



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:04 PM UTC

PDB ID : 3DOK / pdb_00003dok
Title : Crystal structure of K103N mutant HIV-1 reverse transcriptase in complex with GW678248.
Authors : Chamberlain, P.P.; Ren, J.; Stammers, D.K.
Deposited on : 2008-07-04
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

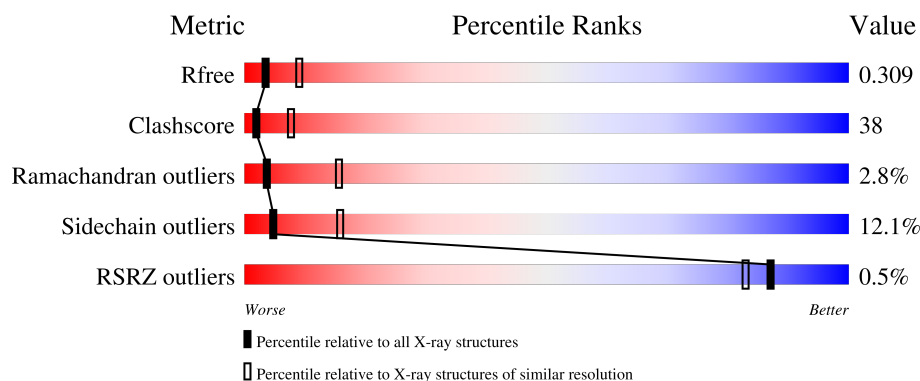
1 Overall quality at a glance

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	440	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7750 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4383	2835	729	811	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	engineered mutation	UNP P04585

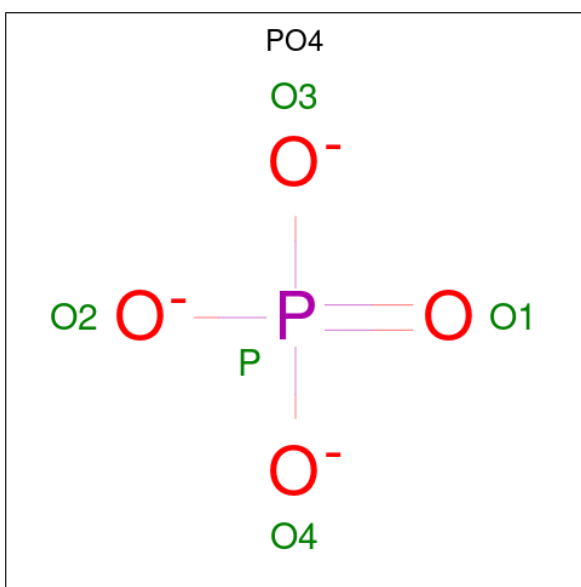
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3320	2158	553	602	7			

There is a discrepancy between the modelled and reference sequences:

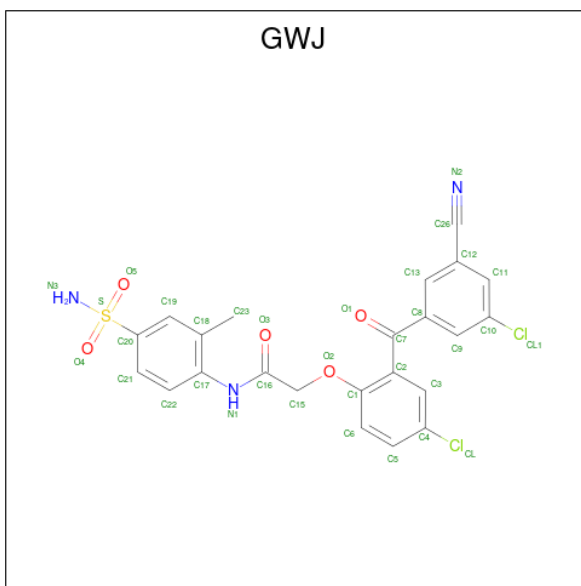
Chain	Residue	Modelled	Actual	Comment	Reference
B	103	ASN	LYS	engineered mutation	UNP P04585

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 2-{4-chloro-2-[(3-chloro-5-cyanophenyl)carbonyl]phenoxy}-N-(2-methyl-4-sulfamoylphenyl)acetamide (CCD ID: GWJ) (formula: $C_{23}H_{17}Cl_2N_3O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	
			34	23	2	3	5	1	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0
5	B	2	Total 2	O 2	0	0

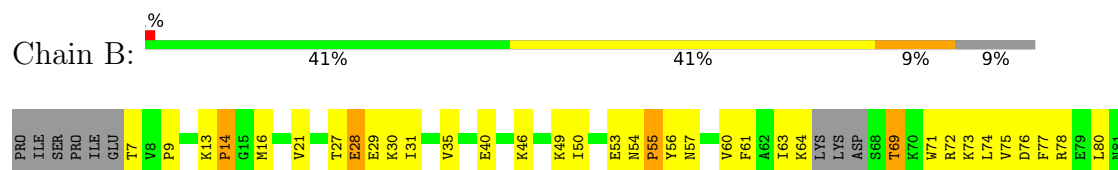
3 Residue-property plots

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/ribonuclease H



• Molecule 2: p51 RT



G384	K82	Q151	HIS	T296	G384
K385	R83	K154	GLN	E297	K385
T386	T84	GLY	LYS	E298	T386
P387	Q85	I159	PRO	E302	P387
F388	D86	F160	PRO	L303	F388
F389	F87	Q161	PHE	L310	F389
T393	W88	S162	LEU	Q331	T393
W398	GLU	S163	TRP	Q332	W398
E399	VAL	M164	GLY	Y319	E399
T400	GLN	T165	MET	D320	T400
W401	LEU	K166	TVR	P321	W401
W402	G93	I167	E233	S322	W402
T403	I94	L168	L234	K323	T403
E404	F95	E169	H235	L324	E404
W410	H96	F170	P236	D237	W410
F416	A98	F171	K238	Q237	F416
V417	G99	R172	W239	Q242	V417
N418	L100	K173	Q242	P243	N418
P421	K101	Q174	L244	V245	P421
K424	V108	N175	D250	K341	K424
L425	L109	F176	V254	Y342	L425
W426	D110	D177	Q258	Q343	W426
Y427	D111	I178	K259	F346	Y427
Q428	V111	V179	L260	L349	Q428
L429	G112	I180	V261	G352	L429
E430	D113	Y181	W266	K353	E430
K431	A114	Q182	A267	Y354	K431
GLU	Y115	D186	Q268	A355	GLU
PRO	F116	L187	S268	K356	PRO
ILE	S117	Y188	Q269	W357	ILE
VAL	V118	L193	L270	H361	VAL
GLY	P119	E194	Y271	T362	GLY
ALA	L120	I195	P272	N363	ALA
GLU	D121	G196	Q273	D364	GLU
THR	E122	Q199	L274	V365	THR
PHE	I123	R199	K275	K366	PHE
	F124	T200	V276	Q367	
	R125	K201	R277	L368	
	K126	L202	Q278	T369	
	Y127	E203	L279	E370	
	T128	E204	K281	Q373	
	A129	L205	L282	T376	
	F130	L206	L283	T377	
	T131	R206	T286	E378	
	I132	Q207	K287	S379	
	F133	H208	L288	T380	
	S134	L209	L289	V381	
	I135	L210	L290	I382	
	N136	R211	T295	W383	
	M137	G213			
	E138	L214			
	T139	T215			
	R143	T216			
	Y144	PRO			
	Q145	ASP			
	L149	LYS			
	P150	LYS			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.94Å 109.77Å 72.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 2.90 29.79 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.79-2.90) 99.5 (29.79-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.312 0.215 , 0.309	Depositor DCC
R_{free} test set	1203 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7750	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: PO4, CSD, GWJ

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	0.75	3/4491 (0.1%)	1.25	42/6107 (0.7%)
2	B	0.69	0/3412	1.19	29/4635 (0.6%)
All	All	0.72	3/7903 (0.0%)	1.23	71/10742 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	MET	SD-CE	5.99	1.94	1.79
1	A	473	THR	N-CA	5.73	1.52	1.46
1	A	108	VAL	CA-CB	5.60	1.60	1.54

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	THR	CA-C-N	11.74	134.52	119.84
1	A	139	THR	C-N-CA	11.74	134.52	119.84
2	B	215	THR	N-CA-C	11.04	134.32	110.80
1	A	118	VAL	CA-C-N	9.95	130.05	119.90
1	A	118	VAL	C-N-CA	9.95	130.05	119.90
2	B	69	THR	N-CA-C	-8.93	102.40	113.38
1	A	239	TRP	N-CA-C	-8.63	96.61	109.81
1	A	386	THR	CA-C-N	8.33	128.38	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	THR	C-N-CA	8.33	128.38	119.89
2	B	250	ASP	N-CA-C	-8.01	102.23	110.97
1	A	137	ASN	N-CA-C	7.99	122.44	111.90
1	A	473	THR	N-CA-C	-7.73	97.09	109.76
1	A	442	VAL	N-CA-C	7.58	121.10	109.12
1	A	140	PRO	N-CA-C	7.56	128.04	112.47
2	B	118	VAL	N-CA-C	7.52	117.15	108.96
1	A	539	HIS	N-CA-C	-7.49	90.03	111.00
1	A	51	GLY	CA-C-N	7.47	127.18	119.56
1	A	51	GLY	C-N-CA	7.47	127.18	119.56
1	A	505	ILE	CB-CA-C	-7.45	99.07	111.29
1	A	443	ASP	N-CA-C	7.42	120.48	108.76
2	B	363	ASN	N-CA-C	7.38	121.68	107.44
2	B	235	HIS	CA-C-N	7.37	129.05	119.84
2	B	235	HIS	C-N-CA	7.37	129.05	119.84
1	A	3	SER	N-CA-C	7.27	125.88	109.81
1	A	245	VAL	N-CA-C	7.26	118.59	107.99
1	A	139	THR	N-CA-C	7.11	125.52	109.81
1	A	388	LYS	N-CA-C	-7.04	97.77	109.46
2	B	428	GLN	N-CA-C	-7.00	104.86	113.19
1	A	218	ASP	N-CA-C	-6.83	99.86	109.69
2	B	353	LYS	N-CA-C	-6.81	98.96	109.24
1	A	124	PHE	N-CA-C	6.70	120.55	112.38
2	B	343	GLN	N-CA-C	-6.64	105.07	113.43
2	B	417	VAL	N-CA-C	6.59	118.21	108.65
1	A	138	GLU	N-CA-C	-6.55	99.63	110.17
1	A	154	LYS	N-CA-C	6.46	119.14	111.33
1	A	197	GLN	N-CA-C	-6.39	104.01	110.97
1	A	368	LEU	N-CA-C	-6.23	103.63	111.11
2	B	215	THR	CB-CA-C	-6.15	98.19	110.42
2	B	28	GLU	N-CA-C	-6.04	104.61	111.07
1	A	222	GLN	N-CA-C	6.01	117.81	109.15
2	B	341	ILE	N-CA-C	-5.87	99.95	108.17
1	A	142	ILE	N-CA-C	5.79	116.54	109.30
2	B	216	THR	N-CA-C	5.76	127.12	111.00
1	A	146	TYR	N-CA-C	5.75	119.00	109.46
2	B	215	THR	CA-C-N	-5.71	111.41	121.70
2	B	215	THR	C-N-CA	-5.71	111.41	121.70
1	A	57	ASN	N-CA-C	5.68	117.76	108.55
1	A	219	LYS	N-CA-C	-5.67	105.54	113.37
2	B	132	ILE	CA-C-N	5.58	125.57	120.21
2	B	132	ILE	C-N-CA	5.58	125.57	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	PHE	N-CA-C	5.55	119.11	110.17
2	B	115	TYR	N-CA-C	5.54	117.40	111.36
2	B	186	ASP	N-CA-C	5.53	119.12	110.32
2	B	295	LEU	N-CA-C	5.50	117.70	108.96
2	B	298	GLU	N-CA-C	-5.47	105.22	111.07
1	A	271	TYR	N-CA-C	5.26	116.45	109.93
1	A	188	TYR	N-CA-C	-5.25	99.22	108.20
1	A	254	VAL	N-CA-C	-5.24	105.42	110.72
2	B	131	THR	N-CA-C	5.22	117.95	109.24
1	A	348	ASN	N-CA-C	5.21	117.78	109.96
2	B	320	ASP	CA-C-N	5.19	124.85	119.56
2	B	320	ASP	C-N-CA	5.19	124.85	119.56
2	B	182	GLN	N-CA-C	5.16	117.15	108.73
2	B	203	GLU	N-CA-C	-5.13	105.81	111.71
1	A	180	ILE	CB-CA-C	-5.12	105.12	111.32
1	A	495	ILE	CB-CA-C	-5.11	103.51	110.77
1	A	216	THR	O-C-N	5.10	125.37	121.65
2	B	177	ASP	N-CA-C	-5.07	106.87	113.16
1	A	495	ILE	CA-C-N	-5.03	116.61	123.10
1	A	495	ILE	C-N-CA	-5.03	116.61	123.10
1	A	110	ASP	N-CA-C	-5.01	101.79	109.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	TYR	Sidechain
1	A	188	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	4383	0	4416	390	0
2	B	3320	0	3346	222	0
3	A	5	0	0	0	0
4	A	34	0	17	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	6	0	0	1	0
5	B	2	0	0	0	0
All	All	7750	0	7779	597	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 38.

All (597) 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:139:THR:HB	1:A:140:PRO:HD2	1.28	1.14
1:A:448:ARG:H	1:A:448:ARG:HD3	0.93	1.09
1:A:49:LYS:H	1:A:49:LYS:HD3	0.97	1.05
1:A:49:LYS:H	1:A:49:LYS:CD	1.64	1.03
1:A:448:ARG:HD3	1:A:448:ARG:N	1.75	0.99
1:A:448:ARG:H	1:A:448:ARG:CD	1.77	0.96
2:B:278:GLN:HE21	2:B:298:GLU:CB	1.77	0.96
1:A:312:GLU:HG2	1:A:313:PRO:HD2	1.48	0.96
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.45	0.95
2:B:84:THR:HG22	2:B:154:LYS:HE2	1.49	0.94
1:A:49:LYS:HD3	1:A:49:LYS:N	1.77	0.93
1:A:139:THR:CB	1:A:140:PRO:HD2	1.95	0.92
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.04	0.92
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.52	0.90
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.08	0.88
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.39	0.87
2:B:138:GLU:HG3	2:B:139:THR:HG22	1.56	0.86
1:A:94:ILE:HG22	1:A:183:TYR:HE2	1.37	0.86
1:A:149:LEU:HD11	1:A:159:ILE:HG21	1.58	0.85
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.12	0.85
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.57	0.85
1:A:335:GLY:HA2	1:A:367:GLN:OE1	1.76	0.84
1:A:489:SER:OG	1:A:493:VAL:HG21	1.77	0.84
1:A:206:ARG:HH11	1:A:206:ARG:HG2	1.43	0.84
1:A:206:ARG:HH11	1:A:206:ARG:CG	1.90	0.84
1:A:149:LEU:HD21	1:A:159:ILE:HG22	1.60	0.84
2:B:163:SER:O	2:B:167:ILE:HG23	1.78	0.83
1:A:518:VAL:O	1:A:522:ILE:HG13	1.79	0.83
1:A:491:LEU:CD1	1:A:492:GLU:HG3	2.10	0.82
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.60	0.81
1:A:465:LYS:O	1:A:466:VAL:HG23	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:ILE:HD12	2:B:135:ILE:H	1.46	0.80
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.61	0.80
1:A:79:GLU:CD	1:A:83:ARG:HH12	1.91	0.79
1:A:308:GLU:OE2	1:A:308:GLU:HA	1.82	0.79
1:A:122:GLU:H	1:A:122:GLU:CD	1.89	0.79
2:B:214:LEU:O	2:B:215:THR:HG23	1.83	0.78
1:A:399:GLU:O	1:A:403:THR:HB	1.84	0.77
1:A:418:ASN:O	1:A:420:PRO:HD3	1.84	0.77
1:A:23:GLN:OE1	1:A:60:VAL:HG12	1.84	0.76
1:A:248:GLU:HG3	1:A:307:ARG:NH2	1.99	0.76
2:B:376:THR:O	2:B:380:ILE:HG13	1.85	0.76
1:A:9:PRO:HG2	2:B:53:GLU:HG3	1.66	0.76
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.86	0.76
1:A:8:VAL:HG13	2:B:53:GLU:OE1	1.87	0.76
1:A:109:LEU:HD23	1:A:216:THR:HG21	1.66	0.74
1:A:218:ASP:C	1:A:220:LYS:H	1.94	0.74
1:A:358:ARG:H	1:A:358:ARG:HD3	1.53	0.73
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.68	0.73
2:B:173:LYS:HD2	2:B:173:LYS:N	2.02	0.73
1:A:129:ALA:HB1	1:A:143:ARG:HH12	1.52	0.73
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.70	0.73
1:A:403:THR:HG23	1:A:404:GLU:OE1	1.89	0.73
1:A:220:LYS:O	1:A:220:LYS:HD3	1.88	0.72
1:A:220:LYS:O	1:A:221:HIS:HB2	1.88	0.72
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.06	0.72
2:B:373:GLN:O	2:B:377:THR:HG23	1.89	0.72
1:A:27:THR:O	1:A:31:ILE:HG13	1.88	0.72
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.70	0.72
1:A:2:ILE:HG22	1:A:3:SER:N	2.02	0.72
1:A:206:ARG:HH11	1:A:206:ARG:CB	2.04	0.71
2:B:61:PHE:CE1	2:B:74:LEU:HD23	2.23	0.71
1:A:474:ASN:O	1:A:477:THR:OG1	2.07	0.71
1:A:17:ASP:O	1:A:83:ARG:HD3	1.89	0.71
1:A:100:LEU:HD23	1:A:181:TYR:HE1	1.57	0.70
1:A:334:GLN:O	1:A:356:ARG:HD2	1.91	0.70
1:A:474:ASN:O	1:A:478:GLU:HG3	1.91	0.70
1:A:307:ARG:HH11	1:A:307:ARG:HG2	1.56	0.70
1:A:102:LYS:HE2	1:A:237:ASP:HA	1.72	0.70
2:B:98:ALA:O	2:B:101:LYS:HG2	1.91	0.70
2:B:169:GLU:HA	2:B:173:LYS:HZ3	1.58	0.69
1:A:478:GLU:O	1:A:481:ALA:HB3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:HG3	1:A:307:ARG:CZ	2.23	0.69
2:B:94:ILE:HD11	2:B:181:TYR:HD2	1.56	0.69
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.28	0.68
2:B:170:PRO:O	2:B:174:GLN:HG3	1.94	0.68
1:A:317:VAL:HG12	1:A:318:TYR:N	2.08	0.68
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.74	0.68
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.28	0.68
1:A:219:LYS:HD2	1:A:222:GLN:NE2	2.08	0.68
1:A:350:LYS:HE3	1:A:378:GLU:OE1	1.93	0.68
2:B:134:SER:CB	2:B:139:THR:HG23	2.24	0.68
2:B:278:GLN:HE21	2:B:298:GLU:HB3	1.58	0.68
1:A:94:ILE:HG22	1:A:183:TYR:CE2	2.26	0.68
1:A:402:TRP:CD1	1:A:402:TRP:C	2.71	0.68
1:A:448:ARG:HG2	1:A:448:ARG:HH11	1.58	0.68
1:A:139:THR:HB	1:A:140:PRO:CD	2.16	0.67
1:A:225:PRO:HA	1:A:226:PRO:C	2.20	0.67
1:A:454:LYS:HA	1:A:467:VAL:O	1.95	0.67
1:A:388:LYS:HZ3	1:A:415:GLU:HB3	1.59	0.67
1:A:112:GLY:O	1:A:114:ALA:N	2.24	0.67
2:B:424:LYS:HD2	2:B:425:LEU:HD13	1.75	0.67
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.29	0.67
1:A:111:VAL:HG22	1:A:185:ASP:HB3	1.77	0.67
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	2.83	0.67
1:A:439:THR:HG22	1:A:439:THR:O	1.95	0.67
1:A:206:ARG:HB3	1:A:206:ARG:NH1	2.10	0.66
2:B:376:THR:CG2	2:B:386:THR:HG22	2.25	0.66
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.24	0.66
1:A:68:SER:C	1:A:70:LYS:H	2.04	0.66
1:A:122:GLU:HB3	1:A:125:ARG:NH1	2.10	0.66
1:A:122:GLU:N	1:A:122:GLU:OE1	2.27	0.66
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.30	0.66
1:A:231:GLY:C	1:A:242:GLN:HG2	2.21	0.65
1:A:491:LEU:HD22	1:A:529:GLU:CD	2.20	0.65
1:A:121:ASP:OD2	1:A:123:ASP:HB2	1.96	0.65
1:A:508:ALA:O	1:A:509:GLN:C	2.39	0.65
2:B:245:VAL:HG13	2:B:431:LYS:HB2	1.79	0.65
1:A:49:LYS:CD	1:A:49:LYS:N	2.46	0.65
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.78	0.65
1:A:491:LEU:HD13	1:A:492:GLU:HG3	1.77	0.65
1:A:218:ASP:C	1:A:220:LYS:N	2.54	0.65
2:B:161:GLN:HE22	2:B:182:GLN:HE22	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:VAL:HG12	1:A:494:ASN:N	2.11	0.64
1:A:516:GLU:O	1:A:519:ASN:HB2	1.97	0.64
1:A:486:LEU:O	1:A:528:LYS:NZ	2.31	0.64
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.78	0.64
1:A:388:LYS:NZ	1:A:415:GLU:HB3	2.12	0.64
2:B:120:LEU:O	2:B:121:ASP:C	2.40	0.63
1:A:317:VAL:HG12	1:A:318:TYR:H	1.63	0.63
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.80	0.63
2:B:13:LYS:HE3	2:B:84:THR:O	1.97	0.63
1:A:79:GLU:OE1	1:A:82:LYS:HD3	1.98	0.63
1:A:178:ILE:HD11	1:A:201:LYS:HG2	1.79	0.63
2:B:169:GLU:O	2:B:173:LYS:HD3	1.98	0.63
2:B:196:GLY:O	2:B:200:THR:HG23	1.98	0.63
1:A:149:LEU:HD21	1:A:159:ILE:CG2	2.28	0.63
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.80	0.62
1:A:445:ALA:HA	5:A:1306:HOH:O	1.99	0.62
2:B:56:TYR:HE2	2:B:126:LYS:HE3	1.63	0.62
2:B:424:LYS:HZ3	2:B:428:GLN:NE2	1.98	0.62
1:A:408:ALA:HB3	2:B:393:ILE:CG1	2.28	0.62
1:A:358:ARG:O	1:A:358:ARG:HG2	1.98	0.62
1:A:43:LYS:C	1:A:45:GLY:H	2.07	0.62
1:A:101:LYS:HA	1:A:319:TYR:O	2.00	0.61
1:A:170:PRO:HA	1:A:173:LYS:HZ1	1.65	0.61
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.82	0.61
1:A:210:LEU:HD22	1:A:214:LEU:O	2.00	0.61
1:A:3:SER:HB3	1:A:5:ILE:CG1	2.29	0.61
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.35	0.61
1:A:43:LYS:C	1:A:45:GLY:N	2.55	0.61
1:A:100:LEU:HD23	1:A:181:TYR:CE1	2.35	0.61
2:B:88:TRP:HZ3	2:B:93:GLY:N	1.99	0.61
1:A:241:VAL:CG2	1:A:270:ILE:HD13	2.31	0.61
2:B:84:THR:CG2	2:B:154:LYS:HE2	2.26	0.61
1:A:2:ILE:HG22	1:A:3:SER:H	1.64	0.61
2:B:161:GLN:HE22	2:B:182:GLN:NE2	1.97	0.61
1:A:118:VAL:HG13	1:A:119:PRO:HD2	1.82	0.60
1:A:241:VAL:HG21	1:A:270:ILE:HD13	1.82	0.60
1:A:31:ILE:O	1:A:35:VAL:HG23	2.02	0.60
1:A:538:ALA:O	1:A:539:HIS:HB3	2.01	0.60
1:A:312:GLU:HG2	1:A:313:PRO:CD	2.28	0.60
2:B:266:TRP:CZ3	2:B:426:TRP:CG	2.89	0.60
1:A:346:PHE:N	1:A:346:PHE:CD2	2.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLN:HB2	2:B:302:GLU:OE1	2.01	0.60
1:A:139:THR:CB	1:A:140:PRO:CD	2.76	0.60
1:A:318:TYR:CD1	4:A:999:GWJ:H15A	2.38	0.59
2:B:27:THR:O	2:B:31:ILE:HG13	2.03	0.59
1:A:115:TYR:O	1:A:117:SER:N	2.35	0.59
1:A:515:SER:OG	1:A:518:VAL:HG23	2.03	0.59
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.84	0.59
1:A:112:GLY:C	1:A:114:ALA:H	2.11	0.59
1:A:206:ARG:HG2	1:A:206:ARG:NH1	2.15	0.59
1:A:220:LYS:HD3	1:A:220:LYS:C	2.27	0.59
1:A:102:LYS:CE	1:A:237:ASP:HA	2.32	0.59
1:A:358:ARG:HD3	1:A:358:ARG:N	2.18	0.58
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.37	0.58
1:A:219:LYS:HA	1:A:222:GLN:HG2	1.86	0.58
1:A:489:SER:CB	1:A:493:VAL:HG21	2.34	0.58
1:A:219:LYS:HD2	1:A:222:GLN:HE21	1.68	0.58
1:A:376:THR:O	1:A:380:ILE:HG12	2.02	0.58
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.38	0.58
2:B:61:PHE:CD1	2:B:403:THR:HG22	2.39	0.58
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.15	0.58
2:B:194:GLU:OE2	2:B:195:ILE:HG22	2.04	0.58
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.85	0.58
1:A:320:ASP:OD1	1:A:323:LYS:HG3	2.04	0.58
1:A:232:TYR:N	1:A:242:GLN:HE21	2.00	0.58
1:A:291:GLU:HG2	1:A:293:ILE:CD1	2.34	0.57
2:B:113:ASP:O	2:B:116:PHE:HD2	1.86	0.57
1:A:98:ALA:HB2	1:A:349:LEU:O	2.04	0.57
2:B:175:ASN:HB3	2:B:178:ILE:HD12	1.86	0.57
1:A:46:LYS:HE2	1:A:116:PHE:HB3	1.86	0.57
2:B:114:ALA:HB2	2:B:214:LEU:HD11	1.87	0.57
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.18	0.57
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.04	0.57
1:A:257:ILE:HD13	1:A:282:LEU:HD23	1.85	0.57
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.87	0.57
1:A:399:GLU:O	1:A:403:THR:CB	2.53	0.57
2:B:331:LYS:NZ	2:B:364:ASP:OD1	2.34	0.57
1:A:438:GLU:OE1	1:A:459:THR:OG1	2.08	0.57
2:B:235:HIS:O	2:B:238:LYS:HG2	2.05	0.57
2:B:339:TYR:CE1	2:B:352:GLY:HA3	2.39	0.57
1:A:308:GLU:OE2	1:A:311:LYS:HE2	2.05	0.56
1:A:420:PRO:HA	1:A:421:PRO:C	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:VAL:O	2:B:258:GLN:HG3	2.05	0.56
1:A:109:LEU:HB3	1:A:216:THR:HG23	1.86	0.56
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.87	0.56
1:A:439:THR:HG22	1:A:441:TYR:HE1	1.70	0.56
2:B:161:GLN:O	2:B:165:THR:HG23	2.06	0.56
2:B:365:VAL:O	2:B:369:THR:HG23	2.04	0.56
1:A:63:ILE:C	1:A:63:ILE:HD12	2.30	0.56
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.87	0.56
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.34	0.56
1:A:268:SER:HB3	1:A:353:LYS:HE2	1.86	0.56
1:A:503:LEU:O	1:A:506:ILE:HB	2.06	0.56
2:B:163:SER:O	2:B:167:ILE:CG2	2.50	0.56
2:B:242:GLN:NE2	2:B:243:PRO:HD2	2.21	0.56
1:A:292:VAL:C	1:A:293:ILE:HD12	2.30	0.56
2:B:111:VAL:HA	2:B:214:LEU:HD22	1.87	0.56
2:B:56:TYR:O	2:B:57:ASN:HB2	2.06	0.55
1:A:68:SER:C	1:A:70:LYS:N	2.64	0.55
1:A:334:GLN:NE2	1:A:512:GLN:HB3	2.20	0.55
2:B:29:GLU:CG	2:B:30:LYS:N	2.70	0.55
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.88	0.55
1:A:506:ILE:HG13	1:A:533:LEU:HD23	1.89	0.55
1:A:43:LYS:O	1:A:45:GLY:N	2.40	0.55
1:A:220:LYS:O	1:A:221:HIS:CB	2.52	0.55
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.36	0.55
1:A:502:ALA:O	1:A:503:LEU:C	2.50	0.55
2:B:376:THR:HG23	2:B:386:THR:HG22	1.87	0.55
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.88	0.55
1:A:111:VAL:HG21	1:A:160:PHE:CZ	2.42	0.55
2:B:278:GLN:HA	2:B:278:GLN:OE1	2.06	0.55
2:B:27:THR:HB	2:B:29:GLU:HG2	1.89	0.55
2:B:195:ILE:HG23	2:B:196:GLY:H	1.72	0.55
1:A:448:ARG:HG2	1:A:448:ARG:NH1	2.22	0.55
2:B:233:GLU:CD	2:B:233:GLU:N	2.65	0.55
1:A:28:GLU:HG3	1:A:29:GLU:N	2.22	0.55
2:B:169:GLU:HB2	2:B:170:PRO:CD	2.31	0.55
1:A:96:HIS:HD2	1:A:98:ALA:H	1.55	0.54
1:A:109:LEU:HD23	1:A:216:THR:CG2	2.35	0.54
1:A:308:GLU:OE2	1:A:308:GLU:CA	2.53	0.54
1:A:170:PRO:HA	1:A:173:LYS:NZ	2.21	0.54
1:A:254:VAL:O	1:A:258:GLN:HG3	2.07	0.54
1:A:440:PHE:HZ	1:A:489:SER:HB3	1.67	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ILE:O	1:A:509:GLN:N	2.39	0.54
2:B:205:LEU:HD13	2:B:205:LEU:C	2.32	0.54
1:A:205:LEU:O	1:A:208:HIS:N	2.40	0.54
2:B:254:VAL:HG21	2:B:287:LYS:HG3	1.89	0.54
1:A:491:LEU:HD12	1:A:492:GLU:HG3	1.90	0.54
1:A:493:VAL:CG1	1:A:494:ASN:N	2.70	0.54
2:B:193:LEU:N	2:B:193:LEU:HD23	2.23	0.54
1:A:206:ARG:HH11	1:A:206:ARG:HB3	1.66	0.54
1:A:332:GLN:O	1:A:332:GLN:HG2	2.07	0.54
2:B:320:ASP:OD1	2:B:320:ASP:C	2.51	0.54
1:A:302:GLU:HA	1:A:305:GLU:OE1	2.07	0.54
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.72	0.54
1:A:268:SER:CB	1:A:353:LYS:HE2	2.37	0.54
1:A:447:ASN:CG	1:A:450:THR:HG23	2.32	0.54
2:B:7:THR:HG22	2:B:119:PRO:CG	2.34	0.54
1:A:331:LYS:NZ	1:A:364:ASP:OD1	2.37	0.53
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.43	0.53
1:A:164:MET:HE1	1:A:214:LEU:CD1	2.38	0.53
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.22	0.53
1:A:84:THR:HG22	1:A:85:GLN:N	2.22	0.53
1:A:418:ASN:C	1:A:420:PRO:HD3	2.33	0.53
1:A:419:THR:HG22	1:A:419:THR:O	2.06	0.53
2:B:337:TRP:O	2:B:353:LYS:HA	2.09	0.53
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.90	0.53
1:A:455:ALA:O	1:A:484:LEU:HD12	2.08	0.53
1:A:434:ILE:HB	1:A:437:ALA:HB3	1.89	0.53
2:B:172:ARG:O	2:B:175:ASN:C	2.52	0.53
1:A:96:HIS:O	1:A:97:PRO:C	2.48	0.53
1:A:179:VAL:HG13	1:A:181:TYR:CE2	2.43	0.53
1:A:451:LYS:O	1:A:471:ASP:N	2.41	0.53
1:A:95:PRO:HA	2:B:136:ASN:OD1	2.09	0.53
1:A:457:TYR:CD1	1:A:457:TYR:C	2.87	0.53
1:A:206:ARG:CB	1:A:206:ARG:NH1	2.71	0.52
2:B:424:LYS:NZ	2:B:428:GLN:NE2	2.57	0.52
1:A:388:LYS:HD3	1:A:413:GLU:OE2	2.10	0.52
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.90	0.52
2:B:175:ASN:HD21	2:B:201:LYS:HD2	1.74	0.52
1:A:42:GLU:OE2	1:A:49:LYS:HG2	2.10	0.52
1:A:199:ARG:HG3	1:A:219:LYS:NZ	2.24	0.52
1:A:416:PHE:HZ	1:A:422:LEU:HD11	1.73	0.52
2:B:245:VAL:CG1	2:B:431:LYS:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.92	0.52
1:A:49:LYS:HG3	1:A:144:TYR:CE2	2.44	0.52
1:A:473:THR:O	1:A:475:GLN:N	2.42	0.52
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.92	0.52
1:A:58:THR:HG23	1:A:76:ASP:O	2.10	0.52
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.44	0.52
1:A:42:GLU:OE2	1:A:49:LYS:CG	2.57	0.52
1:A:216:THR:HG23	1:A:217:PRO:HD2	1.91	0.52
1:A:246:LEU:O	1:A:307:ARG:NH1	2.29	0.52
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.91	0.52
1:A:335:GLY:CA	1:A:367:GLN:OE1	2.56	0.52
1:A:491:LEU:HD22	1:A:529:GLU:OE2	2.10	0.52
1:A:69:THR:O	1:A:69:THR:HG22	2.10	0.52
1:A:170:PRO:O	1:A:173:LYS:HB2	2.10	0.52
2:B:426:TRP:O	2:B:429:LEU:HB2	2.10	0.52
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.38	0.51
1:A:439:THR:CG2	1:A:441:TYR:HE1	2.23	0.51
1:A:465:LYS:O	1:A:466:VAL:CG2	2.56	0.51
1:A:129:ALA:HA	1:A:144:TYR:O	2.11	0.51
1:A:408:ALA:HB3	2:B:393:ILE:CB	2.41	0.51
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.45	0.51
1:A:454:LYS:NZ	1:A:468:THR:HG23	2.26	0.51
2:B:27:THR:CG2	2:B:29:GLU:HG2	2.40	0.51
1:A:476:LYS:O	1:A:480:GLN:HB2	2.10	0.51
1:A:53:GLU:HG3	1:A:53:GLU:O	2.09	0.51
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.93	0.51
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.41	0.51
2:B:72:ARG:NH2	2:B:151:GLN:OE1	2.44	0.51
2:B:173:LYS:N	2:B:173:LYS:CD	2.71	0.51
1:A:377:THR:O	1:A:381:VAL:HG23	2.11	0.51
2:B:169:GLU:CA	2:B:173:LYS:HZ3	2.22	0.51
1:A:254:VAL:HG22	1:A:286:THR:HG21	1.92	0.51
1:A:435:VAL:HA	2:B:290:THR:HG21	1.92	0.50
2:B:361:HIS:C	2:B:361:HIS:CD2	2.88	0.50
1:A:484:LEU:O	1:A:487:GLN:HG3	2.12	0.50
2:B:277:ARG:O	2:B:281:LYS:HG3	2.12	0.50
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.10	0.50
1:A:389:PHE:HB2	1:A:414:TRP:HB3	1.92	0.50
2:B:356:ARG:NH1	2:B:357:MET:O	2.44	0.50
1:A:489:SER:HB2	1:A:493:VAL:CG2	2.42	0.50
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HB3	1:A:216:THR:CG2	2.42	0.50
1:A:110:ASP:OD1	1:A:217:PRO:HG2	2.11	0.50
1:A:427:TYR:C	1:A:427:TYR:CD2	2.89	0.50
1:A:439:THR:CG2	1:A:441:TYR:CE1	2.95	0.50
1:A:84:THR:CG2	1:A:85:GLN:N	2.75	0.50
1:A:253:THR:O	1:A:257:ILE:HG13	2.11	0.50
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.46	0.50
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.46	0.50
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.12	0.49
2:B:173:LYS:HD2	2:B:173:LYS:H	1.76	0.49
2:B:195:ILE:HG23	2:B:196:GLY:N	2.27	0.49
1:A:291:GLU:HG2	1:A:293:ILE:HD12	1.94	0.49
1:A:465:LYS:CG	1:A:466:VAL:N	2.76	0.49
2:B:110:ASP:HB3	2:B:216:THR:CG2	2.43	0.49
2:B:277:ARG:HG2	2:B:278:GLN:H	1.77	0.49
2:B:159:ILE:O	2:B:159:ILE:CG2	2.60	0.49
2:B:343:GLN:HG3	2:B:349:LEU:HD11	1.95	0.49
1:A:77:PHE:O	1:A:78:ARG:C	2.54	0.49
1:A:179:VAL:CG1	1:A:181:TYR:CE2	2.95	0.49
2:B:129:ALA:HA	2:B:144:TYR:O	2.13	0.49
2:B:175:ASN:CB	2:B:178:ILE:HD12	2.43	0.49
2:B:270:ILE:O	2:B:272:PRO:HD3	2.12	0.49
2:B:368:LEU:HD13	2:B:398:TRP:CZ3	2.47	0.49
2:B:98:ALA:O	2:B:101:LYS:CG	2.61	0.48
1:A:113:ASP:O	1:A:117:SER:HB2	2.12	0.48
2:B:208:HIS:C	2:B:208:HIS:CD2	2.89	0.48
2:B:258:GLN:O	2:B:259:LYS:C	2.55	0.48
1:A:399:GLU:O	1:A:403:THR:CG2	2.61	0.48
1:A:105:SER:HA	4:A:999:GWJ:H21	1.94	0.48
1:A:12:LEU:O	1:A:13:LYS:O	2.31	0.48
2:B:53:GLU:O	2:B:55:PRO:HD3	2.13	0.48
1:A:216:THR:HG22	1:A:217:PRO:N	2.29	0.48
1:A:308:GLU:OE2	1:A:311:LYS:CE	2.62	0.48
2:B:276:VAL:O	2:B:280:CYS:HB2	2.14	0.48
1:A:100:LEU:O	1:A:318:TYR:HB3	2.13	0.48
2:B:164:MET:HE3	2:B:187:LEU:HD13	1.95	0.48
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.49	0.48
2:B:46:LYS:HE2	2:B:116:PHE:HD1	1.78	0.48
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.53	0.48
1:A:229:TRP:O	1:A:232:TYR:HB2	2.14	0.48
1:A:287:LYS:N	1:A:291:GLU:OE2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:TRP:CG	1:A:403:THR:N	2.80	0.48
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.28	0.48
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.49	0.47
1:A:317:VAL:CG1	1:A:318:TYR:N	2.76	0.47
2:B:54:ASN:O	2:B:143:ARG:NH2	2.47	0.47
1:A:108:VAL:HG21	1:A:223:LYS:HG3	1.96	0.47
1:A:453:GLY:O	1:A:469:LEU:N	2.28	0.47
1:A:122:GLU:HB3	1:A:125:ARG:HH12	1.77	0.47
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.45	0.47
1:A:205:LEU:O	1:A:206:ARG:C	2.57	0.47
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.46	0.47
1:A:408:ALA:HB3	2:B:393:ILE:HB	1.96	0.47
1:A:427:TYR:CE2	1:A:509:GLN:HB3	2.49	0.47
2:B:16:MET:HE3	2:B:83:ARG:HG2	1.96	0.47
2:B:169:GLU:CB	2:B:170:PRO:HD3	2.34	0.47
1:A:279:LEU:O	1:A:282:LEU:HB2	2.15	0.47
1:A:443:ASP:O	1:A:455:ALA:HA	2.15	0.47
1:A:49:LYS:HG3	1:A:144:TYR:HE2	1.80	0.47
1:A:237:ASP:OD2	1:A:237:ASP:N	2.48	0.47
1:A:473:THR:HG22	1:A:475:GLN:H	1.78	0.47
1:A:489:SER:CB	1:A:493:VAL:CG2	2.93	0.47
2:B:137:ASN:C	2:B:139:THR:H	2.22	0.47
2:B:214:LEU:O	2:B:215:THR:CG2	2.59	0.47
2:B:421:PRO:O	2:B:425:LEU:HD22	2.14	0.47
1:A:111:VAL:HG11	1:A:164:MET:HE3	1.97	0.47
1:A:484:LEU:HA	1:A:484:LEU:HD23	1.71	0.47
2:B:61:PHE:CE1	2:B:74:LEU:CD2	2.94	0.47
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.29	0.47
2:B:239:TRP:CZ3	2:B:378:GLU:HG2	2.50	0.47
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.98	0.46
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.63	0.46
1:A:291:GLU:HG2	1:A:293:ILE:HD11	1.96	0.46
1:A:460:ASN:HA	2:B:286:THR:O	2.15	0.46
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.50	0.46
2:B:108:VAL:HG22	2:B:188:TYR:CE2	2.50	0.46
2:B:173:LYS:CD	2:B:173:LYS:H	2.29	0.46
1:A:11:LYS:O	1:A:85:GLN:HB3	2.16	0.46
1:A:97:PRO:HA	1:A:100:LEU:CD1	2.45	0.46
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.80	0.46
1:A:497:THR:OG1	1:A:498:ASP:N	2.48	0.46
2:B:99:GLY:O	2:B:100:LEU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:TYR:CE2	1:A:487:GLN:NE2	2.83	0.46
2:B:138:GLU:C	2:B:139:THR:HG22	2.40	0.46
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.51	0.46
1:A:477:THR:O	1:A:481:ALA:N	2.31	0.46
1:A:436:GLY:O	1:A:461:ARG:NH2	2.43	0.46
2:B:115:TYR:C	2:B:117:SER:N	2.71	0.46
1:A:57:ASN:HD22	1:A:143:ARG:NH2	2.13	0.46
1:A:341:ILE:O	1:A:349:LEU:HB2	2.16	0.46
1:A:418:ASN:OD1	1:A:420:PRO:HD3	2.15	0.46
2:B:118:VAL:HB	2:B:149:LEU:HG	1.98	0.46
1:A:418:ASN:O	1:A:418:ASN:OD1	2.34	0.46
2:B:425:LEU:HD12	2:B:425:LEU:HA	1.61	0.46
1:A:489:SER:HB2	1:A:493:VAL:HG22	1.96	0.45
1:A:514:GLU:HG3	1:A:515:SER:N	2.31	0.45
2:B:61:PHE:CZ	2:B:74:LEU:HG	2.52	0.45
2:B:114:ALA:N	2:B:214:LEU:HD21	2.31	0.45
2:B:235:HIS:O	2:B:238:LYS:CG	2.64	0.45
2:B:427:TYR:C	2:B:429:LEU:H	2.22	0.45
1:A:115:TYR:C	1:A:117:SER:N	2.74	0.45
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.52	0.45
2:B:369:THR:O	2:B:373:GLN:HG3	2.16	0.45
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.58	0.45
1:A:522:ILE:O	1:A:523:GLU:C	2.59	0.45
1:A:57:ASN:HA	1:A:129:ALA:O	2.17	0.45
2:B:118:VAL:CG1	2:B:119:PRO:HD2	2.47	0.45
1:A:10:VAL:HG11	1:A:153:TRP:CH2	2.52	0.45
1:A:479:LEU:HB2	1:A:517:LEU:HD13	1.98	0.45
1:A:517:LEU:HD23	1:A:517:LEU:HA	1.56	0.45
1:A:3:SER:OG	1:A:212:TRP:O	2.30	0.45
1:A:405:TYR:O	2:B:331:LYS:HE2	2.17	0.45
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.98	0.45
1:A:218:ASP:O	1:A:220:LYS:N	2.49	0.45
1:A:363:ASN:OD1	1:A:363:ASN:C	2.59	0.44
1:A:89:GLU:O	1:A:89:GLU:CD	2.60	0.44
1:A:194:GLU:O	1:A:195:ILE:C	2.60	0.44
2:B:205:LEU:CD1	2:B:209:LEU:HD22	2.47	0.44
2:B:235:HIS:HB2	2:B:238:LYS:HG2	1.99	0.44
2:B:325:LEU:HD12	2:B:325:LEU:HA	1.72	0.44
1:A:112:GLY:C	1:A:114:ALA:N	2.71	0.44
1:A:115:TYR:C	1:A:117:SER:H	2.26	0.44
1:A:255:ASN:CG	1:A:289:LEU:HB3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:TYR:CE2	2:B:289:LEU:HD23	2.53	0.44
2:B:49:LYS:HA	2:B:143:ARG:O	2.17	0.44
1:A:54:ASN:OD1	1:A:56:TYR:HB2	2.18	0.44
1:A:360:ALA:C	1:A:361:HIS:CD2	2.96	0.44
1:A:475:GLN:O	1:A:479:LEU:HG	2.18	0.44
1:A:480:GLN:O	1:A:481:ALA:C	2.60	0.44
1:A:264:LEU:HD13	1:A:264:LEU:HA	1.87	0.44
1:A:317:VAL:CG1	1:A:318:TYR:H	2.29	0.44
1:A:456:GLY:HA3	1:A:466:VAL:HG22	1.98	0.44
1:A:94:ILE:HA	1:A:95:PRO:HD3	1.85	0.44
1:A:257:ILE:CD1	1:A:282:LEU:HD23	2.48	0.44
1:A:149:LEU:HG	1:A:156:SER:HA	1.99	0.44
1:A:439:THR:O	1:A:439:THR:CG2	2.64	0.44
1:A:477:THR:O	1:A:478:GLU:C	2.60	0.44
2:B:27:THR:HG22	2:B:29:GLU:H	1.82	0.44
2:B:206:ARG:O	2:B:207:GLN:C	2.60	0.44
2:B:424:LYS:HD3	2:B:424:LYS:C	2.43	0.44
1:A:19:PRO:O	1:A:56:TYR:HA	2.18	0.44
1:A:122:GLU:CD	1:A:122:GLU:N	2.67	0.44
1:A:175:ASN:OD1	1:A:201:LYS:HE2	2.18	0.44
1:A:253:THR:HA	1:A:291:GLU:O	2.18	0.43
1:A:516:GLU:O	1:A:520:GLN:HG3	2.18	0.43
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.53	0.43
2:B:76:ASP:C	2:B:76:ASP:OD2	2.61	0.43
2:B:179:VAL:HG12	2:B:180:ILE:N	2.33	0.43
2:B:181:TYR:CD2	2:B:182:GLN:N	2.86	0.43
1:A:56:TYR:O	1:A:143:ARG:NH2	2.37	0.43
1:A:68:SER:O	1:A:70:LYS:N	2.52	0.43
1:A:246:LEU:HD22	1:A:260:LEU:HD11	2.00	0.43
1:A:454:LYS:HG3	1:A:468:THR:HA	2.00	0.43
2:B:202:ILE:O	2:B:205:LEU:HB3	2.18	0.43
1:A:283:LEU:HA	1:A:283:LEU:HD12	1.80	0.43
1:A:483:TYR:O	1:A:487:GLN:HG2	2.17	0.43
1:A:382:ILE:O	2:B:135:ILE:HG22	2.19	0.43
2:B:172:ARG:HH21	2:B:180:ILE:HB	1.83	0.43
1:A:319:TYR:OH	1:A:385:LYS:HD3	2.18	0.43
2:B:27:THR:HG22	2:B:28:GLU:N	2.34	0.43
1:A:204:GLU:O	1:A:205:LEU:C	2.62	0.43
1:A:43:LYS:HA	1:A:43:LYS:HD3	1.85	0.43
1:A:345:PRO:C	1:A:347:LYS:H	2.27	0.43
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LYS:NZ	2:B:69:THR:O	2.52	0.43
2:B:113:ASP:O	2:B:116:PHE:CD2	2.70	0.43
2:B:427:TYR:C	2:B:429:LEU:N	2.77	0.43
1:A:318:TYR:CE1	4:A:999:GWJ:H15A	2.53	0.43
1:A:328:GLU:HG3	1:A:390:LYS:CB	2.49	0.43
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.54	0.43
2:B:78:ARG:O	2:B:82:LYS:HG3	2.19	0.43
2:B:332:GLN:NE2	2:B:428:GLN:HB2	2.33	0.43
1:A:42:GLU:HG3	1:A:49:LYS:HD2	2.00	0.42
1:A:409:THR:O	1:A:410:TRP:HB2	2.19	0.42
1:A:417:VAL:O	1:A:417:VAL:HG13	2.20	0.42
2:B:46:LYS:HE2	2:B:116:PHE:CD1	2.53	0.42
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.54	0.42
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.84	0.42
1:A:109:LEU:HD12	1:A:109:LEU:N	2.34	0.42
1:A:122:GLU:CB	1:A:125:ARG:NH1	2.80	0.42
2:B:94:ILE:HD11	2:B:182:GLN:H	1.84	0.42
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.53	0.42
2:B:124:PHE:O	2:B:125:ARG:C	2.61	0.42
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.00	0.42
2:B:400:THR:HG22	2:B:401:TRP:CD2	2.54	0.42
1:A:239:TRP:CE2	1:A:316:GLY:CA	2.96	0.42
2:B:61:PHE:HE1	2:B:74:LEU:HD23	1.79	0.42
2:B:125:ARG:O	2:B:126:LYS:C	2.62	0.42
2:B:128:THR:O	2:B:129:ALA:C	2.61	0.42
2:B:165:THR:O	2:B:166:LYS:C	2.62	0.42
2:B:29:GLU:HG3	2:B:30:LYS:N	2.34	0.42
2:B:169:GLU:CB	2:B:170:PRO:CD	2.95	0.42
1:A:473:THR:O	1:A:474:ASN:C	2.62	0.42
2:B:115:TYR:C	2:B:117:SER:H	2.27	0.42
2:B:167:ILE:HD11	2:B:209:LEU:CD1	2.50	0.42
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.55	0.42
1:A:81:ASN:C	1:A:83:ARG:H	2.27	0.42
1:A:208:HIS:CD2	1:A:208:HIS:C	2.96	0.42
2:B:115:TYR:O	2:B:117:SER:N	2.52	0.42
2:B:208:HIS:HD2	2:B:208:HIS:O	2.03	0.42
1:A:100:LEU:CD2	4:A:999:GWJ:H9	2.49	0.42
1:A:109:LEU:CD2	1:A:216:THR:HG21	2.43	0.42
1:A:415:GLU:HG3	1:A:416:PHE:O	2.20	0.42
1:A:43:LYS:O	1:A:44:GLU:C	2.60	0.42
1:A:175:ASN:OD1	1:A:201:LYS:CE	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ASP:HB2	2:B:214:LEU:HD23	2.01	0.42
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.54	0.42
1:A:97:PRO:HA	1:A:100:LEU:HD12	2.02	0.41
1:A:148:VAL:O	1:A:149:LEU:C	2.62	0.41
1:A:33:ALA:O	1:A:36:GLU:HB3	2.20	0.41
1:A:117:SER:OG	1:A:213:GLY:O	2.38	0.41
1:A:416:PHE:CZ	1:A:422:LEU:HD11	2.54	0.41
2:B:206:ARG:O	2:B:209:LEU:N	2.54	0.41
2:B:235:HIS:N	2:B:236:PRO:HD3	2.35	0.41
2:B:270:ILE:HG12	2:B:346:PHE:HB3	2.03	0.41
1:A:12:LEU:CD2	1:A:83:ARG:O	2.68	0.41
1:A:135:ILE:O	1:A:138:GLU:HG3	2.20	0.41
1:A:194:GLU:OE1	1:A:194:GLU:HA	2.20	0.41
1:A:491:LEU:HD13	1:A:492:GLU:CG	2.48	0.41
2:B:134:SER:HB2	2:B:139:THR:HG23	2.02	0.41
2:B:416:PHE:CD1	2:B:416:PHE:N	2.88	0.41
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.79	0.41
1:A:216:THR:CG2	1:A:217:PRO:N	2.84	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.21	0.41
1:A:483:TYR:HE1	1:A:524:GLN:HG3	1.84	0.41
2:B:214:LEU:HD23	2:B:214:LEU:HA	1.73	0.41
2:B:343:GLN:HG3	2:B:349:LEU:CD1	2.49	0.41
1:A:469:LEU:HD11	1:A:480:GLN:HG2	2.03	0.41
2:B:126:LYS:HE2	2:B:127:TYR:CE1	2.56	0.41
2:B:234:LEU:N	2:B:234:LEU:HD12	2.34	0.41
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.54	0.41
1:A:135:ILE:O	1:A:138:GLU:CG	2.69	0.41
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.56	0.41
1:A:483:TYR:CE1	1:A:524:GLN:HG3	2.56	0.41
2:B:267:ALA:C	2:B:269:GLN:H	2.28	0.41
2:B:377:THR:HG22	2:B:410:TRP:HZ2	1.86	0.41
1:A:168:LEU:O	1:A:169:GLU:C	2.63	0.41
1:A:297:GLU:O	1:A:298:GLU:C	2.63	0.41
1:A:452:LEU:HA	1:A:469:LEU:O	2.21	0.41
1:A:474:ASN:C	1:A:477:THR:HG1	2.19	0.41
2:B:167:ILE:CD1	2:B:209:LEU:HD12	2.50	0.41
2:B:428:GLN:HG2	2:B:428:GLN:O	2.20	0.41
1:A:246:LEU:HD11	1:A:310:LEU:HD12	2.03	0.41
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.81	0.41
2:B:208:HIS:CD2	2:B:208:HIS:O	2.73	0.41
1:A:3:SER:HA	1:A:4:PRO:HD3	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:CD2	1:A:98:ALA:H	2.37	0.41
1:A:135:ILE:HD12	1:A:135:ILE:N	2.35	0.41
1:A:169:GLU:OE2	1:A:173:LYS:HE3	2.21	0.41
1:A:188:TYR:O	4:A:999:GWJ:CL	2.76	0.41
1:A:360:ALA:O	1:A:361:HIS:HB3	2.21	0.41
1:A:386:THR:HA	1:A:387:PRO:HD3	1.87	0.41
1:A:430:GLU:HB2	1:A:532:TYR:HB2	2.03	0.41
1:A:476:LYS:O	1:A:480:GLN:N	2.39	0.41
2:B:50:ILE:HD12	2:B:54:ASN:HB3	2.03	0.41
2:B:96:HIS:CE1	2:B:381:VAL:O	2.74	0.41
2:B:267:ALA:C	2:B:269:GLN:N	2.76	0.41
1:A:8:VAL:O	1:A:121:ASP:HB2	2.21	0.41
1:A:125:ARG:NE	1:A:147:ASN:HA	2.36	0.41
1:A:329:ILE:O	1:A:392:PRO:HD3	2.21	0.41
2:B:85:GLN:HG3	2:B:86:ASP:O	2.21	0.41
1:A:3:SER:HB3	1:A:5:ILE:CD1	2.51	0.40
1:A:79:GLU:O	1:A:80:LEU:C	2.64	0.40
1:A:180:ILE:HG23	1:A:189:VAL:HG22	2.03	0.40
1:A:240:THR:HG22	1:A:315:HIS:CB	2.51	0.40
1:A:474:ASN:HA	1:A:477:THR:OG1	2.21	0.40
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.89	0.40
2:B:169:GLU:C	2:B:173:LYS:HD3	2.45	0.40
1:A:447:ASN:O	1:A:451:LYS:N	2.38	0.40
1:A:29:GLU:O	1:A:30:LYS:C	2.64	0.40
1:A:270:ILE:HG22	1:A:314:VAL:HG21	2.02	0.40
2:B:238:LYS:NZ	2:B:239:TRP:HD1	2.19	0.40
2:B:211:ARG:C	2:B:212:TRP:CD1	3.00	0.40
1:A:132:ILE:HA	1:A:133:PRO:HD2	1.90	0.40
1:A:210:LEU:C	1:A:212:TRP:H	2.30	0.40
1:A:363:ASN:OD1	1:A:365:VAL:N	2.54	0.40
2:B:134:SER:OG	2:B:139:THR:HG23	2.22	0.40
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.57	0.40
2:B:282:LEU:CD2	2:B:296:THR:HG23	2.52	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	531/560 (95%)	441 (83%)	72 (14%)	18 (3%)	3	12
2	B	394/440 (90%)	347 (88%)	39 (10%)	8 (2%)	6	22
All	All	925/1000 (92%)	788 (85%)	111 (12%)	26 (3%)	4	15

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	114	ALA
1	A	116	PHE
1	A	140	PRO
1	A	223	LYS
1	A	474	ASN
1	A	113	ASP
1	A	221	HIS
1	A	358	ARG
1	A	361	HIS
2	B	215	THR
1	A	115	TYR
1	A	139	THR
2	B	14	PRO
2	B	85	GLN
2	B	213	GLY
1	A	230	MET
2	B	116	PHE
2	B	404	GLU
1	A	13	LYS
2	B	166	LYS
1	A	44	GLU
1	A	91	GLN
1	A	14	PRO
1	A	420	PRO

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Mol	Chain	Res	Type
2	B	195	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	480/499 (96%)	409 (85%)	71 (15%)	3	10
2	B	365/400 (91%)	334 (92%)	31 (8%)	10	31
All	All	845/899 (94%)	743 (88%)	102 (12%)	5	16

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	27	THR
1	A	40	GLU
1	A	49	LYS
1	A	73	LYS
1	A	86	ASP
1	A	90	VAL
1	A	92	LEU
1	A	94	ILE
1	A	120	LEU
1	A	122	GLU
1	A	123	ASP
1	A	136	ASN
1	A	138	GLU
1	A	140	PRO
1	A	142	ILE
1	A	143	ARG
1	A	149	LEU
1	A	166	LYS
1	A	179	VAL
1	A	195	ILE
1	A	205	LEU

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Mol	Chain	Res	Type
1	A	206	ARG
1	A	211	ARG
1	A	217	PRO
1	A	220	LYS
1	A	221	HIS
1	A	228	LEU
1	A	244	ILE
1	A	255	ASN
1	A	264	LEU
1	A	266	TRP
1	A	268	SER
1	A	279	LEU
1	A	283	LEU
1	A	290	THR
1	A	308	GLU
1	A	312	GLU
1	A	340	GLN
1	A	344	GLU
1	A	346	PHE
1	A	356	ARG
1	A	362	THR
1	A	368	LEU
1	A	369	THR
1	A	386	THR
1	A	396	GLU
1	A	402	TRP
1	A	403	THR
1	A	404	GLU
1	A	409	THR
1	A	415	GLU
1	A	420	PRO
1	A	422	LEU
1	A	431	LYS
1	A	443	ASP
1	A	448	ARG
1	A	452	LEU
1	A	458	VAL
1	A	459	THR
1	A	473	THR
1	A	475	GLN
1	A	487	GLN
1	A	491	LEU

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Mol	Chain	Res	Type
1	A	496	VAL
1	A	497	THR
1	A	500	GLN
1	A	501	TYR
1	A	515	SER
1	A	517	LEU
1	A	539	HIS
2	B	14	PRO
2	B	21	VAL
2	B	35	VAL
2	B	40	GLU
2	B	55	PRO
2	B	73	LYS
2	B	135	ILE
2	B	138	GLU
2	B	139	THR
2	B	167	ILE
2	B	187	LEU
2	B	193	LEU
2	B	194	GLU
2	B	209	LEU
2	B	211	ARG
2	B	215	THR
2	B	233	GLU
2	B	234	LEU
2	B	238	LYS
2	B	261	VAL
2	B	277	ARG
2	B	280	CYS
2	B	283	LEU
2	B	303	LEU
2	B	323	LYS
2	B	325	LEU
2	B	356	ARG
2	B	368	LEU
2	B	386	THR
2	B	403	THR
2	B	425	LEU

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

Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	96	HIS
1	A	207	GLN
1	A	208	HIS
1	A	222	GLN
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	334	GLN
1	A	336	GLN
1	A	361	HIS
1	A	475	GLN
1	A	487	GLN
1	A	500	GLN
1	A	512	GLN
2	B	57	ASN
2	B	103	ASN
2	B	147	ASN
2	B	161	GLN
2	B	175	ASN
2	B	182	GLN
2	B	197	GLN
2	B	208	HIS
2	B	235	HIS
2	B	255	ASN
2	B	278	GLN
2	B	332	GLN
2	B	336	GLN
2	B	361	HIS
2	B	394	GLN
2	B	418	ASN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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$
1	CSD	A	280	1	4,7,8	1.22	1 (25%)	1,8,10	0.89	0

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
1	CSD	A	280	1	-	1/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	-2.03	1.45	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	PO4	A	1300	-	4,4,4	1.73	2 (50%)	6,6,6	0.46	0
4	GWJ	A	999	-	36,36,36	2.74	9 (25%)	52,52,52	1.58	10 (19%)

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	GWJ	A	999	-	-	4/25/25/25	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	GWJ	C5-C6	7.11	1.50	1.38
4	A	999	GWJ	C17-C18	6.41	1.53	1.40
4	A	999	GWJ	C2-C1	6.27	1.52	1.40
4	A	999	GWJ	C19-C20	5.71	1.49	1.39
4	A	999	GWJ	C22-C21	5.58	1.47	1.38
4	A	999	GWJ	C3-C4	4.27	1.45	1.38
4	A	999	GWJ	C3-C2	-3.68	1.34	1.39
4	A	999	GWJ	C19-C18	-2.79	1.35	1.39
3	A	1300	PO4	P-O2	-2.03	1.48	1.54
3	A	1300	PO4	P-O4	-2.02	1.48	1.54
4	A	999	GWJ	C13-C8	2.02	1.42	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	GWJ	O5-S-O4	-4.55	111.80	118.80
4	A	999	GWJ	O5-S-N3	3.93	113.02	107.35
4	A	999	GWJ	C20-S-N3	-3.28	103.84	108.40
4	A	999	GWJ	C22-C17-C18	-2.92	117.37	120.70
4	A	999	GWJ	C15-O2-C1	2.58	122.99	117.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	GWJ	C15-C16-N1	2.34	120.29	115.62
4	A	999	GWJ	C2-C7-C8	2.30	123.24	119.56
4	A	999	GWJ	C5-C4-CL	2.17	122.56	119.36
4	A	999	GWJ	O4-S-C20	2.16	109.80	107.35
4	A	999	GWJ	C3-C4-CL	-2.05	116.60	119.17

There are no chirality outliers.

All (4) torsion outliers are listed below:

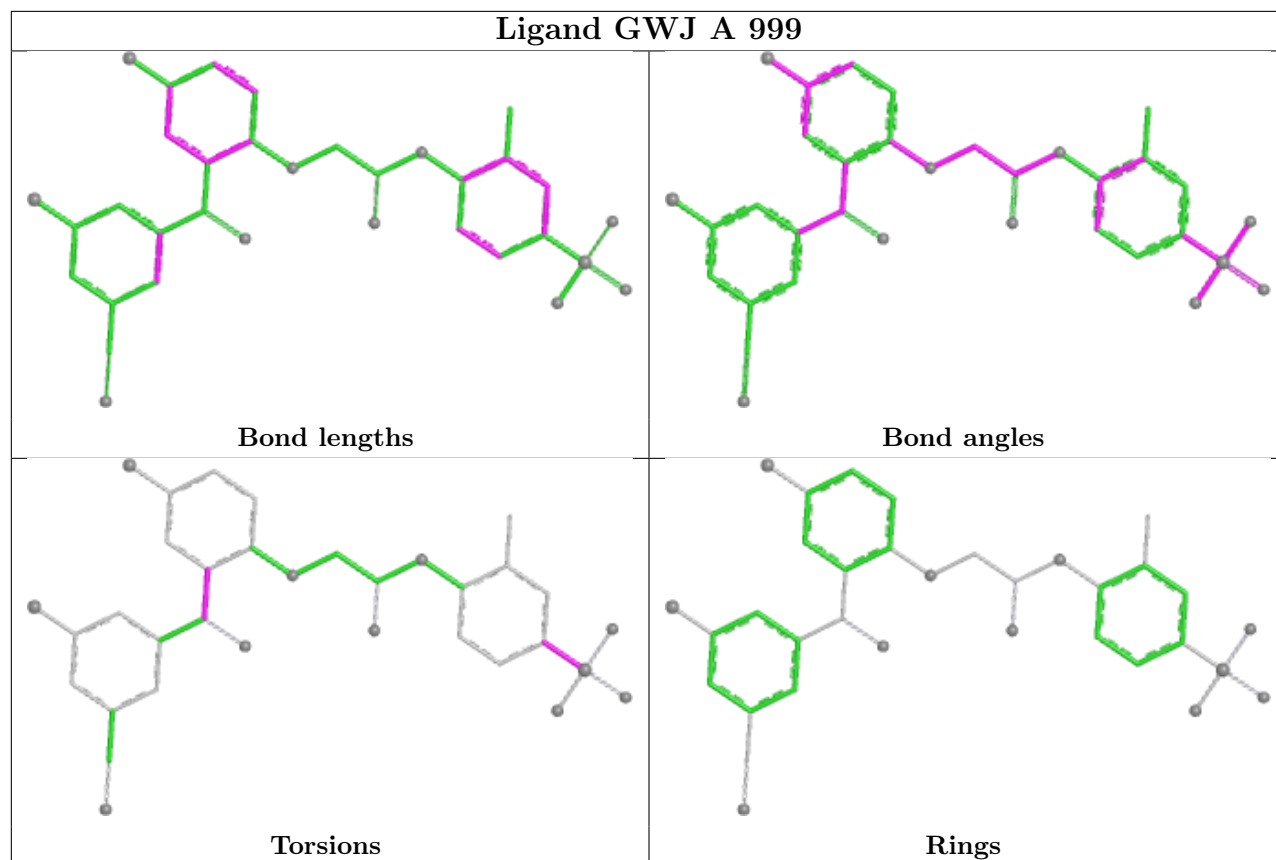
Mol	Chain	Res	Type	Atoms
4	A	999	GWJ	C19-C20-S-O5
4	A	999	GWJ	C21-C20-S-O5
4	A	999	GWJ	C1-C2-C7-O1
4	A	999	GWJ	C1-C2-C7-C8

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	GWJ	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	535/560 (95%)	-0.34	2 (0%) 88 85	37, 72, 116, 174	0
2	B	402/440 (91%)	-0.49	3 (0%) 84 79	32, 69, 120, 148	0
All	All	937/1000 (93%)	-0.40	5 (0%) 87 83	32, 71, 119, 174	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	93	GLY	3.0
1	A	455	ALA	2.9
2	B	215	THR	2.1
1	A	471	ASP	2.0
2	B	426	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CSD	A	280	8/9	0.95	0.08	58,64,81,94	0

6.3 Carbohydrates [i](#)

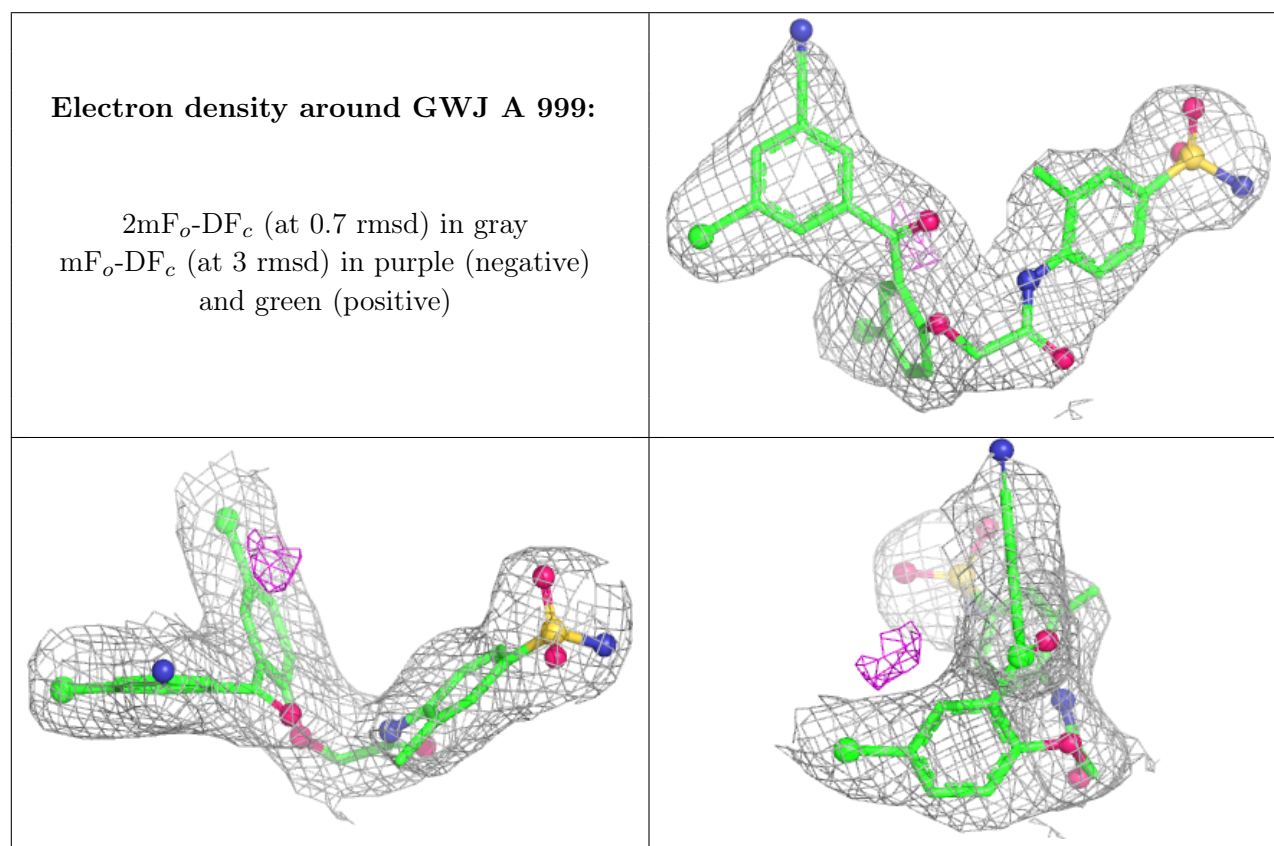
There are no oligosaccharides in this entry.

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	PO4	A	1300	5/5	0.62	0.16	132,137,152,154	0
4	GWJ	A	999	34/34	0.94	0.08	35,59,75,78	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.