:CE2	2.36	0.59
1:A:17:ASP:CG	1:A:18:GLY:H	2.09	0.59
1:A:151:GLN:O	1:A:151:GLN:HG2	2.02	0.59
1:A:235:HIS:HB2	1:A:238:LYS:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLN:O	2:B:89:GLU:N	2.35	0.59
2:B:85:GLN:CA	2:B:88:TRP:HB2	2.21	0.59
2:B:156:SER:O	2:B:157:PRO:C	2.40	0.59
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.37	0.59
1:A:276:VAL:HG12	1:A:276:VAL:O	2.01	0.59
2:B:269:GLN:NE2	2:B:346:PHE:HE2	2.00	0.59
2:B:111:VAL:C	2:B:113:ASP:H	2.09	0.59
2:B:427:TYR:CG	2:B:427:TYR:O	2.55	0.59
1:A:16:MET:CE	1:A:83:ARG:HG2	2.32	0.59
1:A:522:ILE:O	1:A:526:ILE:HD13	2.02	0.59
1:A:542:ILE:HG23	1:A:542:ILE:O	2.03	0.59
2:B:13:LYS:CG	2:B:87:PHE:HB2	2.25	0.59
1:A:101:LYS:CA	3:A:600:65B:N18	2.64	0.59
1:A:134:SER:CB	1:A:140:PRO:HD2	2.32	0.59
2:B:396:GLU:CD	2:B:396:GLU:H	2.11	0.59
1:A:120:LEU:O	1:A:121:ASP:C	2.46	0.58
1:A:241:VAL:CG1	1:A:266:TRP:NE1	2.64	0.58
1:A:453:GLY:C	1:A:454:LYS:HG2	2.28	0.58
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.66	0.58
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.38	0.58
2:B:193:LEU:HD12	2:B:198:HIS:HA	1.85	0.58
2:B:354:TYR:CD1	2:B:354:TYR:C	2.81	0.58
1:A:90:VAL:O	1:A:91:GLN:C	2.43	0.58
1:A:53:GLU:O	1:A:55:PRO:HD3	2.03	0.58
1:A:442:VAL:CG1	1:A:497:THR:HG23	2.33	0.58
1:A:542:ILE:HG12	1:A:546:GLU:HB2	1.86	0.58
2:B:124:PHE:O	2:B:125:ARG:C	2.45	0.58
1:A:442:VAL:HG22	1:A:481:ALA:CB	2.33	0.58
2:B:243:PRO:O	2:B:245:VAL:HG22	2.03	0.58
1:A:161:GLN:O	1:A:162:SER:C	2.43	0.58
1:A:305:GLU:O	1:A:309:ILE:HG13	2.03	0.58
2:B:402:TRP:O	2:B:406:TRP:HB2	2.04	0.58
1:A:140:PRO:CB	1:A:142:ILE:HG13	2.30	0.58
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.39	0.58
1:A:235:HIS:CD2	1:A:238:LYS:HG3	2.39	0.58
2:B:259:LYS:O	2:B:262:GLY:N	2.36	0.57
2:B:269:GLN:CB	2:B:346:PHE:HD2	2.16	0.57
1:A:123:ASP:HA	1:A:126:LYS:HE2	1.85	0.57
2:B:86:ASP:C	2:B:88:TRP:H	2.10	0.57
2:B:401:TRP:O	2:B:404:GLU:N	2.36	0.57
1:A:430:GLU:O	1:A:532:TYR:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:GLN:HG3	2:B:243:PRO:CD	2.27	0.57
2:B:269:GLN:HB3	2:B:346:PHE:HD2	1.69	0.57
1:A:460:ASN:ND2	1:A:460:ASN:C	2.62	0.57
1:A:368:LEU:O	1:A:372:VAL:HG23	2.05	0.57
2:B:50:ILE:CG2	2:B:145:GLN:HB3	2.35	0.57
1:A:480:GLN:O	1:A:483:TYR:HB3	2.04	0.57
2:B:18:GLY:HA3	2:B:56:TYR:CE1	2.40	0.57
1:A:2:ILE:HG23	1:A:3:SER:N	2.19	0.57
1:A:96:HIS:H	2:B:136:ASN:ND2	2.01	0.57
1:A:111:VAL:HG11	1:A:164:MET:CE	2.35	0.57
2:B:88:TRP:HZ3	2:B:159:ILE:CG1	2.17	0.57
1:A:356:ARG:HH12	1:A:359:GLY:HA3	1.70	0.57
1:A:391:LEU:HG	1:A:414:TRP:HB2	1.87	0.57
1:A:395:LYS:HA	1:A:414:TRP:HZ2	1.70	0.56
2:B:66:LYS:HG2	2:B:218:ASP:OD2	2.02	0.56
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.86	0.56
2:B:366:LYS:HE3	2:B:405:TYR:HD2	1.69	0.56
1:A:3:SER:HB3	1:A:119:PRO:CD	2.35	0.56
1:A:56:TYR:O	1:A:143:ARG:NH2	2.38	0.56
1:A:84:THR:HG22	1:A:85:GLN:O	2.06	0.56
1:A:277:ARG:HD3	1:A:334:GLN:HG3	1.87	0.56
1:A:278:GLN:HE21	1:A:298:GLU:CB	2.12	0.56
1:A:350:LYS:NZ	1:A:351:THR:O	2.39	0.56
1:A:448:ARG:HH12	1:A:473:THR:CG2	2.16	0.56
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.40	0.56
2:B:262:GLY:HA2	2:B:265:ASN:HB3	1.87	0.56
2:B:395:LYS:NZ	2:B:399:GLU:OE1	2.38	0.56
1:A:334:GLN:HG3	1:A:334:GLN:O	2.04	0.56
2:B:122:GLU:O	2:B:122:GLU:HG3	2.06	0.56
1:A:283:LEU:HD22	1:A:286:THR:HG21	1.87	0.56
1:A:493:VAL:HG22	1:A:494:ASN:N	2.20	0.56
2:B:87:PHE:C	2:B:88:TRP:CD1	2.84	0.56
2:B:99:GLY:O	2:B:102:LYS:HB3	2.04	0.56
1:A:169:GLU:CB	1:A:170:PRO:HD3	2.34	0.56
2:B:153:TRP:O	2:B:155:GLY:N	2.39	0.56
2:B:154:LYS:O	2:B:154:LYS:HG3	2.05	0.56
1:A:112:GLY:C	1:A:114:ALA:N	2.61	0.56
1:A:296:THR:O	1:A:297:GLU:C	2.48	0.56
2:B:100:LEU:HD12	2:B:100:LEU:C	2.31	0.56
1:A:79:GLU:OE1	1:A:83:ARG:NH1	2.38	0.56
2:B:248:GLU:O	2:B:248:GLU:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:LEU:O	2:B:301:LEU:HD12	2.06	0.56
2:B:393:ILE:HG12	2:B:394:GLN:N	2.21	0.56
2:B:354:TYR:CD2	2:B:374:LYS:HG3	2.41	0.56
2:B:106:VAL:O	2:B:234:LEU:HB2	2.05	0.55
2:B:279:LEU:CA	2:B:299:ALA:HB1	2.35	0.55
2:B:390:LYS:HB3	2:B:417:VAL:HG21	1.88	0.55
2:B:165:THR:HG22	2:B:166:LYS:N	2.20	0.55
2:B:171:PHE:HB2	2:B:208:HIS:CD2	2.40	0.55
1:A:542:ILE:HG12	1:A:546:GLU:CA	2.35	0.55
2:B:150:PRO:HG2	2:B:153:TRP:HB3	1.88	0.55
1:A:503:LEU:HD12	1:A:533:LEU:HD23	1.88	0.55
1:A:390:LYS:C	1:A:391:LEU:HD23	2.30	0.55
2:B:341:ILE:HD11	2:B:375:ILE:CG2	2.36	0.55
2:B:306:ASN:HA	2:B:309:ILE:HG23	1.88	0.55
1:A:200:THR:O	1:A:204:GLU:HB2	2.06	0.55
1:A:140:PRO:HB3	1:A:142:ILE:CG1	2.31	0.55
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.34	0.55
1:A:254:VAL:HG12	1:A:286:THR:HG23	1.88	0.55
1:A:456:GLY:HA2	1:A:484:LEU:HD23	1.88	0.55
1:A:469:LEU:CD1	1:A:480:GLN:HG2	2.19	0.55
2:B:64:LYS:HG3	2:B:71:TRP:CE3	2.42	0.55
1:A:180:ILE:HD11	1:A:187:LEU:HD22	1.89	0.54
1:A:301:LEU:O	1:A:304:ALA:HB3	2.06	0.54
2:B:175:ASN:OD1	2:B:201:LYS:CE	2.55	0.54
2:B:366:LYS:O	2:B:370:GLU:HB2	2.08	0.54
1:A:473:THR:O	1:A:475:GLN:N	2.41	0.54
1:A:356:ARG:NH1	1:A:356:ARG:CG	2.68	0.54
1:A:376:THR:HG23	1:A:386:THR:HG22	1.90	0.54
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.42	0.54
1:A:389:PHE:HB3	1:A:391:LEU:CD2	2.30	0.54
1:A:473:THR:HG22	1:A:475:GLN:N	2.14	0.54
1:A:498:ASP:HB2	1:A:538:ALA:CA	2.32	0.54
2:B:243:PRO:O	2:B:245:VAL:N	2.35	0.54
1:A:254:VAL:HG23	1:A:255:ASN:N	2.22	0.54
1:A:275:LYS:C	1:A:276:VAL:HG23	2.33	0.54
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.36	0.54
1:A:443:ASP:HB3	1:A:548:VAL:HG12	1.90	0.54
1:A:306:ASN:O	1:A:310:LEU:HG	2.07	0.54
1:A:406:TRP:CH2	1:A:407:GLN:OE1	2.61	0.54
2:B:246:LEU:O	2:B:307:ARG:NH2	2.41	0.54
1:A:334:GLN:HG2	1:A:336:GLN:CG	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:HG11	1:A:411:ILE:HG13	1.87	0.54
2:B:352:GLY:O	2:B:353:LYS:CG	2.54	0.54
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.43	0.54
1:A:111:VAL:HB	1:A:114:ALA:HB2	1.90	0.54
1:A:18:GLY:HA3	1:A:127:TYR:HD2	1.73	0.53
1:A:288:ALA:HB1	1:A:291:GLU:HG2	1.89	0.53
1:A:441:TYR:O	1:A:548:VAL:HG21	2.07	0.53
2:B:87:PHE:O	2:B:88:TRP:CD1	2.61	0.53
2:B:253:THR:OG1	2:B:256:ASP:OD2	2.23	0.53
1:A:377:THR:O	1:A:381:VAL:HG23	2.08	0.53
1:A:442:VAL:HG12	1:A:496:VAL:O	2.07	0.53
1:A:498:ASP:HB2	1:A:538:ALA:O	2.08	0.53
2:B:242:GLN:CG	2:B:243:PRO:HD2	2.30	0.53
1:A:54:ASN:ND2	1:A:56:TYR:HD1	2.05	0.53
1:A:275:LYS:O	1:A:276:VAL:CG2	2.56	0.53
1:A:357:MET:C	1:A:359:GLY:H	2.16	0.53
2:B:257:ILE:HG13	2:B:283:LEU:HD11	1.91	0.53
2:B:282:LEU:O	2:B:282:LEU:HD12	2.09	0.53
1:A:181:TYR:HB2	3:A:600:65B:H2'1	1.90	0.53
1:A:257:ILE:HG22	1:A:283:LEU:HD11	1.89	0.53
2:B:254:VAL:O	2:B:255:ASN:C	2.52	0.53
2:B:254:VAL:HA	2:B:257:ILE:HG23	1.89	0.53
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.89	0.53
1:A:65:LYS:HD2	1:A:72:ARG:HH11	1.73	0.53
1:A:164:MET:HE3	1:A:187:LEU:HD11	1.91	0.53
1:A:542:ILE:CG1	1:A:546:GLU:HA	2.38	0.53
2:B:120:LEU:O	2:B:125:ARG:NH1	2.42	0.53
2:B:238:LYS:CG	2:B:239:TRP:H	2.21	0.53
1:A:358:ARG:HG3	1:A:358:ARG:HH11	1.73	0.53
2:B:115:TYR:HE1	2:B:185:ASP:OD1	1.92	0.53
2:B:303:LEU:HD11	2:B:307:ARG:HD2	1.91	0.53
2:B:405:TYR:CD1	2:B:405:TYR:N	2.72	0.53
1:A:539:HIS:CD2	1:A:540:LYS:H	2.25	0.53
1:A:542:ILE:HG22	2:B:277:ARG:HH22	1.73	0.53
2:B:164:MET:HE3	2:B:187:LEU:HD11	1.91	0.53
2:B:303:LEU:CA	2:B:306:ASN:OD1	2.55	0.53
1:A:221:HIS:HD2	1:A:223:LYS:CB	2.21	0.52
1:A:324:ASP:OD2	1:A:388:LYS:NZ	2.39	0.52
1:A:399:GLU:O	1:A:403:THR:HB	2.08	0.52
2:B:238:LYS:O	2:B:239:TRP:C	2.50	0.52
2:B:244:ILE:HG23	2:B:244:ILE:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:O	1:A:272:PRO:HD3	2.10	0.52
1:A:275:LYS:HB2	1:A:302:GLU:HG3	1.91	0.52
2:B:401:TRP:O	2:B:402:TRP:C	2.50	0.52
1:A:137:ASN:O	1:A:140:PRO:HD2	2.10	0.52
1:A:240:THR:OG1	1:A:315:HIS:HA	2.09	0.52
2:B:111:VAL:C	2:B:113:ASP:N	2.67	0.52
2:B:254:VAL:CG2	2:B:288:ALA:O	2.57	0.52
1:A:94:ILE:HG23	1:A:229:TRP:HH2	1.73	0.52
1:A:150:PRO:O	1:A:152:GLY:N	2.41	0.52
1:A:358:ARG:HD2	1:A:358:ARG:N	2.25	0.52
1:A:460:ASN:ND2	1:A:461:LYS:CG	2.72	0.52
1:A:261:VAL:O	1:A:264:LEU:HB2	2.10	0.52
2:B:157:PRO:HG2	2:B:158:ALA:H	1.73	0.52
1:A:3:SER:OG	1:A:5:ILE:CG1	2.54	0.52
1:A:304:ALA:O	1:A:307:ARG:N	2.42	0.52
2:B:254:VAL:HB	2:B:289:LEU:HA	1.91	0.52
2:B:270:ILE:HG22	2:B:271:TYR:H	1.73	0.52
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.90	0.52
2:B:8:VAL:O	2:B:10:VAL:HG23	2.10	0.52
2:B:57:ASN:HA	2:B:129:ALA:O	2.10	0.52
1:A:395:LYS:HD3	1:A:395:LYS:C	2.35	0.52
2:B:78:ARG:HD2	2:B:411:ILE:HB	1.92	0.52
2:B:301:LEU:C	2:B:304:ALA:HB3	2.35	0.52
1:A:53:GLU:OE1	1:A:53:GLU:HA	2.10	0.52
1:A:124:PHE:HE2	1:A:153:TRP:CZ2	2.27	0.52
1:A:132:ILE:HG13	1:A:132:ILE:O	2.10	0.52
1:A:448:ARG:CZ	1:A:473:THR:HG23	2.39	0.52
1:A:460:ASN:HD21	1:A:461:LYS:CG	2.15	0.52
2:B:259:LYS:O	2:B:261:VAL:N	2.43	0.52
2:B:281:LYS:O	2:B:283:LEU:N	2.43	0.52
2:B:302:GLU:C	2:B:306:ASN:ND2	2.68	0.52
2:B:411:ILE:HG22	2:B:412:PRO:O	2.09	0.52
1:A:220:LYS:NZ	1:A:221:HIS:CE1	2.78	0.51
1:A:431:LYS:HE3	1:A:432:GLU:OE1	2.10	0.51
2:B:5:ILE:C	2:B:7:THR:H	2.18	0.51
1:A:2:ILE:HG12	1:A:3:SER:H	1.75	0.51
1:A:107:THR:HG23	1:A:221:HIS:HB2	1.93	0.51
2:B:7:THR:CB	2:B:121:ASP:HA	2.39	0.51
2:B:238:LYS:CG	2:B:239:TRP:N	2.71	0.51
2:B:242:GLN:HE22	2:B:426:TRP:CD1	2.29	0.51
2:B:253:THR:O	2:B:257:ILE:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:GLU:C	2:B:302:GLU:H	2.19	0.51
1:A:271:TYR:O	1:A:274:ILE:HG12	2.10	0.51
1:A:64:LYS:HB2	1:A:71:TRP:CE3	2.46	0.51
1:A:235:HIS:CD2	1:A:238:LYS:CE	2.89	0.51
2:B:60:VAL:O	2:B:60:VAL:HG23	2.09	0.51
2:B:69:THR:HG23	2:B:70:LYS:H	1.75	0.51
2:B:259:LYS:C	2:B:261:VAL:N	2.67	0.51
1:A:47:ILE:HD13	1:A:145:GLN:O	2.10	0.51
1:A:261:VAL:HG12	1:A:265:ASN:HD21	1.74	0.51
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.45	0.51
1:A:126:LYS:H	1:A:126:LYS:CD	2.19	0.51
1:A:450:THR:O	1:A:451:LYS:CG	2.57	0.51
2:B:354:TYR:OH	2:B:370:GLU:OE1	2.29	0.51
1:A:503:LEU:O	1:A:507:GLN:HB2	2.10	0.51
2:B:50:ILE:HD12	2:B:143:ARG:HH21	1.76	0.51
2:B:155:GLY:O	2:B:158:ALA:HB3	2.11	0.51
1:A:16:MET:CE	1:A:83:ARG:HA	2.41	0.51
2:B:101:LYS:O	2:B:236:PRO:HB3	2.11	0.51
2:B:376:THR:HB	2:B:410:TRP:CH2	2.46	0.51
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.46	0.51
1:A:510:PRO:HG2	1:A:522:ILE:HD11	1.92	0.51
2:B:126:LYS:HE2	2:B:127:TYR:CZ	2.46	0.51
2:B:369:THR:O	2:B:373:GLN:NE2	2.44	0.50
1:A:536:VAL:CG1	1:A:537:PRO:HD2	2.40	0.50
1:A:540:LYS:O	1:A:541:GLY:C	2.55	0.50
1:A:288:ALA:HB1	1:A:291:GLU:CG	2.42	0.50
1:A:442:VAL:HG13	1:A:497:THR:HG23	1.91	0.50
2:B:270:ILE:HG22	2:B:271:TYR:N	2.26	0.50
2:B:418:ASN:C	2:B:420:PRO:HD3	2.36	0.50
1:A:47:ILE:HD12	1:A:144:TYR:HB3	1.92	0.50
1:A:481:ALA:O	1:A:482:ILE:C	2.53	0.50
2:B:198:HIS:C	2:B:200:THR:H	2.20	0.50
2:B:300:GLU:C	2:B:302:GLU:N	2.66	0.50
2:B:388:LYS:HE2	2:B:415:GLU:OE1	2.12	0.50
2:B:418:ASN:O	2:B:420:PRO:HD3	2.10	0.50
1:A:365:VAL:HG12	1:A:398:TRP:CD1	2.47	0.50
1:A:442:VAL:HG21	1:A:481:ALA:C	2.37	0.50
2:B:13:LYS:HD3	2:B:87:PHE:N	2.27	0.50
2:B:291:GLU:CG	2:B:292:VAL:N	2.75	0.50
2:B:376:THR:CG2	2:B:410:TRP:CZ3	2.91	0.50
2:B:390:LYS:HB3	2:B:417:VAL:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:HA	1:A:226:PRO:C	2.37	0.50
2:B:66:LYS:HE2	2:B:66:LYS:HA	1.93	0.50
2:B:352:GLY:C	2:B:353:LYS:HG3	2.36	0.50
1:A:106:VAL:HG21	3:A:600:65B:H6'1	1.93	0.50
1:A:434:ILE:H	1:A:494:ASN:HD21	1.59	0.50
1:A:528:LYS:HB3	1:A:531:VAL:HG23	1.94	0.50
2:B:125:ARG:HH11	2:B:125:ARG:CG	2.25	0.50
2:B:243:PRO:C	2:B:245:VAL:N	2.70	0.50
2:B:405:TYR:H	2:B:405:TYR:HD1	1.57	0.50
1:A:447:ASN:CB	1:A:450:THR:HG23	2.41	0.50
1:A:449:GLU:C	1:A:451:LYS:H	2.20	0.50
1:A:470:THR:O	1:A:471:ASN:CG	2.55	0.49
2:B:164:MET:O	2:B:165:THR:C	2.55	0.49
1:A:113:ASP:O	1:A:116:PHE:N	2.41	0.49
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.36	0.49
1:A:546:GLU:HG2	1:A:547:GLN:HE21	1.75	0.49
2:B:366:LYS:HE3	2:B:405:TYR:CD2	2.46	0.49
1:A:42:GLU:HB2	1:A:47:ILE:HG22	1.94	0.49
1:A:498:ASP:C	1:A:535:TRP:HE1	2.20	0.49
2:B:320:ASP:OD1	2:B:320:ASP:C	2.56	0.49
1:A:452:LEU:HD23	1:A:470:THR:CA	2.37	0.49
1:A:467:VAL:HG13	1:A:468:PRO:HD2	1.94	0.49
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.94	0.49
1:A:258:GLN:HG2	1:A:283:LEU:HD13	1.94	0.49
2:B:76:ASP:CG	2:B:78:ARG:HD3	2.37	0.49
2:B:281:LYS:C	2:B:283:LEU:N	2.66	0.49
1:A:334:GLN:CG	1:A:336:GLN:HG3	2.37	0.49
1:A:447:ASN:HB3	1:A:450:THR:HG23	1.93	0.49
1:A:536:VAL:HG12	1:A:537:PRO:HD2	1.95	0.49
2:B:150:PRO:HD2	2:B:153:TRP:HE3	1.78	0.49
1:A:134:SER:CB	1:A:140:PRO:CD	2.90	0.49
1:A:356:ARG:HH22	1:A:359:GLY:CA	2.21	0.49
1:A:443:ASP:O	1:A:552:VAL:HG11	2.12	0.49
1:A:510:PRO:HG2	1:A:522:ILE:CD1	2.42	0.49
1:A:528:LYS:CB	1:A:531:VAL:HG23	2.43	0.49
2:B:243:PRO:C	2:B:245:VAL:H	2.20	0.49
1:A:406:TRP:HE3	1:A:406:TRP:O	1.96	0.48
1:A:475:GLN:O	1:A:476:LYS:C	2.56	0.48
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.53	0.48
2:B:57:ASN:ND2	2:B:57:ASN:C	2.70	0.48
1:A:434:ILE:HD11	1:A:530:LYS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:ALA:O	2:B:291:GLU:HB3	2.13	0.48
1:A:27:THR:C	1:A:29:GLU:H	2.21	0.48
1:A:137:ASN:C	1:A:139:THR:H	2.21	0.48
1:A:457:TYR:C	1:A:457:TYR:CD2	2.91	0.48
2:B:271:TYR:CD1	2:B:310:LEU:HD23	2.49	0.48
1:A:110:ASP:OD1	1:A:110:ASP:O	2.31	0.48
1:A:350:LYS:HB2	1:A:350:LYS:NZ	2.24	0.48
2:B:377:THR:O	2:B:378:GLU:C	2.57	0.48
2:B:401:TRP:O	2:B:403:THR:N	2.46	0.48
1:A:457:TYR:HE2	1:A:464:GLN:C	2.22	0.48
1:A:498:ASP:CB	1:A:538:ALA:HA	2.33	0.48
1:A:418:ASN:O	1:A:420:PRO:CD	2.61	0.48
1:A:516:GLU:O	1:A:520:GLN:HG2	2.14	0.48
1:A:115:TYR:O	1:A:149:LEU:HB2	2.13	0.48
1:A:431:LYS:HD2	1:A:432:GLU:N	2.29	0.48
1:A:108:VAL:HG12	1:A:223:LYS:CB	2.44	0.48
1:A:252:TRP:HE3	1:A:256:ASP:HB3	1.79	0.48
1:A:328:GLU:CG	1:A:329:ILE:N	2.77	0.48
2:B:7:THR:CG2	2:B:121:ASP:HA	2.43	0.48
2:B:153:TRP:C	2:B:155:GLY:N	2.72	0.48
1:A:153:TRP:CG	1:A:154:LYS:N	2.81	0.48
1:A:254:VAL:HG11	1:A:286:THR:HG23	1.96	0.48
2:B:193:LEU:HD12	2:B:198:HIS:CA	2.44	0.48
1:A:80:LEU:O	1:A:84:THR:N	2.46	0.48
1:A:241:VAL:HG12	1:A:242:GLN:N	2.29	0.48
1:A:241:VAL:HG11	1:A:266:TRP:CD1	2.49	0.48
1:A:528:LYS:HG3	1:A:531:VAL:CG2	2.43	0.48
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.95	0.48
1:A:175:ASN:CB	1:A:178:ILE:HG13	2.43	0.47
1:A:276:VAL:HA	1:A:302:GLU:OE1	2.13	0.47
2:B:379:SER:HA	2:B:383:TRP:CZ3	2.49	0.47
1:A:441:TYR:HB3	1:A:548:VAL:HG21	1.96	0.47
1:A:457:TYR:C	1:A:457:TYR:HD2	2.23	0.47
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.40	0.47
1:A:54:ASN:OD1	1:A:129:ALA:HB2	2.13	0.47
1:A:77:PHE:O	1:A:78:ARG:C	2.57	0.47
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.95	0.47
1:A:356:ARG:HB2	1:A:367:GLN:HE21	1.78	0.47
1:A:397:THR:HG21	1:A:424:LYS:HA	1.97	0.47
1:A:497:THR:HB	1:A:499:SER:H	1.80	0.47
2:B:138:GLU:C	2:B:139:THR:HG22	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:GLU:O	1:A:451:LYS:N	2.46	0.47
2:B:153:TRP:CE2	2:B:155:GLY:HA3	2.49	0.47
2:B:330:GLN:NE2	2:B:340:GLN:OE1	2.47	0.47
1:A:221:HIS:C	1:A:223:LYS:H	2.22	0.47
1:A:358:ARG:N	1:A:358:ARG:CD	2.77	0.47
1:A:441:TYR:CB	1:A:548:VAL:HG21	2.43	0.47
2:B:242:GLN:CG	2:B:243:PRO:CD	2.90	0.47
1:A:78:ARG:HG3	1:A:79:GLU:N	2.29	0.47
1:A:328:GLU:HG2	1:A:329:ILE:N	2.29	0.47
1:A:357:MET:O	1:A:359:GLY:N	2.48	0.47
1:A:448:ARG:HH22	1:A:473:THR:CG2	2.21	0.47
2:B:50:ILE:CD1	2:B:143:ARG:HH21	2.28	0.47
1:A:80:LEU:O	1:A:83:ARG:N	2.45	0.47
1:A:94:ILE:HD11	1:A:183:TYR:CE1	2.50	0.47
1:A:94:ILE:HD11	1:A:183:TYR:CZ	2.50	0.47
1:A:175:ASN:HB3	1:A:178:ILE:HG13	1.97	0.47
1:A:278:GLN:NE2	1:A:298:GLU:HB3	2.16	0.47
1:A:411:ILE:O	1:A:411:ILE:CG2	2.60	0.47
2:B:99:GLY:O	2:B:102:LYS:CB	2.63	0.47
2:B:107:THR:HG21	2:B:219:LYS:CD	2.43	0.47
2:B:120:LEU:HD23	2:B:125:ARG:HA	1.96	0.47
2:B:125:ARG:HH11	2:B:125:ARG:HG2	1.80	0.47
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.49	0.47
1:A:19:PRO:HB3	1:A:79:GLU:HB3	1.97	0.47
1:A:106:VAL:CG1	1:A:107:THR:N	2.77	0.47
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.96	0.47
1:A:286:THR:O	1:A:286:THR:CG2	2.59	0.47
2:B:88:TRP:HZ3	2:B:159:ILE:HG13	1.80	0.47
2:B:175:ASN:OD1	2:B:201:LYS:HE3	2.14	0.47
1:A:363:ASN:OD1	1:A:363:ASN:C	2.58	0.47
1:A:394:GLN:HE21	1:A:424:LYS:HZ2	1.63	0.47
2:B:66:LYS:HG3	2:B:218:ASP:CG	2.38	0.47
2:B:85:GLN:O	2:B:88:TRP:C	2.58	0.47
1:A:451:LYS:HD2	1:A:471:ASN:HA	1.97	0.47
1:A:475:GLN:C	1:A:477:THR:N	2.73	0.47
1:A:485:ALA:O	1:A:486:LEU:C	2.58	0.47
2:B:79:GLU:HG3	2:B:83:ARG:NE	2.28	0.47
2:B:242:GLN:NE2	2:B:426:TRP:HD1	2.13	0.46
2:B:260:LEU:HD11	2:B:264:LEU:HD11	1.97	0.46
1:A:359:GLY:O	1:A:360:ALA:C	2.58	0.46
2:B:52:PRO:C	2:B:54:ASN:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:LYS:HA	2:B:184:MET:HE3	1.97	0.46
2:B:201:LYS:HA	2:B:201:LYS:HD3	1.53	0.46
1:A:23:GLN:O	1:A:25:PRO:HD3	2.14	0.46
1:A:78:ARG:HG3	1:A:79:GLU:H	1.80	0.46
1:A:241:VAL:HG11	1:A:244:ILE:HD11	1.96	0.46
2:B:74:LEU:O	2:B:74:LEU:HG	2.16	0.46
2:B:137:ASN:C	2:B:139:THR:N	2.70	0.46
1:A:7:THR:CG2	1:A:119:PRO:CB	2.93	0.46
1:A:122:GLU:C	1:A:124:PHE:H	2.24	0.46
1:A:324:ASP:O	1:A:343:GLN:CG	2.63	0.46
1:A:356:ARG:HG3	1:A:357:MET:O	2.15	0.46
2:B:85:GLN:O	2:B:85:GLN:HG2	2.15	0.46
1:A:175:ASN:C	1:A:177:ASP:H	2.24	0.46
1:A:203:GLU:O	1:A:206:ARG:HB3	2.16	0.46
1:A:518:VAL:HA	1:A:521:ILE:HD12	1.98	0.46
1:A:539:HIS:ND1	1:A:539:HIS:N	2.63	0.46
2:B:65:LYS:HZ2	2:B:72:ARG:NE	2.14	0.46
2:B:88:TRP:CZ3	2:B:92:LEU:HD12	2.51	0.46
2:B:302:GLU:O	2:B:306:ASN:ND2	2.48	0.46
1:A:346:PHE:CD1	1:A:346:PHE:N	2.83	0.46
1:A:406:TRP:CZ2	2:B:419:THR:CG2	2.88	0.46
1:A:447:ASN:C	1:A:449:GLU:H	2.23	0.46
1:A:270:ILE:O	1:A:272:PRO:CD	2.64	0.46
2:B:278:GLN:NE2	2:B:302:GLU:OE2	2.48	0.46
2:B:334:GLN:O	2:B:335:GLY:C	2.59	0.46
1:A:47:ILE:HD13	1:A:145:GLN:C	2.41	0.46
1:A:325:LEU:HD23	1:A:341:ILE:CG2	2.46	0.46
2:B:334:GLN:O	2:B:336:GLN:N	2.48	0.46
1:A:107:THR:HG23	1:A:221:HIS:CB	2.45	0.46
2:B:242:GLN:HE22	2:B:426:TRP:HD1	1.63	0.46
1:A:240:THR:CG2	1:A:241:VAL:N	2.66	0.46
1:A:255:ASN:CG	1:A:259:LYS:HE3	2.41	0.46
2:B:76:ASP:OD1	2:B:76:ASP:C	2.59	0.46
2:B:332:GLN:HB3	2:B:336:GLN:HG3	1.93	0.46
1:A:48:SER:HB2	1:A:147:ASN:ND2	2.22	0.45
1:A:80:LEU:HD23	1:A:153:TRP:CD1	2.51	0.45
2:B:167:ILE:O	2:B:170:PRO:HD2	2.16	0.45
1:A:330:GLN:HE21	1:A:330:GLN:HB3	1.52	0.45
1:A:451:LYS:HD2	1:A:471:ASN:HB3	1.97	0.45
1:A:71:TRP:CD1	1:A:71:TRP:N	2.85	0.45
1:A:545:ASN:OD1	1:A:548:VAL:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:VAL:O	2:B:60:VAL:CG2	2.62	0.45
2:B:279:LEU:HD12	2:B:279:LEU:O	2.17	0.45
2:B:344:GLU:HA	2:B:345:PRO:HD2	1.79	0.45
2:B:402:TRP:O	2:B:403:THR:C	2.59	0.45
1:A:94:ILE:HG23	1:A:229:TRP:CH2	2.50	0.45
1:A:108:VAL:HG11	1:A:227:PHE:CE1	2.52	0.45
1:A:125:ARG:O	1:A:128:THR:N	2.24	0.45
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.80	0.45
1:A:356:ARG:HB2	1:A:367:GLN:NE2	2.31	0.45
1:A:363:ASN:OD1	1:A:365:VAL:HG23	2.15	0.45
1:A:46:LYS:NZ	1:A:113:ASP:OD2	2.48	0.45
1:A:209:LEU:O	1:A:212:TRP:HB2	2.17	0.45
1:A:260:LEU:O	1:A:264:LEU:HG	2.17	0.45
2:B:111:VAL:O	2:B:113:ASP:N	2.49	0.45
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.51	0.45
1:A:417:VAL:CG1	1:A:419:THR:HG23	2.45	0.45
1:A:482:ILE:HD13	1:A:506:ILE:CD1	2.46	0.45
2:B:88:TRP:HZ3	2:B:159:ILE:HG12	1.80	0.45
2:B:116:PHE:CZ	2:B:151:GLN:NE2	2.67	0.45
2:B:242:GLN:HA	2:B:243:PRO:HD3	1.56	0.45
1:A:277:ARG:HB2	1:A:336:GLN:OE1	2.17	0.45
2:B:88:TRP:CZ3	2:B:159:ILE:CG1	2.99	0.45
2:B:205:LEU:O	2:B:208:HIS:HB3	2.16	0.45
2:B:303:LEU:HD12	2:B:307:ARG:HB2	1.99	0.45
1:A:106:VAL:HG12	1:A:107:THR:N	2.31	0.45
1:A:30:LYS:HE2	1:A:71:TRP:HZ3	1.81	0.45
1:A:90:VAL:HG21	1:A:157:PRO:CB	2.38	0.45
1:A:270:ILE:HD11	1:A:316:GLY:CA	2.47	0.45
2:B:7:THR:O	2:B:9:PRO:HD3	2.17	0.45
2:B:60:VAL:CG1	2:B:130:PHE:HB2	2.47	0.45
2:B:203:GLU:OE2	2:B:207:GLN:HG2	2.16	0.45
2:B:363:ASN:O	2:B:367:GLN:CG	2.65	0.45
2:B:369:THR:HB	2:B:398:TRP:CH2	2.51	0.45
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.51	0.45
1:A:115:TYR:HE2	1:A:157:PRO:HA	1.82	0.45
1:A:168:LEU:O	1:A:169:GLU:C	2.59	0.45
1:A:195:ILE:CD1	1:A:199:ARG:HG3	2.47	0.45
1:A:281:LYS:HA	1:A:358:ARG:NH2	2.19	0.45
1:A:283:LEU:CD2	1:A:286:THR:HG21	2.47	0.45
1:A:327:ALA:CB	1:A:341:ILE:HG12	2.47	0.45
1:A:417:VAL:HG12	1:A:419:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:VAL:HG21	1:A:551:LEU:O	2.17	0.45
2:B:366:LYS:HB2	2:B:405:TYR:CZ	2.49	0.45
1:A:241:VAL:HG11	1:A:266:TRP:NE1	2.32	0.44
1:A:426:TRP:O	1:A:427:TYR:HB3	2.17	0.44
2:B:23:GLN:HG3	2:B:24:TRP:O	2.16	0.44
2:B:66:LYS:HG3	2:B:218:ASP:CB	2.46	0.44
1:A:125:ARG:O	1:A:128:THR:OG1	2.26	0.44
1:A:235:HIS:HB2	1:A:238:LYS:CG	2.47	0.44
1:A:255:ASN:ND2	1:A:259:LYS:HE3	2.32	0.44
2:B:214:LEU:HD12	2:B:214:LEU:O	2.18	0.44
2:B:303:LEU:O	2:B:307:ARG:HB2	2.18	0.44
1:A:442:VAL:CG2	1:A:481:ALA:C	2.90	0.44
2:B:164:MET:HE3	2:B:187:LEU:CD1	2.47	0.44
2:B:373:GLN:HE21	2:B:373:GLN:HB2	1.65	0.44
1:A:38:CYS:CB	1:A:144:TYR:CE1	3.00	0.44
1:A:122:GLU:O	1:A:124:PHE:N	2.51	0.44
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.99	0.44
2:B:10:VAL:HG13	2:B:88:TRP:CZ2	2.52	0.44
1:A:32:LYS:HD3	1:A:32:LYS:HA	1.73	0.44
1:A:275:LYS:C	1:A:276:VAL:CG2	2.91	0.44
1:A:510:PRO:O	1:A:522:ILE:HD12	2.18	0.44
2:B:138:GLU:O	2:B:139:THR:HG22	2.17	0.44
2:B:273:GLY:HA3	2:B:309:ILE:HG12	2.00	0.44
1:A:84:THR:O	1:A:154:LYS:NZ	2.45	0.44
1:A:255:ASN:HD21	1:A:259:LYS:HE3	1.82	0.44
1:A:511:ASP:OD1	1:A:512:LYS:N	2.51	0.44
2:B:65:LYS:NZ	2:B:72:ARG:HE	2.16	0.44
2:B:203:GLU:HA	2:B:206:ARG:HB2	2.00	0.44
1:A:54:ASN:O	1:A:55:PRO:C	2.61	0.44
1:A:76:ASP:OD2	1:A:78:ARG:NE	2.51	0.44
1:A:106:VAL:HG13	1:A:189:VAL:O	2.17	0.44
1:A:479:LEU:O	1:A:480:GLN:C	2.59	0.44
2:B:18:GLY:HA3	2:B:56:TYR:CD1	2.52	0.44
2:B:85:GLN:C	2:B:88:TRP:H	2.26	0.44
2:B:366:LYS:HB2	2:B:405:TYR:CD2	2.52	0.44
1:A:61:PHE:HE1	1:A:76:ASP:HB2	1.81	0.44
1:A:64:LYS:HD2	1:A:71:TRP:CZ2	2.52	0.44
1:A:323:LYS:NZ	1:A:344:GLU:OE2	2.32	0.44
1:A:395:LYS:HD3	1:A:395:LYS:O	2.18	0.44
2:B:5:ILE:C	2:B:7:THR:N	2.73	0.44
2:B:65:LYS:HB3	2:B:66:LYS:H	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:LYS:O	2:B:260:LEU:C	2.60	0.44
2:B:273:GLY:O	2:B:274:ILE:HG13	2.18	0.44
1:A:208:HIS:O	1:A:212:TRP:HD1	2.00	0.44
2:B:2:ILE:O	2:B:4:PRO:O	2.36	0.44
2:B:178:ILE:HD11	2:B:201:LYS:HG3	1.98	0.44
1:A:37:ILE:O	1:A:38:CYS:C	2.60	0.43
1:A:485:ALA:C	1:A:487:GLN:N	2.76	0.43
1:A:525:LEU:HD23	1:A:525:LEU:HA	1.81	0.43
2:B:175:ASN:OD1	2:B:201:LYS:HD2	2.17	0.43
2:B:318:TYR:O	2:B:318:TYR:CD1	2.68	0.43
2:B:350:LYS:CE	2:B:378:GLU:OE1	2.66	0.43
1:A:27:THR:HG22	1:A:29:GLU:H	1.82	0.43
1:A:296:THR:H	1:A:299:ALA:HB3	1.83	0.43
1:A:391:LEU:HG	1:A:414:TRP:CB	2.48	0.43
1:A:407:GLN:O	1:A:408:ALA:C	2.61	0.43
1:A:453:GLY:O	1:A:469:LEU:O	2.35	0.43
2:B:43:LYS:C	2:B:45:GLY:H	2.25	0.43
2:B:85:GLN:O	2:B:88:TRP:N	2.47	0.43
2:B:242:GLN:HB2	2:B:351:THR:OG1	2.19	0.43
2:B:302:GLU:C	2:B:304:ALA:H	2.23	0.43
1:A:13:LYS:O	1:A:14:PRO:C	2.61	0.43
1:A:30:LYS:HD3	1:A:62:ALA:O	2.19	0.43
1:A:64:LYS:HA	1:A:71:TRP:HA	2.00	0.43
1:A:248:GLU:HG3	1:A:248:GLU:O	2.19	0.43
2:B:272:PRO:O	2:B:274:ILE:N	2.52	0.43
2:B:291:GLU:CG	2:B:292:VAL:H	2.31	0.43
1:A:246:LEU:CD1	1:A:260:LEU:CD1	2.91	0.43
2:B:282:LEU:O	2:B:283:LEU:HD23	2.19	0.43
1:A:5:ILE:HG22	1:A:6:GLU:N	2.33	0.43
1:A:137:ASN:O	1:A:140:PRO:CD	2.66	0.43
1:A:439:THR:CG2	1:A:441:TYR:CE1	3.00	0.43
1:A:524:GLN:O	1:A:525:LEU:C	2.60	0.43
1:A:548:VAL:HG12	1:A:552:VAL:HG21	1.99	0.43
2:B:340:GLN:HB3	2:B:348:ASN:ND2	2.33	0.43
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.83	0.43
1:A:48:SER:N	1:A:145:GLN:O	2.45	0.43
1:A:108:VAL:CG1	1:A:227:PHE:CE1	3.01	0.43
1:A:416:PHE:HZ	1:A:422:LEU:HD11	1.83	0.43
1:A:420:PRO:HA	1:A:422:LEU:HD23	2.00	0.43
1:A:482:ILE:O	1:A:485:ALA:HB3	2.19	0.43
2:B:161:GLN:O	2:B:162:SER:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HG22	2:B:196:GLY:N	2.34	0.43
2:B:242:GLN:CG	2:B:243:PRO:N	2.82	0.43
2:B:270:ILE:CG2	2:B:271:TYR:H	2.31	0.43
1:A:2:ILE:HG23	1:A:3:SER:H	1.83	0.43
1:A:17:ASP:OD1	1:A:56:TYR:HE2	2.01	0.43
1:A:277:ARG:HB3	1:A:334:GLN:OE1	2.18	0.43
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.49	0.43
1:A:449:GLU:C	1:A:451:LYS:N	2.76	0.43
2:B:278:GLN:O	2:B:299:ALA:HB2	2.18	0.43
2:B:319:TYR:CG	2:B:320:ASP:N	2.87	0.43
1:A:434:ILE:HD13	1:A:530:LYS:CB	2.49	0.43
1:A:480:GLN:NE2	1:A:480:GLN:HA	2.33	0.43
1:A:16:MET:HE1	1:A:83:ARG:HA	2.01	0.43
1:A:17:ASP:CG	1:A:56:TYR:HE2	2.27	0.43
1:A:64:LYS:O	1:A:65:LYS:C	2.62	0.43
1:A:447:ASN:C	1:A:449:GLU:N	2.76	0.43
1:A:453:GLY:O	1:A:469:LEU:HB2	2.19	0.43
2:B:115:TYR:O	2:B:116:PHE:C	2.62	0.43
2:B:131:THR:HG23	2:B:141:GLY:HA3	2.01	0.43
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.92	0.43
2:B:193:LEU:HD12	2:B:198:HIS:N	2.34	0.43
1:A:94:ILE:HD12	1:A:94:ILE:HA	1.78	0.42
1:A:137:ASN:C	1:A:139:THR:N	2.76	0.42
1:A:138:GLU:C	1:A:140:PRO:CD	2.88	0.42
1:A:525:LEU:O	1:A:526:ILE:C	2.60	0.42
2:B:125:ARG:O	2:B:127:TYR:N	2.51	0.42
2:B:265:ASN:O	2:B:266:TRP:C	2.60	0.42
1:A:275:LYS:O	1:A:276:VAL:HG23	2.19	0.42
2:B:131:THR:OG1	2:B:143:ARG:CD	2.60	0.42
1:A:49:LYS:HA	1:A:144:TYR:HD2	1.84	0.42
1:A:113:ASP:O	1:A:114:ALA:C	2.61	0.42
1:A:410:TRP:CZ3	2:B:401:TRP:CE3	3.07	0.42
1:A:548:VAL:O	1:A:552:VAL:CG2	2.67	0.42
1:A:235:HIS:CB	1:A:238:LYS:HG2	2.50	0.42
1:A:337:TRP:O	1:A:354:TYR:N	2.52	0.42
1:A:420:PRO:HB2	1:A:421:PRO:HA	2.02	0.42
1:A:435:VAL:HA	2:B:290:THR:HG21	2.01	0.42
2:B:100:LEU:C	2:B:102:LYS:N	2.76	0.42
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.54	0.42
2:B:191:SER:OG	2:B:198:HIS:ND1	2.39	0.42
2:B:198:HIS:C	2:B:200:THR:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LYS:NZ	2:B:364:ASP:OD2	2.48	0.42
1:A:110:ASP:CB	1:A:222:GLN:NE2	2.82	0.42
1:A:254:VAL:CG2	1:A:255:ASN:N	2.83	0.42
1:A:341:ILE:O	1:A:349:LEU:HB2	2.20	0.42
1:A:391:LEU:O	1:A:416:PHE:HA	2.18	0.42
1:A:261:VAL:O	1:A:262:GLY:C	2.62	0.42
1:A:278:GLN:OE1	1:A:278:GLN:HA	2.20	0.42
1:A:456:GLY:HA2	1:A:484:LEU:CD2	2.50	0.42
2:B:197:GLN:O	2:B:200:THR:HB	2.20	0.42
2:B:279:LEU:HA	2:B:299:ALA:CB	2.47	0.42
1:A:229:TRP:NE1	1:A:230:MET:HG2	2.35	0.42
1:A:279:LEU:HA	1:A:282:LEU:HD12	2.02	0.42
1:A:288:ALA:O	1:A:289:LEU:C	2.63	0.42
1:A:317:VAL:HG22	1:A:318:TYR:H	1.85	0.42
1:A:317:VAL:HG22	1:A:318:TYR:N	2.33	0.42
1:A:406:TRP:CE3	1:A:406:TRP:C	2.98	0.42
2:B:86:ASP:C	2:B:88:TRP:N	2.76	0.42
2:B:142:ILE:H	2:B:142:ILE:HG12	1.72	0.42
1:A:93:GLY:HA3	2:B:137:ASN:ND2	2.35	0.42
2:B:334:GLN:C	2:B:336:GLN:N	2.77	0.42
1:A:338:THR:HA	1:A:353:LYS:HA	2.02	0.42
2:B:66:LYS:HB3	2:B:221:HIS:CE1	2.55	0.42
2:B:156:SER:HB2	2:B:157:PRO:CD	2.50	0.42
2:B:164:MET:HE2	2:B:182:GLN:NE2	2.35	0.42
2:B:282:LEU:HD13	2:B:297:GLU:CD	2.45	0.42
2:B:302:GLU:O	2:B:303:LEU:C	2.63	0.42
1:A:288:ALA:O	1:A:290:THR:N	2.53	0.41
1:A:438:GLU:OE2	1:A:459:THR:HG21	2.20	0.41
1:A:442:VAL:HG21	1:A:482:ILE:HA	2.02	0.41
2:B:65:LYS:O	2:B:67:ASP:N	2.53	0.41
2:B:87:PHE:C	2:B:88:TRP:HD1	2.28	0.41
2:B:242:GLN:HG2	2:B:243:PRO:N	2.34	0.41
2:B:279:LEU:CD1	2:B:282:LEU:HD23	2.50	0.41
2:B:331:LYS:CE	2:B:364:ASP:OD2	2.68	0.41
2:B:363:ASN:ND2	2:B:405:TYR:OH	2.53	0.41
2:B:379:SER:HA	2:B:383:TRP:HZ3	1.83	0.41
1:A:107:THR:HG21	1:A:202:ILE:HG21	2.03	0.41
1:A:206:ARG:NH2	1:A:207:GLN:OE1	2.49	0.41
1:A:324:ASP:O	1:A:343:GLN:NE2	2.47	0.41
1:A:340:GLN:HA	1:A:351:THR:HA	2.02	0.41
2:B:4:PRO:O	2:B:6:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:LEU:HA	2:B:306:ASN:CG	2.44	0.41
1:A:153:TRP:CG	1:A:154:LYS:H	2.38	0.41
1:A:442:VAL:HG21	1:A:482:ILE:N	2.35	0.41
1:A:467:VAL:CG1	1:A:468:PRO:HD2	2.50	0.41
2:B:298:GLU:CG	2:B:299:ALA:N	2.83	0.41
1:A:24:TRP:O	1:A:25:PRO:C	2.63	0.41
1:A:134:SER:O	1:A:136:ASN:N	2.53	0.41
1:A:324:ASP:OD2	1:A:388:LYS:HE3	2.20	0.41
1:A:398:TRP:CH2	1:A:411:ILE:HG22	2.55	0.41
1:A:427:TYR:CE1	1:A:525:LEU:HD13	2.55	0.41
1:A:451:LYS:NZ	1:A:471:ASN:HB3	2.35	0.41
2:B:13:LYS:CE	2:B:86:ASP:HB2	2.50	0.41
1:A:96:HIS:CD2	1:A:96:HIS:C	2.98	0.41
2:B:376:THR:HG21	2:B:410:TRP:CE3	2.55	0.41
1:A:258:GLN:C	1:A:260:LEU:N	2.77	0.41
1:A:296:THR:C	1:A:298:GLU:N	2.74	0.41
1:A:329:ILE:HD12	1:A:391:LEU:HD22	2.03	0.41
1:A:27:THR:HG22	1:A:29:GLU:CB	2.50	0.41
1:A:157:PRO:O	1:A:160:PHE:HB3	2.21	0.41
1:A:397:THR:HG23	1:A:424:LYS:HD2	2.03	0.41
1:A:296:THR:O	1:A:299:ALA:N	2.53	0.41
2:B:363:ASN:OD1	2:B:363:ASN:C	2.64	0.41
1:A:139:THR:O	1:A:140:PRO:C	2.63	0.41
1:A:148:VAL:O	1:A:150:PRO:CD	2.67	0.41
1:A:424:LYS:HG3	1:A:425:LEU:N	2.36	0.41
1:A:517:LEU:O	1:A:521:ILE:HD12	2.21	0.41
2:B:3:SER:CB	2:B:4:PRO:CD	2.98	0.41
2:B:14:PRO:O	2:B:15:GLY:C	2.64	0.41
2:B:46:LYS:CD	2:B:116:PHE:CD2	3.03	0.41
2:B:77:PHE:CD1	2:B:80:LEU:HD23	2.56	0.41
2:B:373:GLN:OE1	2:B:407:GLN:N	2.34	0.41
2:B:394:GLN:O	2:B:395:LYS:C	2.64	0.41
2:B:401:TRP:C	2:B:403:THR:N	2.79	0.41
1:A:134:SER:CB	1:A:140:PRO:HB2	2.51	0.41
1:A:134:SER:C	1:A:136:ASN:N	2.78	0.41
1:A:138:GLU:O	1:A:138:GLU:HG2	2.21	0.41
1:A:482:ILE:HD13	1:A:506:ILE:HD12	2.03	0.41
2:B:12:LEU:HD21	2:B:127:TYR:CD2	2.55	0.41
2:B:260:LEU:CD1	2:B:264:LEU:HD11	2.51	0.41
2:B:331:LYS:HE3	2:B:364:ASP:OD2	2.21	0.41
1:A:221:HIS:CD2	1:A:223:LYS:CB	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:VAL:HG21	1:A:425:LEU:HD21	2.03	0.40
2:B:99:GLY:O	2:B:102:LYS:N	2.48	0.40
2:B:122:GLU:HA	2:B:125:ARG:HG3	2.02	0.40
2:B:298:GLU:H	2:B:298:GLU:HG2	1.62	0.40
1:A:202:ILE:HD13	1:A:202:ILE:HA	1.90	0.40
1:A:390:LYS:HB3	1:A:417:VAL:HG21	2.02	0.40
1:A:396:GLU:O	1:A:396:GLU:HG2	2.21	0.40
1:A:431:LYS:O	1:A:532:TYR:HE2	2.03	0.40
2:B:291:GLU:HG3	2:B:292:VAL:H	1.87	0.40
1:A:66:LYS:HE3	1:A:66:LYS:HB2	1.90	0.40
1:A:379:SER:HB3	1:A:385:LYS:O	2.21	0.40
1:A:520:GLN:HA	1:A:520:GLN:NE2	2.25	0.40
2:B:40:GLU:HB3	2:B:44:GLU:OE2	2.20	0.40
2:B:183:TYR:O	2:B:184:MET:HB2	2.20	0.40
1:A:27:THR:C	1:A:29:GLU:N	2.76	0.40
1:A:416:PHE:CD2	1:A:416:PHE:C	2.91	0.40
1:A:472:THR:OG1	1:A:476:LYS:HB3	2.21	0.40
2:B:350:LYS:HE3	2:B:378:GLU:OE1	2.21	0.40
1:A:16:MET:HE2	1:A:16:MET:HB3	1.87	0.40
1:A:113:ASP:O	1:A:116:PHE:HB2	2.21	0.40
1:A:156:SER:O	1:A:157:PRO:C	2.64	0.40
2:B:158:ALA:O	2:B:159:ILE:C	2.64	0.40
2:B:404:GLU:OE1	2:B:404:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	550/560 (98%)	410 (74%)	94 (17%)	46 (8%)	0 1
2	B	425/430 (99%)	310 (73%)	71 (17%)	44 (10%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	975/990 (98%)	720 (74%)	165 (17%)	90 (9%)	0 1

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	289	LEU
1	A	334	GLN
1	A	360	ALA
1	A	433	PRO
1	A	540	LYS
2	B	5	ILE
2	B	85	GLN
2	B	154	LYS
2	B	195	ILE
2	B	273	GLY
2	B	366	LYS
2	B	404	GLU
1	A	78	ARG
1	A	123	ASP
1	A	137	ASN
1	A	237	ASP
1	A	247	PRO
1	A	276	VAL
1	A	358	ARG
1	A	406	TRP
1	A	450	THR
1	A	476	LYS
1	A	541	GLY
2	B	18	GLY
2	B	66	LYS
2	B	91	GLN
2	B	103	ASN
2	B	116	PHE
2	B	126	LYS
2	B	193	LEU
2	B	217	PRO
2	B	260	LEU
2	B	282	LEU
2	B	345	PRO
2	B	365	VAL
1	A	52	PRO

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Mol	Chain	Res	Type
1	A	126	LYS
1	A	151	GLN
1	A	152	GLY
1	A	169	GLU
1	A	195	ILE
1	A	230	MET
1	A	538	ALA
2	B	77	PHE
2	B	199	ARG
2	B	226	PRO
2	B	287	LYS
2	B	304	ALA
2	B	395	LYS
2	B	421	PRO
1	A	2	ILE
1	A	103	ASN
1	A	114	ALA
1	A	127	TYR
1	A	279	LEU
1	A	304	ALA
1	A	408	ALA
1	A	409	THR
1	A	419	THR
2	B	138	GLU
2	B	229	TRP
2	B	359	GLY
2	B	402	TRP
2	B	419	THR
1	A	25	PRO
1	A	122	GLU
1	A	157	PRO
1	A	184	MET
1	A	259	LYS
1	A	311	LYS
2	B	162	SER
2	B	174	GLN
2	B	270	ILE
2	B	335	GLY
1	A	111	VAL
2	B	173	LYS
2	B	418	ASN
1	A	135	ILE

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Mol	Chain	Res	Type
1	A	217	PRO
2	B	95	PRO
2	B	97	PRO
2	B	276	VAL
2	B	9	PRO
2	B	244	ILE
1	A	55	PRO
1	A	133	PRO
2	B	176	PRO
1	A	243	PRO
2	B	243	PRO

5.3.2 Protein sidechains [i](#)

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	475/500 (95%)	422 (89%)	53 (11%)	6	19
2	B	367/392 (94%)	312 (85%)	55 (15%)	3	10
All	All	842/892 (94%)	734 (87%)	108 (13%)	4	14

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	47	ILE
1	A	50	ILE
1	A	54	ASN
1	A	83	ARG
1	A	84	THR
1	A	89	GLU
1	A	94	ILE
1	A	113	ASP
1	A	119	PRO
1	A	126	LYS
1	A	128	THR

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Mol	Chain	Res	Type
1	A	133	PRO
1	A	140	PRO
1	A	169	GLU
1	A	175	ASN
1	A	178	ILE
1	A	194	GLU
1	A	218	ASP
1	A	228	LEU
1	A	243	PRO
1	A	286	THR
1	A	289	LEU
1	A	325	LEU
1	A	330	GLN
1	A	350	LYS
1	A	353	LYS
1	A	356	ARG
1	A	358	ARG
1	A	362	THR
1	A	363	ASN
1	A	365	VAL
1	A	369	THR
1	A	370	GLU
1	A	387	PRO
1	A	391	LEU
1	A	398	TRP
1	A	409	THR
1	A	422	LEU
1	A	423	VAL
1	A	431	LYS
1	A	450	THR
1	A	454	LYS
1	A	457	TYR
1	A	458	VAL
1	A	460	ASN
1	A	497	THR
1	A	520	GLN
1	A	523	GLU
1	A	529	GLU
1	A	533	LEU
1	A	545	ASN
1	A	551	LEU
2	B	9	PRO

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Mol	Chain	Res	Type
2	B	12	LEU
2	B	16	MET
2	B	17	ASP
2	B	40	GLU
2	B	41	MET
2	B	49	LYS
2	B	57	ASN
2	B	69	THR
2	B	78	ARG
2	B	86	ASP
2	B	100	LEU
2	B	139	THR
2	B	142	ILE
2	B	145	GLN
2	B	151	GLN
2	B	165	THR
2	B	176	PRO
2	B	177	ASP
2	B	187	LEU
2	B	206	ARG
2	B	212	TRP
2	B	215	THR
2	B	216	THR
2	B	218	ASP
2	B	257	ILE
2	B	265	ASN
2	B	274	ILE
2	B	290	THR
2	B	293	ILE
2	B	294	PRO
2	B	297	GLU
2	B	300	GLU
2	B	301	LEU
2	B	302	GLU
2	B	309	ILE
2	B	311	LYS
2	B	317	VAL
2	B	318	TYR
2	B	330	GLN
2	B	336	GLN
2	B	344	GLU
2	B	346	PHE

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Mol	Chain	Res	Type
2	B	354	TYR
2	B	363	ASN
2	B	367	GLN
2	B	369	THR
2	B	373	GLN
2	B	383	TRP
2	B	388	LYS
2	B	393	ILE
2	B	403	THR
2	B	405	TYR
2	B	417	VAL
2	B	420	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	103	ASN
1	A	147	ASN
1	A	161	GLN
1	A	175	ASN
1	A	221	HIS
1	A	222	GLN
1	A	235	HIS
1	A	265	ASN
1	A	269	GLN
1	A	278	GLN
1	A	332	GLN
1	A	394	GLN
1	A	471	ASN
1	A	474	ASN
1	A	480	GLN
1	A	487	GLN
1	A	509	GLN
1	A	519	ASN
1	A	520	GLN
1	A	524	GLN
1	A	547	GLN
2	B	136	ASN
2	B	182	GLN
2	B	208	HIS
2	B	269	GLN

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Mol	Chain	Res	Type
2	B	336	GLN
2	B	348	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	65B	A	600	-	30,30,30	2.98	16 (53%)	40,42,42	2.39	7 (17%)

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	65B	A	600	-	-	4/12/12/12	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	65B	C22-C21	7.91	1.52	1.39
3	A	600	65B	C1-C2	4.69	1.48	1.40
3	A	600	65B	C13-N12	4.65	1.39	1.32
3	A	600	65B	C1-C6	4.56	1.48	1.40
3	A	600	65B	C23-C22	4.29	1.45	1.38
3	A	600	65B	BR-C14	-3.90	1.80	1.89
3	A	600	65B	O17-C13	3.44	1.48	1.36
3	A	600	65B	C23-C24	3.12	1.45	1.39
3	A	600	65B	C5-C6	3.12	1.43	1.39
3	A	600	65B	C26-C25	2.93	1.43	1.38
3	A	600	65B	C3-C2	2.91	1.43	1.39
3	A	600	65B	C11-N12	2.81	1.42	1.34
3	A	600	65B	C15-N16	2.74	1.38	1.35
3	A	600	65B	C25-C24	2.38	1.44	1.39
3	A	600	65B	C13-C14	2.35	1.41	1.38
3	A	600	65B	C6'-C6	2.06	1.54	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	65B	C1-O17-C13	-5.88	110.71	116.84
3	A	600	65B	C14-C13-N12	-5.77	117.57	123.78
3	A	600	65B	O17-C13-C14	5.72	121.58	117.89
3	A	600	65B	C11-N16-C15	5.65	121.17	116.59
3	A	600	65B	N16-C11-N12	-5.27	117.63	126.26
3	A	600	65B	C11-N12-C13	4.83	123.70	115.38
3	A	600	65B	C22-C23-C24	-2.39	117.30	120.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

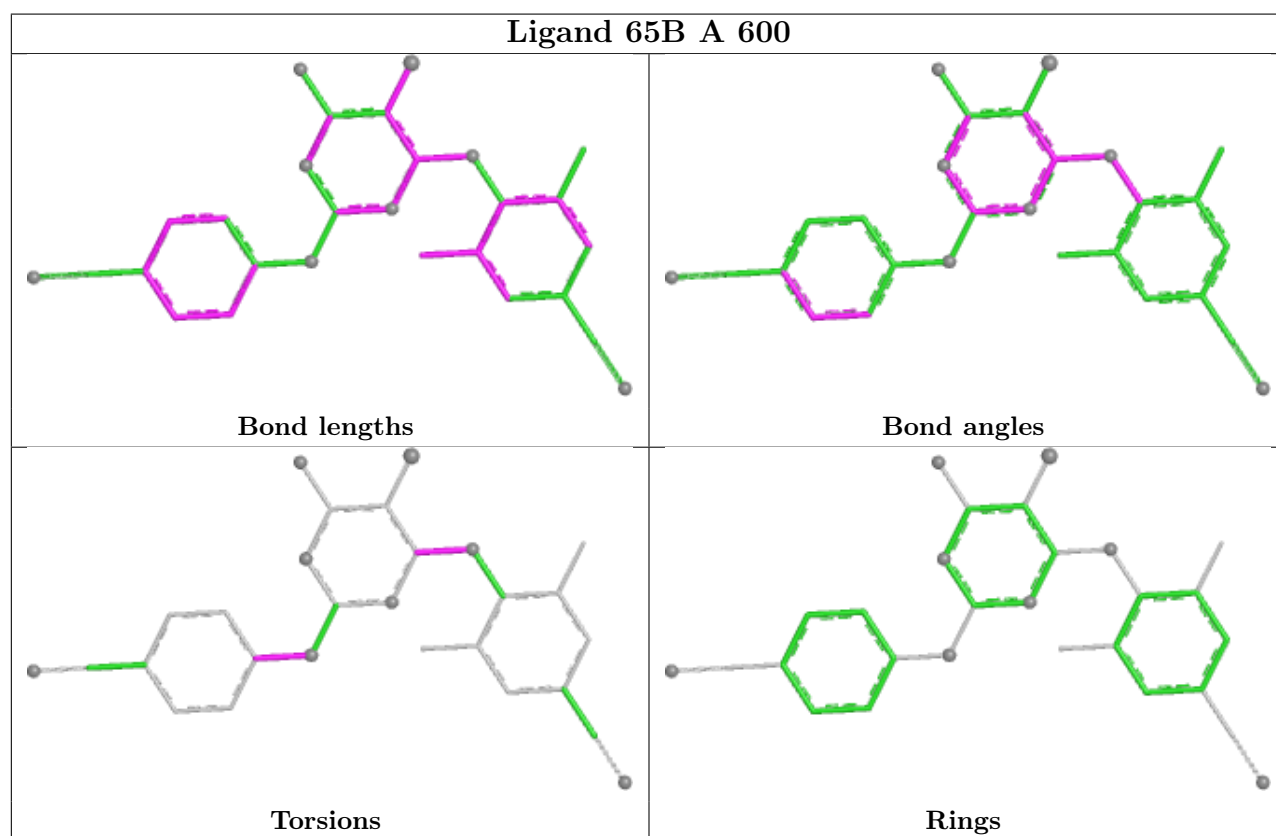
Mol	Chain	Res	Type	Atoms
3	A	600	65B	C14-C13-O17-C1
3	A	600	65B	C26-C21-N5-C11
3	A	600	65B	C22-C21-N5-C11
3	A	600	65B	N12-C13-O17-C1

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	65B	9	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	552/560 (98%)	-0.02	11 (1%) 65 56	47, 87, 120, 120	0
2	B	427/430 (99%)	0.03	15 (3%) 47 38	36, 77, 120, 120	0
All	All	979/990 (98%)	0.00	26 (2%) 56 47	36, 83, 120, 120	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	28	GLU	4.0
2	B	228	LEU	4.0
2	B	218	ASP	3.6
2	B	227	PHE	3.4
2	B	358	ARG	3.3
2	B	285	GLY	3.2
2	B	317	VAL	3.1
1	A	218	ASP	2.8
1	A	253	THR	2.8
1	A	549	ASP	2.6
1	A	29	GLU	2.6
2	B	5	ILE	2.5
2	B	219	LYS	2.5
1	A	544	GLY	2.4
1	A	139	THR	2.4
1	A	362	THR	2.4
2	B	306	ASN	2.4
1	A	270	ILE	2.3
2	B	251	SER	2.2
1	A	271	TYR	2.2
2	B	229	TRP	2.2
2	B	240	THR	2.1
1	A	335	GLY	2.1
1	A	541	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	324	ASP	2.0
2	B	231	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

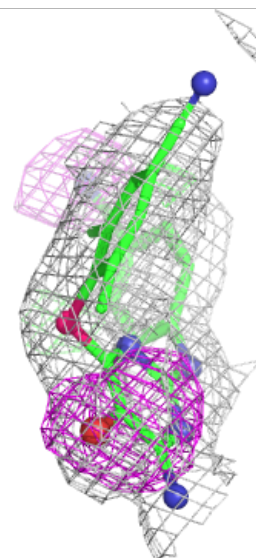
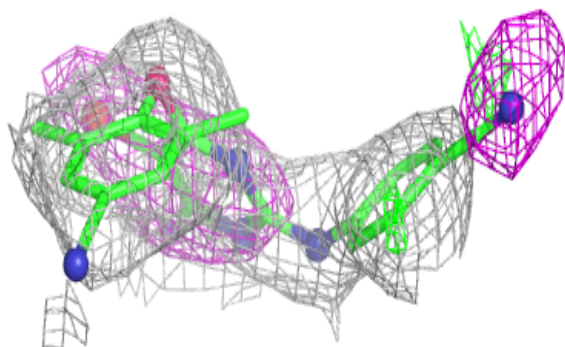
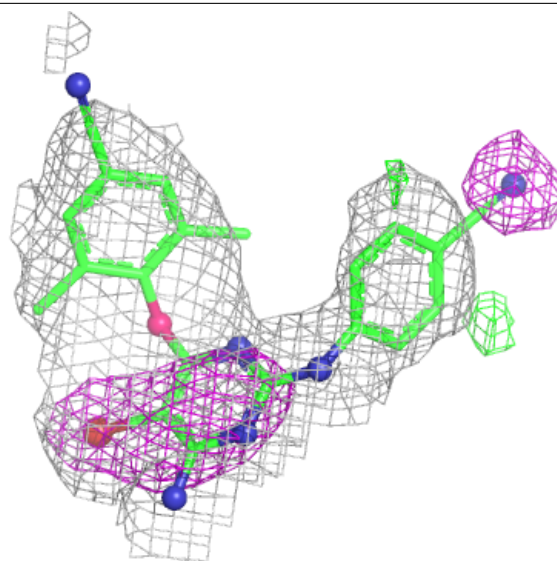
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	65B	A	600	28/28	0.78	0.13	58,72,83,108	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 65B A 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.