



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:11 AM UTC

PDB ID : 1S6P / pdb_00001s6p
Title : CRYSTAL STRUCTURE OF HUMAN IMMUNODEFICIENCY VIRUS
TYPE 1 REVERSE TRANSCRIPTASE (RT) IN COMPLEX WITH
JANSSEN-R100943
Authors : Das, K.; Arnold, E.
Deposited on : 2004-01-26
Resolution : 2.90 Å(reported)

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

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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

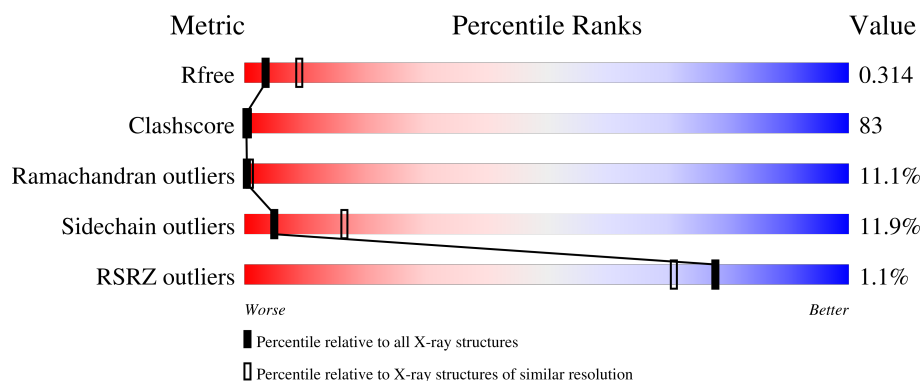
1 Overall quality at a glance

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	19%58%20%..
2	B	430	14%54%28%..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8202 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 POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	18	0	0
			4498	2913	748	830	7			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	17	0	0
			3529	2300	584	638	7			

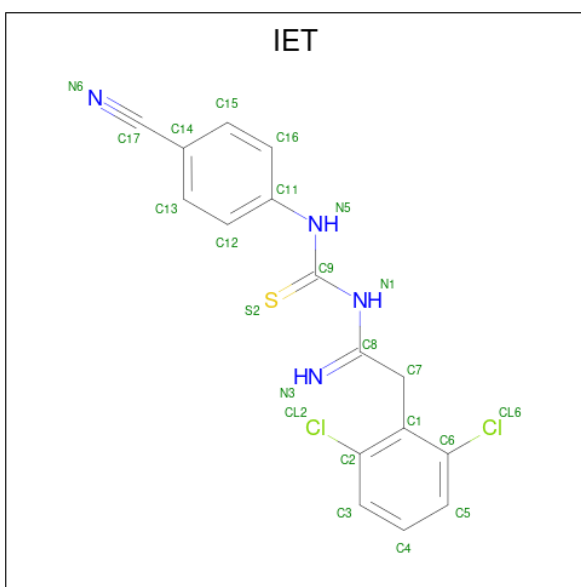
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 1-(4-CYANO-PHENYL)-3-[2-(2,6-DICHLORO-PHENYL)-1-IMINO-ETHYL]-THIOUREA (CCD ID: IET) (formula: C₁₆H₁₂Cl₂N₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	S	0	0
			23	16	2	4	1		

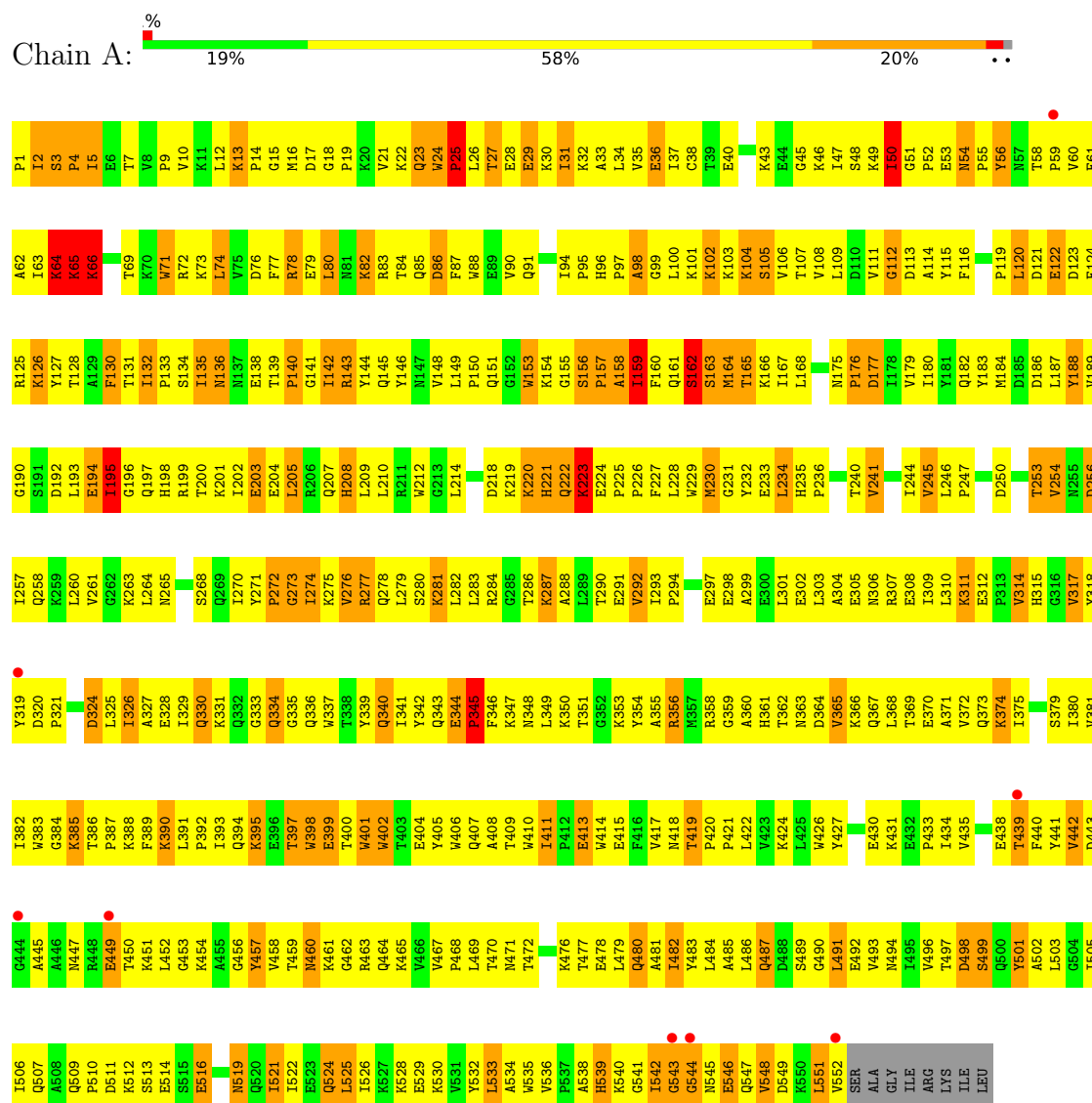
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total	O	0	0
			81	81		
5	B	70	Total	O	0	0
			70	70		

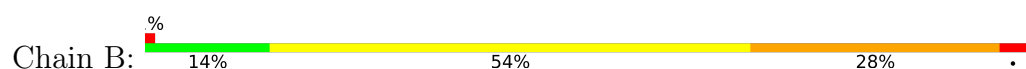
3 Residue-property plots

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: POL polyprotein [Contains: Reverse transcriptase]



- Molecule 2: POL polyprotein [Contains: Reverse transcriptase]



P1	K65	G190	D250	P313	I375
I2	K66	S191	S251	V314	I376
I5	D67	D192	W252	H315	I377
E6	S68	L193	T253	G316	E378
T7	T69	E194	V254	V317	S379
V8	K70	I195	W255	Y318	I380
P9	W71	G196	D256	Y319	W381
V10	R72	Q197	I257	D320	I382
K11	K73	H198	Q258	P321	W383
L12	L74	R199	K259	S322	G384
K13	V75	T200	L260	K323	K385
P14	D76	K201	V261	D324	T386
G15	F77	I202	G262	L325	P387
M16	R78	E203	K263	I326	K388
D17	E79	E204	L264	A327	F389
G18	L80	L205	N265	E328	K390
K22	N81	R206	W266	I329	L391
Q23	K82	Q207	A267	Q330	P392
W24	R83	H208	S268	K331	I393
T27	T84	L209	Q269	Q332	Q394
E28	Q85	L210	I270	G333	K395
E29	D86	R211	Y271	Q334	W398
K30	F87	W212	P272	G335	E399
I31	W88	G213	G273	Q336	T400
K32	W89	L214	I274	W337	W401
A33	V90	T215	K275	T338	W402
L34	Q91	T216	V276	Y339	T403
V35	L92	P217	Q277	Q340	E404
E36	H96	D218	Q278	I341	Y405
I37	P97	K219	L279	Y342	W406
C38	L100	K220	S280	Q343	
K101	K101	H221	K281	E344	
T39	K102	Q222	L282	P345	T409
E40	K103	K223	L283	F346	W410
M41	K104	E224	R284		I411
E42	T107	P225	Q285	L349	P412
K43	V108	P226		K350	
E44	L108	F227	L289	T351	F416
G45	L109	L228	T290		W417
K46	D110	W229	E291	Y354	M418
I47	V111	M230	V292	A355	T419
S48	G112	G231	I293	K356	P420
K49	D113	Y232	P294	M357	P421
I50	A114	E233	L295	R358	L422
G51	Y115	L234	T296	G359	V423
P52	F116	H235	E297	A360	K424
E53	D117	P236	E298	H361	L425
N54	S117	D237	A299	T362	W426
P55	W118	K238	E300	N363	Y427
Y56	P119	W239	L301	D364	GLN
N57		T240	E302	V365	LEU
T58	E122	Y241	E305	K366	GLU
P59	D123	Q242	N306	Q367	
V60	F124	P243	R307	L368	
F61	R125	I244	E308	T369	
A62	K126	Y245	I309	E370	
I63	Y127	L246	L310	A371	
K64	T128	P247	K311	V372	
	A129	K249	E312	K374	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.70Å 67.40Å 104.30Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.8 (20.00-2.90) 91.8 (20.00-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.83Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.312 0.252 , 0.314	Depositor DCC
R_{free} test set	1616 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 100.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8202	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.95	7/4616 (0.2%)	1.27	52/6271 (0.8%)
2	B	0.81	7/3634 (0.2%)	1.41	60/4940 (1.2%)
All	All	0.89	14/8250 (0.2%)	1.33	112/11211 (1.0%)

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

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	ILE	CG1-CD1	40.87	3.11	1.51
1	A	221	HIS	CA-C	9.78	1.57	1.52
2	B	224	GLU	C-N	-7.84	1.24	1.33
1	A	498	ASP	C-N	-6.97	1.24	1.33
2	B	225	PRO	CA-C	6.73	1.58	1.52
2	B	37	ILE	CA-CB	-6.26	1.46	1.54
2	B	226	PRO	CA-C	5.81	1.58	1.53
2	B	419	THR	CA-CB	5.60	1.62	1.53
1	A	223	LYS	N-CA	5.36	1.53	1.46
2	B	47	ILE	CA-CB	-5.28	1.47	1.55
1	A	69	THR	C-N	5.15	1.37	1.33
1	A	71	TRP	NE1-CE2	-5.13	1.31	1.37
1	A	65	LYS	C-N	-5.09	1.26	1.33
2	B	225	PRO	N-CD	-5.07	1.40	1.47

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ILE	CB-CG1-CD1	-27.80	55.42	113.80
2	B	419	THR	CA-C-N	-13.21	106.77	120.38
2	B	419	THR	C-N-CA	-13.21	106.77	120.38
2	B	225	PRO	CB-CA-C	-11.61	96.76	110.92
2	B	156	SER	N-CA-C	-10.50	98.28	112.35
2	B	225	PRO	N-CA-C	10.47	123.47	110.70
2	B	417	VAL	N-CA-C	10.40	122.73	108.17
2	B	225	PRO	O-C-N	-10.13	109.51	121.46
2	B	242	GLN	N-CA-C	9.24	130.24	109.81
2	B	89	GLU	N-CA-C	-9.22	101.30	114.12
2	B	240	THR	N-CA-C	9.19	122.83	109.14
2	B	241	VAL	N-CA-C	8.98	128.01	109.34
1	A	344	GLU	CA-C-N	8.94	131.01	119.84
1	A	344	GLU	C-N-CA	8.94	131.01	119.84
2	B	29	GLU	N-CA-C	-8.88	101.29	110.97
2	B	226	PRO	CB-CA-C	-8.73	100.48	112.97
2	B	411	ILE	CA-C-N	-8.40	109.34	119.84
2	B	411	ILE	C-N-CA	-8.40	109.34	119.84
2	B	307	ARG	N-CA-C	-8.38	102.08	113.30
1	A	287	LYS	O-C-N	8.29	133.61	122.59
2	B	58	THR	CA-C-N	8.26	128.29	119.78
2	B	58	THR	C-N-CA	8.26	128.29	119.78
1	A	544	GLY	N-CA-C	-8.17	104.53	114.66
2	B	401	TRP	N-CA-C	8.12	123.73	112.45
2	B	130	PHE	N-CA-C	-8.07	97.05	109.24
2	B	389	PHE	N-CA-C	8.06	122.39	109.24
2	B	27	THR	N-CA-C	-7.92	100.32	110.53
1	A	349	LEU	N-CA-C	-7.71	102.42	112.68
1	A	480	GLN	N-CA-C	-7.66	102.53	111.03
1	A	80	LEU	N-CA-C	-7.64	102.52	112.68
1	A	91	GLN	N-CA-C	-7.55	103.79	113.16
2	B	194	GLU	N-CA-C	-7.36	99.13	110.10
1	A	460	ASN	N-CA-C	-7.26	103.36	111.28
1	A	525	LEU	N-CA-C	-7.11	102.94	111.69
2	B	333	GLY	N-CA-C	-7.08	100.92	111.19
1	A	143	ARG	N-CA-C	6.96	120.31	107.99
1	A	221	HIS	N-CA-CB	-6.94	99.38	111.04
2	B	87	PHE	N-CA-C	-6.92	104.83	113.28
2	B	172	LYS	N-CA-C	-6.90	103.81	111.82
1	A	524	GLN	N-CA-C	-6.78	105.30	113.97
2	B	400	THR	N-CA-C	6.72	119.96	111.69
1	A	162	SER	N-CA-C	-6.70	96.54	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	VAL	CB-CA-C	-6.65	103.46	111.97
2	B	311	LYS	N-CA-C	-6.63	107.06	114.62
1	A	208	HIS	N-CA-C	-6.44	104.19	111.14
2	B	366	LYS	N-CA-C	-6.42	104.39	112.93
2	B	186	ASP	N-CA-C	6.41	119.85	109.40
1	A	241	VAL	N-CA-C	6.40	117.03	110.05
1	A	220	LYS	O-C-N	6.38	131.07	122.59
2	B	12	LEU	N-CA-C	-6.30	101.79	110.35
1	A	40	GLU	N-CA-C	-6.24	105.15	112.89
1	A	487	GLN	N-CA-C	6.24	117.74	111.07
1	A	499	SER	N-CA-C	6.17	119.58	107.98
1	A	273	GLY	N-CA-C	6.16	127.78	113.18
2	B	11	LYS	N-CA-C	6.15	118.55	108.52
2	B	309	ILE	N-CA-C	-6.14	105.01	113.00
1	A	234	LEU	N-CA-C	6.09	118.61	108.20
1	A	29	GLU	N-CA-C	-6.07	104.29	111.03
1	A	65	LYS	O-C-N	6.06	130.65	122.59
1	A	345	PRO	N-CA-C	6.04	124.92	112.47
2	B	230	MET	CA-C-O	5.97	126.89	120.38
1	A	203	GLU	N-CA-C	-5.93	104.40	111.69
2	B	107	THR	N-CA-C	-5.92	101.76	110.52
2	B	242	GLN	CA-C-N	-5.88	110.77	120.88
2	B	242	GLN	C-N-CA	-5.88	110.77	120.88
2	B	386	THR	CA-C-N	5.86	127.17	119.84
2	B	386	THR	C-N-CA	5.86	127.17	119.84
2	B	235	HIS	CA-C-N	5.72	126.99	119.84
2	B	235	HIS	C-N-CA	5.72	126.99	119.84
2	B	225	PRO	CA-N-CD	5.70	119.98	112.00
2	B	245	VAL	N-CA-C	5.70	121.19	109.34
1	A	346	PHE	N-CA-C	5.67	118.98	112.57
1	A	498	ASP	N-CA-C	-5.67	106.03	113.17
2	B	48	SER	N-CA-C	5.62	117.79	109.69
1	A	250	ASP	N-CA-C	-5.62	105.02	113.89
1	A	281	LYS	N-CA-C	-5.59	105.73	112.54
2	B	137	ASN	CB-CA-C	-5.58	102.26	111.36
2	B	45	GLY	N-CA-C	-5.57	108.18	115.47
2	B	142	ILE	N-CA-C	-5.54	101.67	109.21
2	B	279	LEU	N-CA-C	-5.53	105.66	112.90
1	A	519	ASN	N-CA-C	-5.50	106.56	113.28
2	B	281	LYS	N-CA-C	-5.48	105.86	112.54
2	B	357	MET	N-CA-C	5.47	118.58	110.48
1	A	205	LEU	N-CA-C	-5.45	105.24	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	326	ILE	CB-CA-C	-5.45	103.08	111.31
2	B	418	ASN	N-CA-C	5.43	122.36	110.80
1	A	50	ILE	N-CA-C	5.41	115.49	108.35
1	A	442	VAL	N-CA-C	5.39	117.56	109.20
2	B	370	GLU	N-CA-C	-5.38	105.52	112.68
1	A	13	LYS	CA-C-N	5.36	126.54	119.84
1	A	13	LYS	C-N-CA	5.36	126.54	119.84
1	A	431	LYS	N-CA-C	-5.36	105.48	112.23
1	A	82	LYS	N-CA-C	-5.34	106.73	113.20
1	A	72	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	69	THR	N-CA-C	5.33	117.51	111.11
1	A	390	LYS	N-CA-C	-5.31	98.61	107.80
1	A	105	SER	N-CA-C	5.29	116.93	108.41
2	B	219	LYS	N-CA-C	-5.29	99.54	110.80
1	A	157	PRO	N-CA-C	-5.28	106.16	113.81
2	B	231	GLY	N-CA-C	-5.28	100.68	113.18
2	B	316	GLY	N-CA-C	-5.16	107.89	114.85
1	A	365	VAL	N-CA-C	-5.15	105.69	110.53
2	B	210	LEU	N-CA-C	5.14	116.57	111.07
1	A	221	HIS	CA-CB-CG	5.13	118.93	113.80
1	A	292	VAL	CA-C-N	-5.10	119.13	122.60
1	A	292	VAL	C-N-CA	-5.10	119.13	122.60
1	A	501	TYR	N-CA-C	-5.08	105.43	110.97
2	B	234	LEU	N-CA-C	-5.08	102.94	110.46
2	B	10	VAL	N-CA-C	5.03	115.22	107.77
1	A	140	PRO	N-CA-C	-5.02	107.50	113.98
2	B	243	PRO	N-CA-C	5.01	119.25	112.48
1	A	4	PRO	N-CA-C	-5.00	102.17	112.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	31	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	PHE	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	4498	0	4560	724	0
2	B	3529	0	3568	649	0
3	A	1	0	0	0	0
4	A	23	0	12	5	0
5	A	81	0	0	8	0
5	B	70	0	0	5	0
All	All	8202	0	8140	1338	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 83.

All (1338) 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:64:LYS:O	1:A:66:LYS:HG2	1.34	1.25
2:B:139:THR:CG2	2:B:140:PRO:HD2	1.66	1.24
1:A:222:GLN:O	1:A:224:GLU:HG3	1.41	1.16
1:A:497:THR:HG22	1:A:499:SER:H	1.09	1.16
2:B:358:ARG:HG2	2:B:359:GLY:H	1.09	1.16
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.23	1.15
2:B:206:ARG:HE	2:B:218:ASP:HB2	1.09	1.14
2:B:296:THR:HG22	2:B:297:GLU:H	1.10	1.14
1:A:90:VAL:HG11	1:A:161:GLN:HE22	1.13	1.13
1:A:362:THR:HG22	1:A:363:ASN:H	0.97	1.13
2:B:135:ILE:H	2:B:135:ILE:CD1	1.61	1.12
2:B:195:ILE:HG23	2:B:196:GLY:H	1.10	1.11
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.28	1.10
2:B:135:ILE:HD12	2:B:135:ILE:N	1.66	1.09
1:A:454:LYS:HB2	1:A:552:VAL:HG13	1.16	1.07
2:B:220:LYS:HE3	2:B:231:GLY:HA2	1.35	1.07
1:A:64:LYS:C	1:A:66:LYS:HG2	1.78	1.06
1:A:288:ALA:HB1	1:A:291:GLU:HB2	1.38	1.06
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.33	1.06
1:A:442:VAL:HG22	1:A:481:ALA:HB1	1.38	1.05
1:A:397:THR:HG21	1:A:424:LYS:HA	1.36	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:THR:HG23	1:A:154:LYS:HE2	1.35	1.03
1:A:411:ILE:HD13	1:A:411:ILE:H	1.23	1.02
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.42	1.02
2:B:297:GLU:HG3	2:B:298:GLU:H	1.22	1.00
2:B:326:ILE:HB	2:B:342:TYR:CE1	1.96	1.00
2:B:295:LEU:HD12	2:B:300:GLU:HG2	1.43	1.00
1:A:492:GLU:HG3	1:A:530:LYS:HB2	1.44	0.99
2:B:216:THR:HB	2:B:218:ASP:OD2	1.62	0.98
2:B:74:LEU:HD21	2:B:411:ILE:HD11	1.47	0.97
1:A:108:VAL:HG12	1:A:188:TYR:CG	1.99	0.97
2:B:221:HIS:ND1	2:B:229:TRP:HB2	1.80	0.97
2:B:358:ARG:HA	2:B:362:THR:HB	1.47	0.96
2:B:135:ILE:H	2:B:135:ILE:HD12	0.81	0.95
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.44	0.95
2:B:326:ILE:HB	2:B:342:TYR:HE1	1.30	0.94
1:A:362:THR:HG22	1:A:363:ASN:N	1.80	0.94
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.30	0.94
1:A:19:PRO:O	1:A:56:TYR:HB3	1.67	0.93
2:B:253:THR:O	2:B:257:ILE:HG22	1.68	0.93
1:A:362:THR:CG2	1:A:363:ASN:H	1.80	0.92
2:B:363:ASN:O	2:B:367:GLN:HG3	1.68	0.92
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.49	0.92
2:B:296:THR:CG2	2:B:297:GLU:H	1.82	0.92
1:A:411:ILE:H	1:A:411:ILE:CD1	1.82	0.91
2:B:174:GLN:O	2:B:176:PRO:HD3	1.70	0.91
1:A:90:VAL:HG11	1:A:161:GLN:NE2	1.85	0.91
1:A:422:LEU:HD23	1:A:424:LYS:HD3	1.51	0.91
2:B:171:PHE:HB2	2:B:208:HIS:HD2	1.35	0.90
1:A:449:GLU:HG3	1:A:450:THR:N	1.83	0.90
2:B:31:ILE:O	2:B:35:VAL:HG23	1.72	0.90
2:B:275:LYS:HG2	2:B:277:ARG:HH21	1.35	0.90
2:B:139:THR:CG2	2:B:140:PRO:CD	2.50	0.88
1:A:53:GLU:HG3	1:A:54:ASN:H	1.38	0.88
1:A:288:ALA:CB	1:A:291:GLU:HB2	2.04	0.88
1:A:442:VAL:CG2	1:A:481:ALA:HB1	2.02	0.88
2:B:12:LEU:HD12	2:B:83:ARG:O	1.73	0.88
1:A:64:LYS:O	1:A:66:LYS:N	2.06	0.88
1:A:115:TYR:OH	1:A:151:GLN:HG3	1.74	0.88
2:B:115:TYR:HE2	2:B:157:PRO:HA	1.37	0.88
2:B:260:LEU:HG	2:B:264:LEU:HD11	1.56	0.87
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.10	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:HG22	1:A:241:VAL:N	1.90	0.87
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.05	0.86
1:A:134:SER:OG	1:A:139:THR:HB	1.75	0.86
1:A:258:GLN:HG2	1:A:283:LEU:HD22	1.56	0.86
1:A:441:TYR:HB3	1:A:548:VAL:HG11	1.56	0.86
1:A:254:VAL:HG23	1:A:293:ILE:HD11	1.58	0.86
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.56	0.86
2:B:248:GLU:HG2	2:B:307:ARG:HH12	1.39	0.85
2:B:373:GLN:NE2	2:B:406:TRP:HA	1.90	0.85
2:B:183:TYR:HD1	2:B:380:ILE:HG23	1.40	0.85
2:B:221:HIS:CE1	2:B:229:TRP:HB2	2.11	0.85
2:B:296:THR:HG22	2:B:297:GLU:N	1.89	0.85
2:B:358:ARG:HG2	2:B:359:GLY:N	1.87	0.85
1:A:291:GLU:O	1:A:293:ILE:HD12	1.77	0.85
1:A:497:THR:HG22	1:A:499:SER:N	1.92	0.84
1:A:195:ILE:O	1:A:199:ARG:HG2	1.74	0.84
1:A:483:TYR:HB2	1:A:521:ILE:CG1	2.07	0.84
2:B:380:ILE:O	2:B:384:GLY:HA2	1.78	0.84
2:B:298:GLU:O	2:B:302:GLU:N	2.11	0.84
1:A:240:THR:HG22	1:A:241:VAL:H	1.39	0.84
1:A:254:VAL:HA	1:A:257:ILE:HG22	1.57	0.84
2:B:1:PRO:HD3	2:B:117:SER:HA	1.59	0.84
2:B:195:ILE:HG23	2:B:196:GLY:N	1.91	0.84
2:B:104:LYS:CB	2:B:192:ASP:HA	2.07	0.83
1:A:218:ASP:O	1:A:221:HIS:HB2	1.77	0.83
1:A:27:THR:HB	1:A:29:GLU:HG2	1.61	0.83
1:A:545:ASN:O	1:A:548:VAL:HG22	1.79	0.82
1:A:479:LEU:O	1:A:521:ILE:HD11	1.79	0.82
2:B:174:GLN:HA	2:B:174:GLN:HE21	1.44	0.82
2:B:101:LYS:O	2:B:236:PRO:HB2	1.80	0.82
1:A:164:MET:HE3	1:A:168:LEU:HD11	1.60	0.82
2:B:206:ARG:NE	2:B:218:ASP:HB2	1.93	0.82
1:A:31:ILE:O	1:A:35:VAL:HG23	1.79	0.81
1:A:60:VAL:HG22	1:A:130:PHE:HB2	1.62	0.81
1:A:447:ASN:HB3	1:A:450:THR:HB	1.60	0.81
2:B:332:GLN:HG2	2:B:338:THR:HG23	1.60	0.81
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.16	0.81
2:B:206:ARG:HB3	2:B:206:ARG:NH1	1.95	0.81
1:A:79:GLU:HG3	1:A:83:ARG:HH12	1.45	0.81
2:B:178:ILE:HD13	2:B:191:SER:HB3	1.61	0.81
1:A:356:ARG:CZ	1:A:358:ARG:HG3	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLN:HG2	1:A:283:LEU:CD2	2.09	0.81
1:A:368:LEU:O	1:A:372:VAL:HG23	1.80	0.81
1:A:96:HIS:HB3	1:A:382:ILE:HD12	1.63	0.81
1:A:288:ALA:HB1	1:A:291:GLU:CB	2.11	0.81
1:A:108:VAL:CG1	1:A:188:TYR:CD2	2.64	0.81
1:A:320:ASP:H	1:A:343:GLN:HE22	1.27	0.81
1:A:441:TYR:HB3	1:A:548:VAL:CG1	2.10	0.80
2:B:27:THR:HG22	2:B:29:GLU:H	1.47	0.80
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.47	0.80
2:B:171:PHE:HB2	2:B:208:HIS:CD2	2.16	0.80
1:A:29:GLU:HG3	1:A:30:LYS:N	1.97	0.79
2:B:326:ILE:CB	2:B:342:TYR:HE1	1.94	0.79
1:A:434:ILE:HG21	1:A:492:GLU:HG2	1.61	0.79
2:B:103:LYS:HG3	2:B:190:GLY:O	1.83	0.79
1:A:64:LYS:O	1:A:66:LYS:CG	2.26	0.79
1:A:23:GLN:O	1:A:25:PRO:HD3	1.81	0.79
2:B:201:LYS:HE2	2:B:201:LYS:HA	1.64	0.79
1:A:540:LYS:HD3	2:B:265:ASN:HD21	1.48	0.78
1:A:476:LYS:HE3	1:A:516:GLU:OE2	1.83	0.78
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.12	0.78
1:A:28:GLU:HG2	1:A:135:ILE:O	1.83	0.78
2:B:295:LEU:HG	2:B:295:LEU:O	1.83	0.78
2:B:339:TYR:CG	2:B:375:ILE:HD11	2.19	0.78
2:B:103:LYS:HG3	2:B:190:GLY:C	2.09	0.77
1:A:2:ILE:HG22	1:A:3:SER:H	1.47	0.77
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.64	0.77
2:B:376:THR:HG22	2:B:380:ILE:CD1	2.14	0.77
1:A:132:ILE:CG2	1:A:142:ILE:HB	2.15	0.77
2:B:195:ILE:CG2	2:B:196:GLY:H	1.96	0.77
2:B:335:GLY:O	2:B:355:ALA:HA	1.85	0.77
1:A:12:LEU:HG	1:A:124:PHE:HE1	1.47	0.77
2:B:175:ASN:H	2:B:175:ASN:HD22	1.31	0.77
1:A:28:GLU:HA	1:A:31:ILE:CG2	2.14	0.77
1:A:189:VAL:HG21	1:A:205:LEU:CD2	2.15	0.77
1:A:439:THR:O	1:A:459:THR:HG22	1.85	0.77
2:B:69:THR:O	2:B:70:LYS:HG3	1.84	0.76
2:B:139:THR:HG23	2:B:140:PRO:CD	2.12	0.76
2:B:23:GLN:CG	2:B:133:PRO:HG3	2.14	0.76
1:A:331:LYS:HE2	1:A:333:GLY:HA2	1.68	0.76
2:B:261:VAL:HG13	2:B:276:VAL:CG1	2.14	0.76
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LYS:HD3	2:B:69:THR:HB	1.67	0.76
1:A:23:GLN:CD	1:A:23:GLN:H	1.93	0.76
1:A:104:LYS:HD3	1:A:192:ASP:O	1.84	0.76
1:A:354:TYR:HB2	1:A:374:LYS:HZ1	1.48	0.76
2:B:23:GLN:HG2	2:B:133:PRO:HG3	1.68	0.76
2:B:221:HIS:N	2:B:221:HIS:CD2	2.53	0.76
1:A:156:SER:H	1:A:157:PRO:HD2	1.51	0.76
1:A:193:LEU:HB3	1:A:197:GLN:HB3	1.65	0.76
2:B:131:THR:OG1	2:B:143:ARG:HG2	1.86	0.75
1:A:286:THR:HG22	1:A:287:LYS:N	2.00	0.75
2:B:267:ALA:HB2	2:B:426:TRP:CZ2	2.21	0.75
1:A:29:GLU:HG3	1:A:30:LYS:H	1.51	0.75
1:A:399:GLU:CD	1:A:402:TRP:HE1	1.92	0.75
2:B:76:ASP:OD1	2:B:78:ARG:NE	2.17	0.75
2:B:282:LEU:O	2:B:293:ILE:HD11	1.85	0.75
1:A:101:LYS:O	1:A:103:LYS:HG2	1.86	0.75
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.20	0.75
1:A:132:ILE:HG22	1:A:142:ILE:HB	1.68	0.75
1:A:286:THR:CG2	1:A:287:LYS:N	2.49	0.75
2:B:91:GLN:HE21	2:B:91:GLN:C	1.95	0.75
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.69	0.75
1:A:195:ILE:HD12	1:A:199:ARG:HH21	1.51	0.75
1:A:53:GLU:HG3	1:A:54:ASN:N	2.00	0.75
1:A:34:LEU:HD21	1:A:62:ALA:CB	2.16	0.74
1:A:209:LEU:HD22	1:A:214:LEU:HD12	1.69	0.74
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.12	0.74
2:B:271:TYR:HB3	2:B:274:ILE:HD13	1.67	0.74
1:A:331:LYS:HE3	1:A:364:ASP:OD1	1.87	0.74
2:B:139:THR:HG22	2:B:140:PRO:CD	2.14	0.74
2:B:351:THR:HG22	2:B:351:THR:O	1.87	0.74
2:B:31:ILE:HG22	2:B:35:VAL:CG2	2.18	0.74
1:A:84:THR:CG2	1:A:154:LYS:HE2	2.17	0.74
2:B:33:ALA:O	2:B:37:ILE:HG13	1.88	0.74
1:A:108:VAL:CG1	1:A:188:TYR:CG	2.70	0.73
1:A:222:GLN:O	1:A:223:LYS:C	2.31	0.73
1:A:339:TYR:O	1:A:340:GLN:HG3	1.88	0.73
2:B:69:THR:HG23	2:B:70:LYS:N	2.03	0.73
2:B:358:ARG:CG	2:B:359:GLY:H	1.96	0.73
1:A:108:VAL:HG12	1:A:188:TYR:CB	2.18	0.73
1:A:132:ILE:HD13	1:A:133:PRO:HD2	1.70	0.73
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:ASP:CG	2:B:78:ARG:HH21	1.96	0.73
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.22	0.73
1:A:240:THR:CG2	1:A:241:VAL:H	2.00	0.73
2:B:244:ILE:HD13	2:B:244:ILE:H	1.53	0.73
2:B:393:ILE:HG12	2:B:398:TRP:HB2	1.70	0.73
2:B:61:PHE:HE1	2:B:76:ASP:HB2	1.54	0.73
2:B:369:THR:O	2:B:373:GLN:HG3	1.89	0.73
1:A:64:LYS:HA	1:A:66:LYS:HD3	1.70	0.73
2:B:80:LEU:HD11	2:B:124:PHE:HZ	1.54	0.73
2:B:277:ARG:H	2:B:277:ARG:HD3	1.53	0.73
2:B:302:GLU:O	2:B:306:ASN:HB2	1.89	0.73
2:B:380:ILE:HD12	2:B:380:ILE:H	1.54	0.73
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.23	0.72
1:A:442:VAL:HG12	1:A:496:VAL:O	1.87	0.72
1:A:17:ASP:O	1:A:83:ARG:HD3	1.89	0.72
1:A:64:LYS:HG3	1:A:66:LYS:HG3	1.71	0.72
2:B:358:ARG:CA	2:B:362:THR:HB	2.19	0.72
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.71	0.72
1:A:427:TYR:CE1	1:A:525:LEU:HD13	2.25	0.72
1:A:483:TYR:HB2	1:A:521:ILE:HG12	1.70	0.72
1:A:64:LYS:O	1:A:64:LYS:CG	2.37	0.72
1:A:84:THR:HG21	1:A:154:LYS:HB3	1.71	0.72
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.69	0.72
1:A:356:ARG:NE	1:A:358:ARG:HG3	2.05	0.72
2:B:278:GLN:NE2	2:B:297:GLU:HG3	2.04	0.72
2:B:311:LYS:O	2:B:313:PRO:HD3	1.89	0.72
2:B:257:ILE:HG23	2:B:283:LEU:HD21	1.71	0.72
1:A:3:SER:OG	1:A:5:ILE:HG13	1.90	0.71
2:B:96:HIS:HD1	2:B:181:TYR:HE2	1.38	0.71
2:B:297:GLU:CG	2:B:298:GLU:H	2.01	0.71
2:B:377:THR:O	2:B:378:GLU:C	2.30	0.71
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.54	0.71
1:A:30:LYS:O	1:A:33:ALA:HB3	1.91	0.71
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.25	0.71
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.56	0.71
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.71	0.71
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.26	0.71
2:B:109:LEU:HB2	2:B:218:ASP:OD2	1.91	0.71
1:A:50:ILE:HA	5:A:1095:HOH:O	1.91	0.71
2:B:109:LEU:HD13	2:B:206:ARG:HG2	1.73	0.71
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:TYR:CD1	2:B:150:PRO:HB3	2.26	0.71
2:B:365:VAL:HG12	2:B:365:VAL:O	1.90	0.70
2:B:174:GLN:HA	2:B:174:GLN:NE2	2.06	0.70
1:A:96:HIS:HB3	1:A:382:ILE:CD1	2.21	0.70
1:A:219:LYS:O	1:A:220:LYS:C	2.34	0.70
2:B:1:PRO:HD3	2:B:117:SER:CA	2.20	0.70
2:B:109:LEU:HB2	2:B:218:ASP:CG	2.17	0.70
2:B:266:TRP:CD1	2:B:422:LEU:HD23	2.27	0.70
2:B:278:GLN:NE2	2:B:297:GLU:CG	2.54	0.70
2:B:297:GLU:HG3	2:B:298:GLU:N	2.02	0.70
2:B:332:GLN:O	2:B:424:LYS:HE2	1.90	0.70
1:A:64:LYS:O	1:A:64:LYS:HG2	1.92	0.70
2:B:339:TYR:CD1	2:B:375:ILE:HD11	2.26	0.70
1:A:55:PRO:HG2	1:A:143:ARG:HH22	1.57	0.70
2:B:1:PRO:O	2:B:2:ILE:HD13	1.91	0.70
1:A:124:PHE:CE2	1:A:153:TRP:CZ2	2.79	0.69
1:A:290:THR:O	1:A:290:THR:HG22	1.91	0.69
2:B:168:LEU:HD11	2:B:180:ILE:HG21	1.74	0.69
1:A:34:LEU:HD12	1:A:132:ILE:HG12	1.75	0.69
1:A:326:ILE:HD12	1:A:326:ILE:N	2.07	0.69
2:B:340:GLN:HE21	2:B:340:GLN:N	1.90	0.69
2:B:69:THR:HG23	2:B:70:LYS:H	1.57	0.69
1:A:491:LEU:O	1:A:529:GLU:HB3	1.93	0.69
1:A:84:THR:HG23	1:A:154:LYS:CE	2.19	0.69
1:A:363:ASN:ND2	1:A:365:VAL:H	1.90	0.69
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.28	0.69
2:B:271:TYR:HB3	2:B:274:ILE:CD1	2.22	0.69
2:B:295:LEU:O	2:B:295:LEU:CG	2.41	0.69
2:B:241:VAL:O	2:B:243:PRO:HD3	1.91	0.69
1:A:108:VAL:HG23	1:A:222:GLN:HB3	1.75	0.69
1:A:128:THR:HB	1:A:146:TYR:HB2	1.75	0.69
1:A:197:GLN:O	1:A:200:THR:HG22	1.92	0.69
2:B:260:LEU:HG	2:B:264:LEU:CD1	2.23	0.69
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.18	0.69
1:A:74:LEU:HD23	1:A:74:LEU:O	1.92	0.69
1:A:388:LYS:HE2	5:A:1092:HOH:O	1.93	0.69
1:A:395:LYS:HA	1:A:414:TRP:HZ2	1.56	0.69
1:A:483:TYR:HB2	1:A:521:ILE:HG13	1.74	0.69
2:B:376:THR:HG22	2:B:380:ILE:HD11	1.74	0.69
2:B:393:ILE:HG23	2:B:416:PHE:HD1	1.57	0.68
1:A:420:PRO:HA	1:A:421:PRO:C	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PRO:HB3	2:B:255:ASN:ND2	2.08	0.68
1:A:76:ASP:OD2	1:A:78:ARG:NH1	2.27	0.68
1:A:87:PHE:CE2	1:A:159:ILE:HD11	2.29	0.68
2:B:31:ILE:C	2:B:35:VAL:HG23	2.18	0.68
1:A:97:PRO:HA	1:A:100:LEU:CD1	2.24	0.68
1:A:282:LEU:C	1:A:284:ARG:H	2.02	0.68
2:B:110:ASP:C	2:B:110:ASP:OD1	2.36	0.68
2:B:181:TYR:HD1	2:B:182:GLN:N	1.92	0.68
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.11	0.68
2:B:111:VAL:O	2:B:113:ASP:N	2.27	0.68
2:B:125:ARG:O	2:B:127:TYR:N	2.27	0.68
2:B:248:GLU:HB2	5:B:1086:HOH:O	1.95	0.67
1:A:34:LEU:HD22	1:A:73:LYS:HB2	1.76	0.67
1:A:96:HIS:HD1	1:A:97:PRO:N	1.92	0.67
1:A:193:LEU:HD22	1:A:197:GLN:NE2	2.09	0.67
2:B:206:ARG:HH11	2:B:206:ARG:CB	2.07	0.67
1:A:17:ASP:OD2	1:A:56:TYR:HE2	1.77	0.67
1:A:64:LYS:HB3	1:A:71:TRP:CD1	2.29	0.67
1:A:406:TRP:CZ2	2:B:418:ASN:O	2.47	0.67
1:A:422:LEU:CD2	1:A:424:LYS:HD3	2.24	0.67
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.28	0.67
2:B:254:VAL:O	2:B:258:GLN:HG3	1.95	0.67
1:A:95:PRO:HG2	1:A:229:TRP:HH2	1.59	0.67
1:A:497:THR:CG2	1:A:499:SER:HB3	2.25	0.67
1:A:87:PHE:HE2	1:A:159:ILE:HD11	1.59	0.67
2:B:175:ASN:H	2:B:175:ASN:ND2	1.92	0.67
1:A:453:GLY:O	1:A:454:LYS:HD3	1.95	0.66
1:A:96:HIS:HD1	1:A:98:ALA:H	1.42	0.66
1:A:430:GLU:HB2	1:A:532:TYR:HB2	1.76	0.66
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.34	0.66
2:B:260:LEU:CG	2:B:264:LEU:HD11	2.25	0.66
1:A:38:CYS:HB3	1:A:144:TYR:HE1	1.58	0.66
2:B:69:THR:CG2	2:B:70:LYS:H	2.08	0.66
2:B:168:LEU:CD1	2:B:180:ILE:HG21	2.25	0.66
2:B:206:ARG:HE	2:B:218:ASP:CB	1.99	0.66
2:B:277:ARG:O	2:B:281:LYS:HG3	1.96	0.66
2:B:326:ILE:CG2	2:B:342:TYR:HE1	2.08	0.66
1:A:108:VAL:HG11	1:A:188:TYR:CD2	2.30	0.66
1:A:298:GLU:N	1:A:298:GLU:CD	2.53	0.66
2:B:206:ARG:NH1	2:B:206:ARG:CB	2.58	0.66
1:A:363:ASN:HB3	1:A:366:LYS:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:PRO:O	2:B:178:ILE:N	2.28	0.66
1:A:435:VAL:HA	2:B:290:THR:OG1	1.96	0.65
2:B:340:GLN:HG2	2:B:427:TYR:CE1	2.31	0.65
2:B:341:ILE:O	2:B:349:LEU:HB2	1.96	0.65
1:A:29:GLU:CG	1:A:30:LYS:H	2.08	0.65
2:B:194:GLU:O	2:B:195:ILE:C	2.37	0.65
2:B:252:TRP:O	2:B:292:VAL:HG13	1.95	0.65
1:A:254:VAL:HG23	1:A:293:ILE:CD1	2.26	0.65
1:A:254:VAL:O	1:A:258:GLN:HG3	1.96	0.65
1:A:340:GLN:HA	1:A:351:THR:HA	1.78	0.65
2:B:100:LEU:HD13	2:B:179:VAL:HG21	1.79	0.65
2:B:202:ILE:O	2:B:205:LEU:N	2.30	0.65
2:B:358:ARG:H	2:B:358:ARG:HE	1.43	0.65
2:B:376:THR:CG2	2:B:380:ILE:HD11	2.26	0.65
2:B:308:GLU:HG3	2:B:309:ILE:N	2.12	0.65
2:B:364:ASP:C	2:B:366:LYS:H	2.05	0.65
1:A:539:HIS:O	1:A:542:ILE:HG12	1.97	0.65
2:B:60:VAL:CG1	2:B:130:PHE:HB2	2.27	0.65
1:A:434:ILE:HG12	1:A:530:LYS:HB3	1.79	0.65
2:B:115:TYR:HE2	2:B:157:PRO:CA	2.09	0.65
2:B:220:LYS:HE3	2:B:231:GLY:CA	2.21	0.65
1:A:27:THR:CB	1:A:29:GLU:HG2	2.27	0.65
1:A:28:GLU:HA	1:A:31:ILE:HG23	1.78	0.65
1:A:64:LYS:C	1:A:66:LYS:N	2.50	0.65
1:A:64:LYS:C	1:A:66:LYS:H	2.05	0.65
2:B:324:ASP:O	2:B:343:GLN:HG2	1.96	0.65
1:A:10:VAL:HG21	1:A:153:TRP:CH2	2.31	0.65
1:A:94:ILE:HG12	1:A:230:MET:HE2	1.79	0.65
2:B:232:TYR:HE2	2:B:234:LEU:HD21	1.60	0.65
1:A:254:VAL:HG13	1:A:283:LEU:HD13	1.79	0.65
1:A:356:ARG:HD2	1:A:362:THR:OG1	1.97	0.65
1:A:398:TRP:CZ2	1:A:411:ILE:HD12	2.32	0.65
1:A:397:THR:CG2	1:A:424:LYS:HA	2.23	0.64
2:B:66:LYS:HD3	2:B:69:THR:CB	2.27	0.64
2:B:191:SER:OG	2:B:198:HIS:ND1	2.30	0.64
1:A:542:ILE:O	1:A:546:GLU:HB2	1.98	0.64
2:B:299:ALA:HA	2:B:302:GLU:HB2	1.78	0.64
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.32	0.64
1:A:406:TRP:CE3	2:B:420:PRO:HD2	2.33	0.64
2:B:78:ARG:HD3	2:B:412:PRO:O	1.96	0.64
2:B:161:GLN:O	2:B:162:SER:C	2.40	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LEU:O	2:B:100:LEU:HD12	1.98	0.64
1:A:108:VAL:CG2	1:A:222:GLN:HB3	2.27	0.64
2:B:76:ASP:CG	2:B:76:ASP:O	2.39	0.64
2:B:342:TYR:HD1	2:B:342:TYR:O	1.81	0.64
2:B:426:TRP:CD1	2:B:427:TYR:H	2.15	0.64
1:A:95:PRO:HG2	1:A:229:TRP:CH2	2.33	0.63
2:B:358:ARG:O	2:B:362:THR:CB	2.45	0.63
2:B:364:ASP:O	2:B:366:LYS:N	2.31	0.63
1:A:64:LYS:HG3	1:A:66:LYS:CG	2.29	0.63
2:B:85:GLN:O	2:B:89:GLU:HB2	1.98	0.63
1:A:130:PHE:HD1	1:A:130:PHE:H	1.46	0.63
1:A:224:GLU:O	1:A:226:PRO:O	2.17	0.63
1:A:301:LEU:O	1:A:304:ALA:HB3	1.97	0.63
2:B:85:GLN:CG	2:B:154:LYS:HB3	2.22	0.63
2:B:197:GLN:O	2:B:200:THR:HB	1.97	0.63
1:A:175:ASN:N	1:A:176:PRO:CD	2.60	0.63
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.34	0.63
1:A:443:ASP:HB2	1:A:548:VAL:HG23	1.81	0.63
1:A:539:HIS:O	1:A:542:ILE:HG23	1.98	0.63
2:B:273:GLY:C	2:B:274:ILE:HD12	2.23	0.63
2:B:220:LYS:HG3	2:B:231:GLY:HA3	1.79	0.63
1:A:99:GLY:HA3	1:A:382:ILE:CG2	2.29	0.63
1:A:163:SER:O	1:A:167:ILE:HG12	1.99	0.63
2:B:5:ILE:HB	2:B:119:PRO:HD2	1.80	0.63
2:B:221:HIS:HD1	2:B:229:TRP:HB2	1.61	0.62
1:A:276:VAL:HG12	1:A:276:VAL:O	1.99	0.62
1:A:51:GLY:O	1:A:53:GLU:N	2.31	0.62
1:A:319:TYR:OH	1:A:385:LYS:HD3	1.98	0.62
2:B:342:TYR:CD1	2:B:342:TYR:C	2.77	0.62
1:A:55:PRO:HG2	1:A:143:ARG:NH2	2.14	0.62
1:A:198:HIS:CD2	1:A:202:ILE:HD11	2.35	0.62
2:B:275:LYS:HA	2:B:277:ARG:NH2	2.14	0.62
2:B:223:LYS:O	2:B:224:GLU:OE1	2.17	0.62
2:B:379:SER:O	2:B:380:ILE:C	2.43	0.62
1:A:254:VAL:H	1:A:293:ILE:HD13	1.64	0.62
1:A:297:GLU:CD	1:A:297:GLU:H	2.07	0.62
2:B:169:GLU:C	2:B:171:PHE:H	2.06	0.62
1:A:142:ILE:HD12	1:A:142:ILE:H	1.63	0.62
1:A:319:TYR:CD1	1:A:325:LEU:HD21	2.35	0.62
2:B:65:LYS:HD3	2:B:72:ARG:HD2	1.80	0.62
2:B:175:ASN:ND2	2:B:175:ASN:N	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:LYS:CE	2:B:231:GLY:HA2	2.22	0.61
1:A:32:LYS:HA	1:A:35:VAL:CG2	2.31	0.61
1:A:244:ILE:HG23	1:A:263:LYS:HE2	1.82	0.61
1:A:434:ILE:HD13	1:A:494:ASN:ND2	2.14	0.61
1:A:479:LEU:HD21	1:A:502:ALA:HA	1.83	0.61
2:B:24:TRP:HE1	2:B:399:GLU:HG3	1.63	0.61
2:B:90:VAL:O	2:B:91:GLN:C	2.43	0.61
2:B:115:TYR:O	2:B:117:SER:N	2.29	0.61
1:A:33:ALA:O	1:A:37:ILE:HG12	2.01	0.61
1:A:189:VAL:HG21	1:A:205:LEU:HD23	1.81	0.61
1:A:434:ILE:HB	1:A:494:ASN:HD21	1.63	0.61
1:A:493:VAL:C	1:A:494:ASN:HD22	2.09	0.61
1:A:360:ALA:HA	1:A:514:GLU:CD	2.26	0.61
2:B:195:ILE:HG13	2:B:199:ARG:CD	2.30	0.61
1:A:97:PRO:HA	1:A:100:LEU:HG	1.83	0.61
1:A:142:ILE:HD12	1:A:142:ILE:N	2.16	0.61
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.36	0.61
2:B:195:ILE:O	2:B:197:GLN:N	2.33	0.61
2:B:111:VAL:C	2:B:113:ASP:N	2.58	0.61
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.83	0.61
2:B:281:LYS:O	2:B:284:ARG:HB2	1.99	0.61
1:A:164:MET:HE2	1:A:187:LEU:HD13	1.82	0.60
2:B:402:TRP:CH2	2:B:411:ILE:HD12	2.36	0.60
1:A:2:ILE:HG22	1:A:3:SER:N	2.14	0.60
1:A:98:ALA:CB	1:A:350:LYS:HB2	2.31	0.60
1:A:121:ASP:C	1:A:123:ASP:H	2.09	0.60
1:A:122:GLU:HA	1:A:125:ARG:CD	2.31	0.60
1:A:226:PRO:HB2	1:A:233:GLU:HG2	1.84	0.60
2:B:111:VAL:O	2:B:112:GLY:C	2.44	0.60
2:B:160:PHE:O	2:B:161:GLN:O	2.19	0.60
2:B:252:TRP:HA	2:B:252:TRP:CE3	2.37	0.60
1:A:417:VAL:HG12	1:A:419:THR:H	1.66	0.60
2:B:115:TYR:OH	2:B:184:MET:O	2.16	0.60
2:B:221:HIS:N	2:B:221:HIS:HD2	1.98	0.60
2:B:282:LEU:HD11	2:B:293:ILE:HG12	1.83	0.60
1:A:56:TYR:N	1:A:56:TYR:CD1	2.70	0.60
1:A:253:THR:OG1	1:A:290:THR:HA	2.01	0.60
2:B:242:GLN:CG	2:B:242:GLN:O	2.49	0.60
1:A:23:GLN:H	1:A:23:GLN:NE2	1.98	0.60
1:A:317:VAL:HG21	1:A:347:LYS:HD3	1.83	0.60
2:B:391:LEU:HB3	2:B:393:ILE:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:LEU:CD1	2:B:159:ILE:HB	2.32	0.60
2:B:349:LEU:HD12	2:B:383:TRP:CZ2	2.37	0.60
1:A:286:THR:CG2	1:A:287:LYS:H	2.14	0.60
2:B:30:LYS:HG3	2:B:62:ALA:HB3	1.82	0.60
1:A:282:LEU:C	1:A:284:ARG:N	2.59	0.59
2:B:252:TRP:HA	2:B:252:TRP:HE3	1.66	0.59
2:B:336:GLN:HA	2:B:354:TYR:O	2.02	0.59
1:A:126:LYS:HG3	1:A:127:TYR:CE2	2.38	0.59
2:B:194:GLU:O	2:B:195:ILE:O	2.20	0.59
2:B:198:HIS:O	2:B:201:LYS:N	2.35	0.59
2:B:244:ILE:HG12	2:B:244:ILE:O	2.01	0.59
1:A:433:PRO:HB3	2:B:255:ASN:HD22	1.65	0.59
2:B:183:TYR:CD2	2:B:183:TYR:C	2.78	0.59
2:B:282:LEU:HD11	2:B:294:PRO:HD2	1.83	0.59
2:B:332:GLN:HA	2:B:332:GLN:OE1	2.01	0.59
1:A:109:LEU:HD21	1:A:202:ILE:CG2	2.33	0.59
2:B:38:CYS:O	2:B:39:THR:C	2.45	0.59
2:B:66:LYS:HB3	2:B:69:THR:HG22	1.84	0.59
2:B:80:LEU:HD11	2:B:124:PHE:CZ	2.36	0.59
1:A:73:LYS:NZ	1:A:130:PHE:CE2	2.70	0.59
1:A:116:PHE:O	1:A:148:VAL:HG21	2.03	0.59
2:B:326:ILE:HB	2:B:342:TYR:CD1	2.38	0.59
1:A:128:THR:CB	1:A:146:TYR:HB2	2.33	0.59
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.38	0.59
1:A:490:GLY:C	1:A:492:GLU:H	2.11	0.59
2:B:69:THR:CG2	2:B:70:LYS:N	2.63	0.59
2:B:277:ARG:H	2:B:277:ARG:CD	2.11	0.59
1:A:254:VAL:H	1:A:293:ILE:CD1	2.16	0.59
2:B:13:LYS:HG3	2:B:14:PRO:HD2	1.85	0.59
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.38	0.59
2:B:282:LEU:HG	2:B:293:ILE:HD13	1.84	0.59
2:B:385:LYS:HB3	2:B:385:LYS:NZ	2.17	0.59
1:A:108:VAL:HA	1:A:188:TYR:HA	1.84	0.59
1:A:543:GLY:C	2:B:284:ARG:HA	2.28	0.59
2:B:10:VAL:HG22	2:B:88:TRP:CH2	2.38	0.59
2:B:242:GLN:O	2:B:242:GLN:HG2	2.02	0.59
1:A:356:ARG:HG3	1:A:367:GLN:HG2	1.85	0.58
1:A:58:THR:HG22	1:A:76:ASP:O	2.03	0.58
1:A:134:SER:HB3	1:A:138:GLU:HB3	1.84	0.58
1:A:513:SER:N	1:A:519:ASN:HD21	2.01	0.58
2:B:206:ARG:HB3	2:B:206:ARG:CZ	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TRP:HD1	2:B:422:LEU:HD23	1.65	0.58
1:A:261:VAL:HG22	1:A:279:LEU:HD22	1.86	0.58
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.38	0.58
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.38	0.58
1:A:200:THR:HG23	1:A:201:LYS:N	2.18	0.58
1:A:229:TRP:CE3	1:A:234:LEU:HD11	2.37	0.58
1:A:410:TRP:HB3	2:B:365:VAL:HG21	1.85	0.58
1:A:430:GLU:OE1	1:A:430:GLU:HA	2.03	0.58
2:B:46:LYS:NZ	2:B:116:PHE:HD2	2.01	0.58
2:B:198:HIS:O	2:B:199:ARG:C	2.44	0.58
2:B:340:GLN:N	2:B:340:GLN:NE2	2.51	0.58
1:A:61:PHE:HB2	1:A:74:LEU:O	2.04	0.58
1:A:342:TYR:OH	1:A:390:LYS:HD2	2.04	0.58
1:A:132:ILE:HG22	1:A:142:ILE:O	2.04	0.58
1:A:24:TRP:O	1:A:25:PRO:C	2.45	0.58
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.39	0.58
1:A:298:GLU:CD	1:A:298:GLU:H	2.11	0.58
1:A:130:PHE:HD1	1:A:130:PHE:N	2.02	0.58
1:A:245:VAL:H	1:A:263:LYS:NZ	2.01	0.58
1:A:506:ILE:HG21	1:A:533:LEU:CD1	2.33	0.58
2:B:217:PRO:O	2:B:219:LYS:N	2.36	0.57
2:B:366:LYS:O	2:B:370:GLU:HG3	2.04	0.57
1:A:363:ASN:HD22	1:A:365:VAL:H	1.52	0.57
2:B:149:LEU:HD23	2:B:149:LEU:H	1.69	0.57
2:B:206:ARG:NH2	2:B:216:THR:O	2.37	0.57
1:A:402:TRP:HE3	1:A:402:TRP:O	1.88	0.57
1:A:162:SER:O	1:A:163:SER:C	2.46	0.57
2:B:192:ASP:O	2:B:193:LEU:HD23	2.03	0.57
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.68	0.57
2:B:168:LEU:O	2:B:172:LYS:HG3	2.04	0.57
2:B:395:LYS:O	2:B:399:GLU:HB2	2.04	0.57
2:B:80:LEU:HD12	2:B:80:LEU:O	2.03	0.57
2:B:161:GLN:O	2:B:164:MET:N	2.35	0.57
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.39	0.57
1:A:179:VAL:HG21	4:A:701:IET:N3	2.20	0.57
1:A:203:GLU:OE2	1:A:207:GLN:NE2	2.37	0.57
1:A:353:LYS:O	1:A:374:LYS:NZ	2.38	0.57
1:A:447:ASN:CB	1:A:450:THR:HB	2.32	0.57
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.19	0.57
1:A:195:ILE:HG13	1:A:196:GLY:N	2.19	0.57
1:A:411:ILE:HD13	1:A:411:ILE:N	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:ARG:HH11	2:B:206:ARG:HB2	1.70	0.57
1:A:497:THR:HG21	1:A:499:SER:HB3	1.87	0.57
2:B:238:LYS:O	2:B:240:THR:N	2.38	0.57
2:B:241:VAL:C	2:B:243:PRO:HD3	2.29	0.57
1:A:77:PHE:CZ	1:A:150:PRO:HB3	2.40	0.56
1:A:254:VAL:N	1:A:293:ILE:HD13	2.20	0.56
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.87	0.56
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.41	0.56
2:B:253:THR:HA	2:B:292:VAL:HA	1.86	0.56
2:B:376:THR:O	2:B:379:SER:HB2	2.05	0.56
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.87	0.56
1:A:438:GLU:OE2	1:A:461:LYS:HB2	2.05	0.56
1:A:492:GLU:OE2	1:A:530:LYS:HD2	2.05	0.56
1:A:524:GLN:O	1:A:528:LYS:HG2	2.06	0.56
2:B:149:LEU:HD23	2:B:149:LEU:N	2.20	0.56
2:B:198:HIS:O	2:B:200:THR:N	2.39	0.56
2:B:201:LYS:HE2	2:B:201:LYS:CA	2.34	0.56
1:A:7:THR:HG22	1:A:119:PRO:CB	2.36	0.56
1:A:182:GLN:HB3	5:A:1044:HOH:O	2.05	0.56
1:A:28:GLU:HA	1:A:31:ILE:HG21	1.87	0.56
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.87	0.56
1:A:32:LYS:HA	1:A:35:VAL:HG23	1.86	0.56
1:A:218:ASP:O	1:A:221:HIS:CB	2.50	0.56
1:A:454:LYS:HB2	1:A:552:VAL:CG1	2.11	0.56
1:A:511:ASP:OD1	1:A:512:LYS:HG2	2.05	0.56
2:B:402:TRP:CZ3	2:B:411:ILE:HD12	2.40	0.56
1:A:180:ILE:N	1:A:180:ILE:HD12	2.21	0.56
1:A:545:ASN:O	1:A:549:ASP:OD2	2.24	0.56
2:B:279:LEU:HD13	2:B:299:ALA:HB1	1.87	0.56
1:A:130:PHE:N	1:A:130:PHE:CD1	2.73	0.56
1:A:198:HIS:CE1	1:A:202:ILE:HD11	2.40	0.56
1:A:369:THR:O	1:A:370:GLU:C	2.49	0.56
1:A:460:ASN:C	1:A:462:GLY:H	2.14	0.56
2:B:13:LYS:HG2	2:B:14:PRO:O	2.06	0.56
1:A:96:HIS:HD1	1:A:96:HIS:C	2.13	0.56
1:A:101:LYS:O	1:A:102:LYS:C	2.49	0.56
2:B:328:GLU:HG2	2:B:390:LYS:HD3	1.86	0.56
1:A:244:ILE:HA	1:A:263:LYS:HE2	1.87	0.56
1:A:543:GLY:HA2	2:B:284:ARG:HA	1.88	0.56
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.41	0.56
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ALA:O	1:A:482:ILE:C	2.48	0.55
2:B:377:THR:HA	2:B:380:ILE:HD13	1.88	0.55
2:B:205:LEU:O	2:B:208:HIS:HB3	2.05	0.55
2:B:315:HIS:HB3	5:B:1076:HOH:O	2.06	0.55
1:A:324:ASP:OD2	1:A:324:ASP:N	2.38	0.55
2:B:393:ILE:HG23	2:B:416:PHE:CD1	2.41	0.55
1:A:339:TYR:CD1	1:A:375:ILE:HD11	2.41	0.55
2:B:332:GLN:OE1	2:B:424:LYS:HG2	2.06	0.55
1:A:3:SER:OG	1:A:4:PRO:HD2	2.05	0.55
1:A:277:ARG:HB2	1:A:336:GLN:CD	2.31	0.55
1:A:543:GLY:O	2:B:284:ARG:HA	2.07	0.55
1:A:426:TRP:O	1:A:427:TYR:HB3	2.06	0.55
1:A:183:TYR:N	1:A:186:ASP:O	2.40	0.55
2:B:342:TYR:HD1	2:B:342:TYR:C	2.14	0.55
1:A:51:GLY:C	1:A:53:GLU:H	2.13	0.55
1:A:86:ASP:OD2	1:A:86:ASP:N	2.40	0.55
1:A:112:GLY:O	1:A:115:TYR:CE2	2.60	0.55
1:A:226:PRO:CB	1:A:233:GLU:HG2	2.36	0.55
1:A:320:ASP:N	1:A:343:GLN:HE22	2.02	0.55
1:A:434:ILE:H	1:A:434:ILE:HD12	1.71	0.55
1:A:401:TRP:HA	1:A:401:TRP:CE3	2.42	0.55
1:A:1:PRO:HA	1:A:46:LYS:NZ	2.22	0.55
1:A:244:ILE:CG2	1:A:310:LEU:HD21	2.37	0.55
1:A:457:TYR:C	1:A:457:TYR:CD2	2.86	0.54
1:A:532:TYR:HE1	2:B:255:ASN:HD21	1.52	0.54
2:B:283:LEU:O	2:B:285:GLY:N	2.40	0.54
1:A:258:GLN:HE21	1:A:283:LEU:HD11	1.73	0.54
2:B:149:LEU:HB2	2:B:156:SER:HB3	1.89	0.54
2:B:345:PRO:HB2	2:B:346:PHE:HD1	1.72	0.54
2:B:168:LEU:CD2	2:B:209:LEU:HD21	2.38	0.54
1:A:106:VAL:HA	1:A:190:GLY:HA2	1.89	0.54
2:B:193:LEU:HD12	2:B:198:HIS:HA	1.90	0.54
1:A:509:GLN:N	1:A:510:PRO:HD3	2.21	0.54
2:B:100:LEU:HD13	2:B:179:VAL:CG2	2.38	0.54
2:B:169:GLU:O	2:B:171:PHE:N	2.34	0.54
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	2.95	0.54
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.36	0.54
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.90	0.54
1:A:325:LEU:HD13	1:A:383:TRP:CE3	2.42	0.54
1:A:339:TYR:C	1:A:340:GLN:HG3	2.33	0.54
2:B:156:SER:N	2:B:157:PRO:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:O	1:A:197:GLN:N	2.41	0.54
1:A:224:GLU:O	1:A:225:PRO:C	2.50	0.54
1:A:401:TRP:CZ3	1:A:509:GLN:NE2	2.76	0.54
2:B:160:PHE:O	2:B:161:GLN:C	2.49	0.54
2:B:183:TYR:O	2:B:184:MET:HB2	2.07	0.54
2:B:214:LEU:N	2:B:214:LEU:HD23	2.23	0.54
1:A:55:PRO:HG2	1:A:143:ARG:HH12	1.73	0.54
2:B:47:ILE:CG2	2:B:146:TYR:CD1	2.91	0.54
2:B:371:ALA:O	2:B:375:ILE:HD12	2.08	0.54
1:A:179:VAL:C	1:A:180:ILE:HD12	2.32	0.54
1:A:363:ASN:HB3	1:A:366:LYS:CG	2.38	0.54
1:A:434:ILE:HD13	1:A:494:ASN:HD21	1.73	0.54
1:A:450:THR:HG22	1:A:452:LEU:CG	2.38	0.54
2:B:12:LEU:CD1	2:B:83:ARG:O	2.53	0.54
2:B:180:ILE:CG2	2:B:187:LEU:HD22	2.37	0.54
2:B:358:ARG:O	2:B:359:GLY:C	2.51	0.54
1:A:373:GLN:HG2	2:B:394:GLN:NE2	2.23	0.53
2:B:183:TYR:CE2	2:B:184:MET:HE3	2.42	0.53
2:B:183:TYR:CE1	2:B:380:ILE:HG13	2.43	0.53
2:B:314:VAL:O	2:B:314:VAL:HG23	2.08	0.53
1:A:288:ALA:CB	1:A:291:GLU:CB	2.78	0.53
1:A:503:LEU:HD12	1:A:507:GLN:HG2	1.90	0.53
2:B:110:ASP:HA	2:B:186:ASP:HA	1.90	0.53
2:B:171:PHE:CE2	2:B:205:LEU:HA	2.42	0.53
2:B:220:LYS:HG3	2:B:231:GLY:CA	2.39	0.53
2:B:257:ILE:CD1	2:B:279:LEU:HG	2.38	0.53
2:B:326:ILE:HG22	2:B:327:ALA:N	2.23	0.53
2:B:331:LYS:HE3	2:B:364:ASP:OD1	2.08	0.53
1:A:47:ILE:HG22	1:A:146:TYR:HA	1.89	0.53
1:A:82:LYS:O	1:A:82:LYS:HD3	2.08	0.53
1:A:272:PRO:O	1:A:274:ILE:N	2.41	0.53
1:A:401:TRP:HA	1:A:401:TRP:HE3	1.72	0.53
1:A:108:VAL:HG12	1:A:188:TYR:HA	1.90	0.53
2:B:205:LEU:O	2:B:208:HIS:N	2.35	0.53
2:B:248:GLU:O	2:B:249:LYS:C	2.52	0.53
2:B:261:VAL:O	2:B:265:ASN:HB2	2.08	0.53
1:A:253:THR:HG22	1:A:256:ASP:OD2	2.08	0.53
1:A:369:THR:O	1:A:372:VAL:N	2.42	0.53
2:B:32:LYS:O	2:B:36:GLU:HG3	2.09	0.53
2:B:73:LYS:HE2	2:B:75:VAL:CG2	2.39	0.53
2:B:116:PHE:HE1	2:B:151:GLN:HG3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LEU:HD13	2:B:180:ILE:HD12	1.91	0.53
2:B:183:TYR:CE2	2:B:184:MET:CE	2.92	0.53
1:A:43:LYS:C	1:A:45:GLY:H	2.16	0.53
1:A:201:LYS:HD3	1:A:204:GLU:OE1	2.09	0.53
2:B:111:VAL:O	2:B:114:ALA:N	2.36	0.53
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.91	0.53
1:A:12:LEU:HD21	1:A:127:TYR:CD1	2.44	0.53
1:A:279:LEU:N	1:A:302:GLU:OE2	2.32	0.53
1:A:458:VAL:HG23	1:A:551:LEU:HD11	1.90	0.53
2:B:57:ASN:C	2:B:57:ASN:ND2	2.66	0.53
1:A:94:ILE:HD12	1:A:94:ILE:N	2.24	0.53
2:B:150:PRO:O	2:B:156:SER:OG	2.19	0.53
1:A:84:THR:O	1:A:154:LYS:NZ	2.33	0.53
2:B:164:MET:O	2:B:166:LYS:N	2.42	0.53
2:B:174:GLN:HE21	2:B:174:GLN:CA	2.11	0.53
2:B:366:LYS:HG3	2:B:405:TYR:CE2	2.44	0.53
1:A:194:GLU:O	1:A:196:GLY:N	2.42	0.52
1:A:244:ILE:HG23	1:A:263:LYS:HG2	1.89	0.52
1:A:398:TRP:O	1:A:400:THR:N	2.42	0.52
1:A:179:VAL:HG11	4:A:701:IET:N3	2.25	0.52
1:A:331:LYS:HG2	1:A:333:GLY:H	1.75	0.52
1:A:402:TRP:CE3	1:A:402:TRP:C	2.86	0.52
1:A:363:ASN:HD22	1:A:365:VAL:N	2.08	0.52
1:A:545:ASN:ND2	1:A:549:ASP:OD2	2.42	0.52
2:B:421:PRO:HG2	2:B:422:LEU:H	1.74	0.52
1:A:19:PRO:O	1:A:56:TYR:CB	2.49	0.52
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.40	0.52
1:A:275:LYS:O	1:A:276:VAL:HG23	2.09	0.52
1:A:331:LYS:HE2	1:A:333:GLY:CA	2.36	0.52
1:A:434:ILE:HD12	1:A:434:ILE:N	2.24	0.52
2:B:183:TYR:C	2:B:183:TYR:HD2	2.17	0.52
2:B:263:LYS:HB3	2:B:426:TRP:CE3	2.45	0.52
2:B:277:ARG:HA	2:B:280:SER:OG	2.10	0.52
1:A:254:VAL:HA	1:A:257:ILE:CG2	2.32	0.52
2:B:282:LEU:O	2:B:293:ILE:CD1	2.55	0.52
1:A:120:LEU:O	1:A:121:ASP:C	2.52	0.52
1:A:485:ALA:O	1:A:486:LEU:C	2.50	0.52
1:A:540:LYS:HD3	2:B:265:ASN:ND2	2.21	0.52
2:B:56:TYR:O	2:B:57:ASN:HB2	2.10	0.52
2:B:149:LEU:HD13	2:B:159:ILE:HB	1.91	0.52
2:B:278:GLN:HG2	2:B:299:ALA:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG12	1:A:188:TYR:CA	2.40	0.52
1:A:121:ASP:O	1:A:123:ASP:N	2.41	0.52
1:A:139:THR:C	1:A:141:GLY:N	2.65	0.52
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.45	0.52
2:B:268:SER:HA	2:B:271:TYR:O	2.09	0.52
2:B:23:GLN:HE21	2:B:24:TRP:N	2.07	0.52
2:B:46:LYS:CE	2:B:116:PHE:HD2	2.23	0.52
2:B:216:THR:C	2:B:218:ASP:H	2.17	0.52
2:B:217:PRO:C	2:B:219:LYS:H	2.18	0.52
2:B:391:LEU:HB3	2:B:393:ILE:CG2	2.39	0.52
1:A:208:HIS:O	1:A:212:TRP:HD1	1.91	0.52
1:A:371:ALA:O	1:A:375:ILE:HD13	2.10	0.52
2:B:376:THR:HG21	2:B:410:TRP:CH2	2.45	0.52
1:A:96:HIS:CE1	1:A:98:ALA:H	2.28	0.52
1:A:271:TYR:CE2	1:A:314:VAL:HG23	2.45	0.52
1:A:276:VAL:O	1:A:276:VAL:CG1	2.58	0.52
1:A:456:GLY:HA2	1:A:484:LEU:HD23	1.91	0.52
2:B:17:ASP:O	2:B:18:GLY:O	2.27	0.52
1:A:164:MET:CE	1:A:187:LEU:HD13	2.39	0.51
2:B:16:MET:HE3	2:B:16:MET:HA	1.91	0.51
2:B:401:TRP:O	2:B:402:TRP:C	2.50	0.51
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.93	0.51
1:A:151:GLN:O	1:A:151:GLN:HG2	2.09	0.51
1:A:450:THR:HG22	1:A:452:LEU:HB2	1.92	0.51
2:B:295:LEU:O	2:B:295:LEU:CD2	2.59	0.51
1:A:258:GLN:HG2	1:A:283:LEU:HD21	1.91	0.51
1:A:329:ILE:HG12	1:A:391:LEU:CD2	2.40	0.51
2:B:247:PRO:HB2	2:B:252:TRP:CZ2	2.45	0.51
2:B:253:THR:H	2:B:256:ASP:HB2	1.74	0.51
2:B:379:SER:HA	2:B:383:TRP:CE3	2.45	0.51
1:A:406:TRP:HZ2	2:B:418:ASN:O	1.93	0.51
1:A:490:GLY:O	1:A:492:GLU:N	2.44	0.51
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.45	0.51
2:B:361:HIS:O	2:B:363:ASN:N	2.43	0.51
2:B:395:LYS:NZ	2:B:399:GLU:OE1	2.34	0.51
1:A:506:ILE:HG21	1:A:533:LEU:HD11	1.92	0.51
1:A:125:ARG:O	1:A:145:GLN:HG3	2.10	0.51
1:A:244:ILE:HG22	1:A:310:LEU:HD21	1.92	0.51
1:A:411:ILE:CD1	1:A:411:ILE:N	2.59	0.51
1:A:513:SER:CA	1:A:519:ASN:HD21	2.24	0.51
2:B:76:ASP:C	2:B:78:ARG:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:O	1:A:198:HIS:HB3	2.10	0.51
1:A:298:GLU:O	1:A:299:ALA:C	2.53	0.51
2:B:41:MET:HE3	2:B:46:LYS:HD3	1.92	0.51
2:B:263:LYS:HB3	2:B:426:TRP:HE3	1.75	0.51
1:A:32:LYS:O	1:A:36:GLU:HG2	2.11	0.51
1:A:64:LYS:O	1:A:65:LYS:C	2.52	0.51
1:A:408:ALA:CB	2:B:337:TRP:HH2	2.24	0.51
1:A:450:THR:O	1:A:451:LYS:C	2.53	0.51
2:B:63:ILE:O	2:B:71:TRP:HE3	1.93	0.51
2:B:124:PHE:O	2:B:125:ARG:C	2.54	0.51
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.46	0.51
2:B:104:LYS:HB2	2:B:192:ASP:CA	2.21	0.51
2:B:263:LYS:HE2	2:B:425:LEU:HD13	1.92	0.51
2:B:275:LYS:O	2:B:276:VAL:HG23	2.11	0.51
2:B:317:VAL:HG23	2:B:317:VAL:O	2.11	0.51
1:A:27:THR:C	1:A:29:GLU:H	2.18	0.51
1:A:55:PRO:HG2	1:A:143:ARG:NH1	2.26	0.51
2:B:66:LYS:CB	2:B:69:THR:CG2	2.89	0.51
2:B:84:THR:O	2:B:87:PHE:N	2.43	0.51
2:B:178:ILE:CG2	2:B:189:VAL:HG12	2.41	0.51
2:B:221:HIS:CD2	2:B:221:HIS:H	2.26	0.51
1:A:38:CYS:CB	1:A:144:TYR:HE1	2.23	0.50
1:A:162:SER:O	1:A:164:MET:N	2.44	0.50
1:A:318:TYR:CE1	4:A:701:IET:H16	2.45	0.50
1:A:480:GLN:O	1:A:481:ALA:C	2.54	0.50
1:A:501:TYR:O	1:A:505:ILE:HG12	2.11	0.50
2:B:295:LEU:O	2:B:295:LEU:HD23	2.11	0.50
2:B:380:ILE:HD11	2:B:386:THR:HG22	1.93	0.50
1:A:34:LEU:CG	1:A:62:ALA:HB2	2.40	0.50
2:B:8:VAL:O	2:B:10:VAL:HG23	2.11	0.50
2:B:257:ILE:CG2	2:B:283:LEU:HD21	2.40	0.50
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.77	0.50
1:A:450:THR:HG22	1:A:452:LEU:HG	1.93	0.50
1:A:457:TYR:C	1:A:457:TYR:HD2	2.18	0.50
1:A:490:GLY:C	1:A:492:GLU:N	2.70	0.50
2:B:49:LYS:HE2	2:B:142:ILE:HG22	1.93	0.50
2:B:278:GLN:HG3	2:B:299:ALA:HB2	1.92	0.50
1:A:28:GLU:CG	1:A:135:ILE:O	2.57	0.50
1:A:318:TYR:OH	4:A:701:IET:H15	2.11	0.50
1:A:360:ALA:O	1:A:514:GLU:HG2	2.11	0.50
2:B:257:ILE:HD11	2:B:279:LEU:HG	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:365:VAL:O	2:B:365:VAL:CG1	2.59	0.50
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.46	0.50
1:A:153:TRP:CE3	1:A:155:GLY:O	2.65	0.50
2:B:115:TYR:C	2:B:117:SER:H	2.19	0.50
2:B:325:LEU:HD23	2:B:343:GLN:HG3	1.94	0.50
1:A:55:PRO:CG	1:A:143:ARG:NH1	2.75	0.50
1:A:77:PHE:CZ	1:A:150:PRO:CB	2.94	0.50
1:A:391:LEU:O	1:A:393:ILE:N	2.41	0.50
2:B:79:GLU:C	2:B:81:ASN:N	2.64	0.50
2:B:156:SER:H	2:B:157:PRO:HD2	1.77	0.50
2:B:329:ILE:HD11	2:B:389:PHE:CD2	2.47	0.50
1:A:97:PRO:HA	1:A:100:LEU:CG	2.41	0.50
1:A:150:PRO:HG2	1:A:153:TRP:HB2	1.94	0.50
1:A:430:GLU:HG3	1:A:434:ILE:HD11	1.94	0.50
1:A:497:THR:HG22	1:A:498:ASP:N	2.26	0.50
2:B:31:ILE:O	2:B:32:LYS:C	2.55	0.50
2:B:181:TYR:C	2:B:181:TYR:CD1	2.88	0.50
2:B:183:TYR:HE2	2:B:184:MET:HG3	1.74	0.50
2:B:149:LEU:HB3	2:B:156:SER:HA	1.94	0.50
2:B:169:GLU:CB	2:B:170:PRO:HD3	2.42	0.50
2:B:181:TYR:CD1	2:B:182:GLN:N	2.77	0.50
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.12	0.50
1:A:55:PRO:CG	1:A:143:ARG:HH12	2.24	0.49
1:A:261:VAL:HG21	1:A:280:SER:HB3	1.93	0.49
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.93	0.49
2:B:18:GLY:HA3	2:B:127:TYR:HD1	1.76	0.49
1:A:135:ILE:O	1:A:136:ASN:ND2	2.44	0.49
1:A:307:ARG:O	1:A:308:GLU:C	2.55	0.49
1:A:356:ARG:NH1	1:A:358:ARG:HB2	2.26	0.49
1:A:481:ALA:O	1:A:484:LEU:HB3	2.12	0.49
1:A:513:SER:HB3	1:A:519:ASN:ND2	2.27	0.49
1:A:50:ILE:N	1:A:50:ILE:HD12	2.26	0.49
1:A:229:TRP:O	1:A:231:GLY:N	2.44	0.49
1:A:319:TYR:CE2	1:A:321:PRO:HA	2.47	0.49
2:B:164:MET:C	2:B:166:LYS:N	2.70	0.49
2:B:245:VAL:HG13	2:B:245:VAL:O	2.12	0.49
2:B:385:LYS:HB3	2:B:385:LYS:HZ3	1.77	0.49
2:B:402:TRP:O	2:B:403:THR:C	2.54	0.49
1:A:139:THR:HG22	1:A:141:GLY:H	1.77	0.49
1:A:200:THR:HG23	1:A:201:LYS:H	1.76	0.49
1:A:543:GLY:CA	2:B:284:ARG:HA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TRP:C	2:B:268:SER:H	2.20	0.49
2:B:372:VAL:HG12	2:B:373:GLN:N	2.27	0.49
1:A:77:PHE:O	1:A:78:ARG:C	2.56	0.49
1:A:121:ASP:C	1:A:123:ASP:N	2.71	0.49
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.78	0.49
2:B:66:LYS:CB	2:B:69:THR:HG22	2.42	0.49
2:B:374:LYS:O	2:B:375:ILE:C	2.54	0.49
1:A:1:PRO:HA	1:A:46:LYS:HZ1	1.77	0.49
1:A:90:VAL:HG22	1:A:90:VAL:O	2.12	0.49
1:A:134:SER:HG	1:A:139:THR:HB	1.77	0.49
2:B:46:LYS:HZ3	2:B:116:PHE:HD2	1.56	0.49
1:A:38:CYS:CB	1:A:144:TYR:CE1	2.92	0.49
1:A:384:GLY:HA3	2:B:135:ILE:CG2	2.43	0.49
2:B:47:ILE:HG13	2:B:47:ILE:O	2.12	0.49
2:B:125:ARG:HD3	2:B:146:TYR:O	2.12	0.49
2:B:205:LEU:O	2:B:206:ARG:C	2.53	0.49
2:B:255:ASN:HB2	2:B:289:LEU:O	2.12	0.49
1:A:12:LEU:HB3	1:A:83:ARG:O	2.13	0.49
1:A:413:GLU:H	1:A:413:GLU:HG2	1.33	0.49
2:B:282:LEU:CD1	2:B:293:ILE:HG12	2.41	0.49
1:A:96:HIS:C	1:A:96:HIS:ND1	2.71	0.49
1:A:104:LYS:HG3	1:A:192:ASP:HA	1.95	0.49
1:A:194:GLU:O	1:A:195:ILE:C	2.56	0.49
1:A:290:THR:O	1:A:290:THR:CG2	2.61	0.49
1:A:402:TRP:O	1:A:402:TRP:CE3	2.65	0.49
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.47	0.49
2:B:191:SER:HG	2:B:198:HIS:HD1	1.53	0.49
1:A:97:PRO:HA	1:A:100:LEU:HD12	1.95	0.49
2:B:195:ILE:O	2:B:196:GLY:C	2.54	0.49
2:B:274:ILE:HA	2:B:306:ASN:HD21	1.78	0.49
1:A:17:ASP:CG	1:A:18:GLY:H	2.21	0.48
1:A:49:LYS:HG2	1:A:144:TYR:CE2	2.48	0.48
1:A:58:THR:CG2	1:A:76:ASP:O	2.61	0.48
1:A:149:LEU:HA	1:A:150:PRO:HD2	1.72	0.48
2:B:172:LYS:NZ	5:B:1070:HOH:O	2.46	0.48
2:B:305:GLU:HA	2:B:308:GLU:HG2	1.95	0.48
1:A:478:GLU:HB3	1:A:499:SER:HB2	1.95	0.48
2:B:84:THR:HG22	2:B:85:GLN:N	2.28	0.48
2:B:111:VAL:HG21	2:B:164:MET:HE1	1.94	0.48
1:A:27:THR:C	1:A:29:GLU:N	2.71	0.48
1:A:200:THR:O	1:A:204:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ALA:O	1:A:506:ILE:HG12	2.12	0.48
2:B:76:ASP:O	2:B:78:ARG:N	2.42	0.48
2:B:319:TYR:OH	2:B:385:LYS:HD2	2.13	0.48
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.14	0.48
2:B:37:ILE:O	2:B:40:GLU:HB3	2.12	0.48
2:B:354:TYR:CG	2:B:355:ALA:N	2.81	0.48
2:B:364:ASP:C	2:B:366:LYS:N	2.65	0.48
1:A:64:LYS:HA	1:A:66:LYS:CD	2.41	0.48
1:A:139:THR:C	1:A:141:GLY:H	2.21	0.48
1:A:218:ASP:N	5:A:1036:HOH:O	2.36	0.48
1:A:260:LEU:HD23	1:A:279:LEU:HD21	1.95	0.48
1:A:320:ASP:H	1:A:343:GLN:NE2	2.02	0.48
1:A:379:SER:HA	1:A:383:TRP:CE3	2.48	0.48
1:A:458:VAL:CG2	1:A:551:LEU:HD11	2.44	0.48
1:A:19:PRO:CG	1:A:80:LEU:HA	2.44	0.48
1:A:161:GLN:O	1:A:161:GLN:HG2	2.13	0.48
1:A:283:LEU:O	1:A:283:LEU:HD12	2.14	0.48
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.96	0.48
2:B:425:LEU:HD23	2:B:425:LEU:O	2.14	0.48
1:A:43:LYS:C	1:A:45:GLY:N	2.71	0.48
1:A:64:LYS:CA	1:A:66:LYS:HG2	2.44	0.48
1:A:156:SER:O	1:A:157:PRO:C	2.56	0.48
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.43	0.48
2:B:198:HIS:C	2:B:198:HIS:CD2	2.90	0.48
2:B:332:GLN:HG2	2:B:338:THR:CG2	2.39	0.48
1:A:175:ASN:C	1:A:177:ASP:H	2.22	0.48
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.14	0.48
2:B:426:TRP:HD1	2:B:427:TYR:CD2	2.32	0.48
1:A:34:LEU:HD12	1:A:132:ILE:CG1	2.44	0.48
1:A:111:VAL:O	1:A:114:ALA:N	2.47	0.48
1:A:162:SER:HB2	2:B:52:PRO:HG3	1.95	0.48
1:A:331:LYS:CE	1:A:333:GLY:HA2	2.42	0.48
1:A:97:PRO:C	1:A:99:GLY:H	2.22	0.48
1:A:406:TRP:CE3	1:A:406:TRP:C	2.91	0.48
1:A:441:TYR:CE1	1:A:544:GLY:HA3	2.49	0.48
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.48	0.48
2:B:115:TYR:CE2	2:B:157:PRO:HA	2.30	0.47
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.94	0.47
2:B:54:ASN:ND2	2:B:126:LYS:HA	2.29	0.47
1:A:270:ILE:HD12	1:A:351:THR:HG23	1.95	0.47
1:A:410:TRP:HB3	2:B:365:VAL:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASN:HD22	1:A:494:ASN:N	2.12	0.47
2:B:354:TYR:CD1	2:B:355:ALA:N	2.83	0.47
1:A:122:GLU:O	1:A:122:GLU:CG	2.62	0.47
1:A:334:GLN:C	1:A:336:GLN:N	2.69	0.47
1:A:334:GLN:C	1:A:336:GLN:H	2.21	0.47
1:A:375:ILE:HG21	1:A:389:PHE:CE1	2.48	0.47
2:B:79:GLU:O	2:B:80:LEU:C	2.57	0.47
2:B:267:ALA:O	2:B:271:TYR:HB2	2.15	0.47
1:A:107:THR:CB	1:A:202:ILE:HD13	2.45	0.47
1:A:134:SER:O	1:A:135:ILE:C	2.58	0.47
1:A:160:PHE:CE1	1:A:182:GLN:OE1	2.68	0.47
1:A:458:VAL:HG11	1:A:547:GLN:HG2	1.96	0.47
1:A:541:GLY:C	1:A:543:GLY:H	2.23	0.47
1:A:188:TYR:CD2	4:A:701:IET:H5	2.50	0.47
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.31	0.47
1:A:445:ALA:H	1:A:552:VAL:HG11	1.80	0.47
1:A:513:SER:H	1:A:519:ASN:HD21	1.62	0.47
2:B:202:ILE:O	2:B:203:GLU:C	2.57	0.47
2:B:358:ARG:C	2:B:362:THR:HB	2.39	0.47
1:A:244:ILE:HA	1:A:263:LYS:CE	2.44	0.47
1:A:274:ILE:HG23	1:A:306:ASN:OD1	2.14	0.47
1:A:281:LYS:O	1:A:284:ARG:HB3	2.15	0.47
1:A:406:TRP:CZ3	2:B:420:PRO:HD2	2.49	0.47
1:A:439:THR:HG21	1:A:441:TYR:CE2	2.49	0.47
1:A:506:ILE:HD11	1:A:521:ILE:HG21	1.96	0.47
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.97	0.47
2:B:111:VAL:C	2:B:113:ASP:H	2.23	0.47
2:B:320:ASP:OD1	2:B:322:SER:HB3	2.13	0.47
2:B:369:THR:O	2:B:369:THR:HG22	2.14	0.47
2:B:418:ASN:O	2:B:419:THR:HB	2.15	0.47
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.49	0.47
1:A:102:LYS:N	1:A:318:TYR:HD1	2.13	0.47
1:A:108:VAL:HG12	1:A:188:TYR:CD2	2.35	0.47
1:A:139:THR:HG22	1:A:140:PRO:CD	2.45	0.47
1:A:253:THR:O	1:A:254:VAL:C	2.56	0.47
1:A:363:ASN:ND2	1:A:365:VAL:HB	2.29	0.47
2:B:68:SER:O	2:B:69:THR:C	2.57	0.47
2:B:130:PHE:CZ	2:B:144:TYR:CB	2.97	0.47
2:B:208:HIS:ND1	2:B:208:HIS:C	2.73	0.47
1:A:164:MET:HE1	1:A:187:LEU:HD22	1.96	0.47
2:B:179:VAL:HG23	2:B:179:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:CG1	2:B:199:ARG:NE	2.77	0.47
2:B:198:HIS:C	2:B:200:THR:N	2.71	0.47
2:B:307:ARG:O	2:B:307:ARG:HG2	2.14	0.47
2:B:380:ILE:O	2:B:384:GLY:CA	2.58	0.47
2:B:380:ILE:HD12	2:B:380:ILE:N	2.28	0.47
1:A:7:THR:HG22	1:A:119:PRO:CG	2.45	0.47
1:A:34:LEU:CD1	1:A:132:ILE:HG12	2.44	0.47
1:A:124:PHE:CD2	1:A:124:PHE:O	2.68	0.47
2:B:157:PRO:HG3	2:B:184:MET:HA	1.96	0.47
1:A:229:TRP:O	1:A:232:TYR:N	2.48	0.46
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.40	0.46
2:B:168:LEU:HD23	2:B:209:LEU:HD21	1.97	0.46
2:B:195:ILE:HG13	2:B:199:ARG:HD2	1.96	0.46
2:B:345:PRO:C	2:B:346:PHE:HD1	2.22	0.46
1:A:85:GLN:HE22	2:B:53:GLU:HA	1.80	0.46
1:A:208:HIS:CE1	1:A:212:TRP:NE1	2.82	0.46
1:A:309:ILE:HG22	1:A:310:LEU:N	2.30	0.46
1:A:326:ILE:HB	1:A:342:TYR:CD1	2.50	0.46
1:A:458:VAL:HG21	1:A:547:GLN:HG3	1.97	0.46
2:B:195:ILE:HD11	2:B:233:GLU:OE1	2.15	0.46
1:A:301:LEU:O	1:A:305:GLU:HG3	2.16	0.46
2:B:13:LYS:CG	2:B:14:PRO:N	2.78	0.46
2:B:274:ILE:HA	2:B:306:ASN:ND2	2.30	0.46
1:A:418:ASN:O	1:A:420:PRO:HD3	2.16	0.46
2:B:151:GLN:O	2:B:152:GLY:C	2.57	0.46
2:B:178:ILE:HG23	2:B:189:VAL:HG12	1.98	0.46
2:B:223:LYS:HA	2:B:223:LYS:HD3	1.70	0.46
2:B:366:LYS:HB2	2:B:405:TYR:CZ	2.50	0.46
1:A:373:GLN:HG2	2:B:394:GLN:HE21	1.80	0.46
2:B:47:ILE:HG22	2:B:146:TYR:CD1	2.50	0.46
2:B:221:HIS:HD2	2:B:221:HIS:H	1.61	0.46
1:A:9:PRO:O	1:A:9:PRO:HG2	2.16	0.46
1:A:180:ILE:CG2	1:A:187:LEU:HD11	2.46	0.46
1:A:228:LEU:HD23	1:A:232:TYR:O	2.15	0.46
1:A:433:PRO:CB	2:B:255:ASN:ND2	2.78	0.46
2:B:168:LEU:HD13	2:B:180:ILE:CD1	2.45	0.46
2:B:245:VAL:O	2:B:245:VAL:HG22	2.15	0.46
1:A:24:TRP:O	1:A:26:LEU:N	2.49	0.46
1:A:175:ASN:O	1:A:177:ASP:N	2.48	0.46
1:A:440:PHE:CD2	1:A:459:THR:HG23	2.51	0.46
1:A:470:THR:O	1:A:471:ASN:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ILE:HG22	2:B:35:VAL:HG22	1.97	0.46
2:B:109:LEU:HD12	2:B:218:ASP:OD2	2.14	0.46
2:B:161:GLN:O	2:B:163:SER:N	2.48	0.46
2:B:308:GLU:C	2:B:310:LEU:N	2.71	0.46
1:A:98:ALA:HB2	1:A:350:LYS:HB2	1.98	0.46
1:A:335:GLY:O	1:A:355:ALA:HA	2.15	0.46
1:A:401:TRP:HE3	1:A:404:GLU:HG3	1.81	0.46
1:A:482:ILE:O	1:A:483:TYR:C	2.57	0.46
2:B:54:ASN:OD1	2:B:56:TYR:HB2	2.16	0.46
2:B:263:LYS:O	2:B:426:TRP:CZ3	2.68	0.46
2:B:331:LYS:O	2:B:424:LYS:HG3	2.16	0.46
1:A:339:TYR:CE2	1:A:375:ILE:HG13	2.51	0.46
2:B:201:LYS:O	2:B:205:LEU:N	2.49	0.46
2:B:330:GLN:N	2:B:330:GLN:OE1	2.49	0.46
2:B:358:ARG:H	2:B:358:ARG:NE	2.13	0.46
2:B:378:GLU:O	2:B:382:ILE:HG13	2.16	0.46
1:A:111:VAL:O	1:A:113:ASP:N	2.49	0.46
1:A:219:LYS:HB3	5:A:1088:HOH:O	2.16	0.46
1:A:325:LEU:C	1:A:326:ILE:HD12	2.41	0.46
1:A:348:ASN:ND2	1:A:351:THR:HG22	2.31	0.46
1:A:361:HIS:CD2	1:A:505:ILE:HD12	2.51	0.46
2:B:66:LYS:HB2	2:B:69:THR:CG2	2.46	0.46
2:B:202:ILE:O	2:B:205:LEU:HB3	2.16	0.46
2:B:254:VAL:O	2:B:257:ILE:HG23	2.16	0.46
2:B:329:ILE:CD1	2:B:389:PHE:HD2	2.29	0.46
1:A:62:ALA:C	1:A:63:ILE:HG23	2.41	0.45
1:A:64:LYS:CA	1:A:66:LYS:HD3	2.43	0.45
1:A:319:TYR:CE1	1:A:325:LEU:HD21	2.52	0.45
1:A:379:SER:OG	1:A:387:PRO:HD3	2.16	0.45
1:A:394:GLN:O	1:A:397:THR:N	2.44	0.45
1:A:503:LEU:HD23	1:A:535:TRP:HB2	1.98	0.45
2:B:22:LYS:HA	2:B:22:LYS:HD3	1.68	0.45
2:B:61:PHE:CE1	2:B:76:ASP:HB2	2.42	0.45
2:B:72:ARG:NH2	2:B:409:THR:HG22	2.31	0.45
1:A:12:LEU:HG	1:A:124:PHE:CE1	2.38	0.45
1:A:229:TRP:C	1:A:231:GLY:H	2.24	0.45
1:A:229:TRP:C	1:A:231:GLY:N	2.73	0.45
1:A:434:ILE:CG1	1:A:530:LYS:HD3	2.46	0.45
2:B:23:GLN:HG2	2:B:133:PRO:CG	2.43	0.45
1:A:12:LEU:HD12	1:A:12:LEU:H	1.80	0.45
1:A:107:THR:HG21	1:A:202:ILE:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PHE:CE2	1:A:153:TRP:CE2	3.04	0.45
1:A:306:ASN:O	1:A:310:LEU:HB2	2.15	0.45
1:A:307:ARG:C	1:A:309:ILE:N	2.74	0.45
1:A:354:TYR:CB	1:A:374:LYS:HZ1	2.22	0.45
1:A:408:ALA:HB2	2:B:337:TRP:CH2	2.52	0.45
1:A:491:LEU:HD12	1:A:491:LEU:H	1.80	0.45
1:A:513:SER:N	1:A:519:ASN:ND2	2.64	0.45
2:B:85:GLN:O	2:B:88:TRP:C	2.59	0.45
2:B:91:GLN:C	2:B:91:GLN:NE2	2.71	0.45
2:B:227:PHE:O	2:B:228:LEU:HG	2.16	0.45
2:B:308:GLU:C	2:B:310:LEU:H	2.24	0.45
1:A:34:LEU:CD2	1:A:62:ALA:CB	2.85	0.45
1:A:203:GLU:O	1:A:207:GLN:HG2	2.16	0.45
1:A:491:LEU:O	1:A:529:GLU:CB	2.63	0.45
2:B:146:TYR:CE1	2:B:150:PRO:HB3	2.52	0.45
2:B:266:TRP:O	2:B:268:SER:N	2.49	0.45
2:B:376:THR:CG2	2:B:380:ILE:CD1	2.87	0.45
1:A:134:SER:HB3	1:A:138:GLU:OE1	2.16	0.45
1:A:409:THR:OG1	1:A:410:TRP:N	2.48	0.45
1:A:438:GLU:CD	1:A:463:ARG:HH21	2.23	0.45
2:B:169:GLU:C	2:B:171:PHE:N	2.73	0.45
2:B:279:LEU:HD12	2:B:279:LEU:HA	1.82	0.45
2:B:358:ARG:O	2:B:362:THR:HB	2.16	0.45
1:A:12:LEU:HD12	1:A:12:LEU:N	2.31	0.45
1:A:15:GLY:O	1:A:16:MET:C	2.60	0.45
2:B:139:THR:HG22	2:B:140:PRO:N	2.29	0.45
2:B:220:LYS:CB	2:B:221:HIS:HD2	2.29	0.45
1:A:265:ASN:O	1:A:268:SER:N	2.47	0.45
1:A:286:THR:HG23	1:A:287:LYS:H	1.81	0.45
1:A:450:THR:HG22	1:A:450:THR:O	2.17	0.45
1:A:477:THR:C	1:A:479:LEU:N	2.72	0.45
2:B:47:ILE:HG21	2:B:146:TYR:CD1	2.52	0.45
2:B:66:LYS:HB2	2:B:69:THR:HG21	1.98	0.45
2:B:85:GLN:C	2:B:85:GLN:CD	2.85	0.45
1:A:229:TRP:HE3	1:A:234:LEU:HD11	1.82	0.45
1:A:354:TYR:HB2	1:A:374:LYS:NZ	2.25	0.45
1:A:379:SER:CB	1:A:387:PRO:HD3	2.47	0.45
1:A:398:TRP:CD1	1:A:399:GLU:N	2.85	0.45
1:A:483:TYR:HA	1:A:486:LEU:HD12	1.98	0.45
2:B:54:ASN:HD21	2:B:126:LYS:CA	2.30	0.45
2:B:60:VAL:HG23	2:B:60:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:LEU:C	2:B:150:PRO:O	2.60	0.45
2:B:208:HIS:CE1	2:B:212:TRP:HD1	2.34	0.45
1:A:105:SER:OG	1:A:198:HIS:CG	2.70	0.45
1:A:195:ILE:HA	1:A:198:HIS:HB3	1.97	0.45
1:A:270:ILE:O	1:A:272:PRO:HD3	2.17	0.45
1:A:379:SER:O	1:A:380:ILE:C	2.59	0.45
1:A:426:TRP:HB3	1:A:526:ILE:HD12	1.99	0.45
2:B:41:MET:HE2	2:B:41:MET:HB3	1.73	0.45
2:B:125:ARG:O	2:B:126:LYS:C	2.58	0.45
2:B:320:ASP:OD2	2:B:323:LYS:HE2	2.17	0.45
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.52	0.45
1:A:477:THR:C	1:A:479:LEU:H	2.25	0.45
1:A:120:LEU:HD23	1:A:125:ARG:CG	2.48	0.44
1:A:467:VAL:HA	1:A:468:PRO:HD3	1.79	0.44
2:B:38:CYS:O	2:B:40:GLU:N	2.50	0.44
2:B:66:LYS:HA	5:B:1037:HOH:O	2.17	0.44
2:B:88:TRP:HZ3	2:B:159:ILE:HG13	1.81	0.44
2:B:112:GLY:HA2	2:B:115:TYR:CE1	2.52	0.44
2:B:168:LEU:HD21	2:B:209:LEU:HD21	1.99	0.44
2:B:200:THR:O	2:B:204:GLU:N	2.34	0.44
2:B:376:THR:HG22	2:B:380:ILE:HD13	1.97	0.44
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.53	0.44
2:B:27:THR:HG22	2:B:28:GLU:N	2.32	0.44
2:B:58:THR:HG22	2:B:59:PRO:HD2	1.98	0.44
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.88	0.44
2:B:109:LEU:HD12	2:B:216:THR:HG21	1.99	0.44
2:B:220:LYS:HB2	2:B:221:HIS:HD2	1.83	0.44
2:B:346:PHE:N	2:B:346:PHE:CD1	2.85	0.44
1:A:161:GLN:O	1:A:162:SER:O	2.36	0.44
1:A:362:THR:CG2	1:A:363:ASN:N	2.51	0.44
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.99	0.44
2:B:54:ASN:HD21	2:B:126:LYS:HA	1.82	0.44
1:A:62:ALA:O	1:A:63:ILE:CG2	2.66	0.44
1:A:196:GLY:C	1:A:198:HIS:N	2.74	0.44
2:B:38:CYS:C	2:B:40:GLU:N	2.75	0.44
2:B:200:THR:O	2:B:201:LYS:C	2.60	0.44
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.53	0.44
1:A:13:LYS:HB2	1:A:16:MET:HE3	2.00	0.44
1:A:127:TYR:CD2	1:A:127:TYR:N	2.84	0.44
1:A:132:ILE:HD13	1:A:133:PRO:CD	2.44	0.44
1:A:148:VAL:O	1:A:150:PRO:CD	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLU:HG2	1:A:390:LYS:CB	2.44	0.44
1:A:536:VAL:HG12	1:A:541:GLY:HA3	1.99	0.44
2:B:72:ARG:NH2	2:B:409:THR:CG2	2.81	0.44
1:A:452:LEU:HD23	1:A:470:THR:HA	1.99	0.44
1:A:460:ASN:C	1:A:462:GLY:N	2.73	0.44
1:A:482:ILE:CD1	1:A:502:ALA:HB1	2.47	0.44
2:B:53:GLU:OE1	2:B:53:GLU:N	2.37	0.44
2:B:169:GLU:O	2:B:172:LYS:N	2.50	0.44
1:A:2:ILE:HD11	1:A:45:GLY:O	2.18	0.44
1:A:86:ASP:HA	1:A:154:LYS:HZ2	1.82	0.44
1:A:254:VAL:CA	1:A:257:ILE:HG22	2.38	0.44
1:A:282:LEU:O	1:A:284:ARG:N	2.51	0.44
1:A:450:THR:O	1:A:452:LEU:HG	2.17	0.44
1:A:499:SER:OG	1:A:502:ALA:CB	2.65	0.44
2:B:79:GLU:O	2:B:81:ASN:N	2.51	0.44
2:B:86:ASP:O	2:B:89:GLU:HB3	2.17	0.44
2:B:107:THR:HA	2:B:232:TYR:O	2.18	0.44
2:B:228:LEU:HD23	2:B:228:LEU:HA	1.85	0.44
1:A:297:GLU:CD	1:A:297:GLU:N	2.73	0.44
1:A:469:LEU:CD1	1:A:477:THR:HG22	2.46	0.44
2:B:13:LYS:HG2	2:B:14:PRO:N	2.30	0.44
2:B:73:LYS:HE2	2:B:75:VAL:HG23	1.99	0.44
2:B:128:THR:O	2:B:129:ALA:C	2.60	0.44
2:B:140:PRO:O	2:B:141:GLY:C	2.61	0.44
1:A:19:PRO:HG3	1:A:80:LEU:HA	2.00	0.44
1:A:55:PRO:HG2	1:A:143:ARG:CZ	2.48	0.44
1:A:122:GLU:O	1:A:122:GLU:HG2	2.17	0.44
1:A:244:ILE:CA	1:A:263:LYS:HE2	2.48	0.44
2:B:60:VAL:HG11	2:B:130:PHE:HD2	1.76	0.44
2:B:114:ALA:O	2:B:115:TYR:C	2.59	0.44
1:A:292:VAL:O	1:A:294:PRO:HD3	2.18	0.43
1:A:513:SER:H	1:A:519:ASN:ND2	2.16	0.43
2:B:58:THR:HA	2:B:59:PRO:HD3	1.75	0.43
2:B:278:GLN:HE22	2:B:297:GLU:CG	2.30	0.43
2:B:1:PRO:C	2:B:2:ILE:HD13	2.43	0.43
2:B:72:ARG:HH21	2:B:151:GLN:HE22	1.65	0.43
2:B:173:LYS:O	2:B:174:GLN:C	2.61	0.43
2:B:235:HIS:C	2:B:237:ASP:H	2.26	0.43
1:A:102:LYS:O	1:A:103:LYS:HD3	2.18	0.43
1:A:326:ILE:N	1:A:326:ILE:CD1	2.76	0.43
1:A:433:PRO:CB	2:B:255:ASN:HD22	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:LYS:HE3	2:B:179:VAL:HG13	1.98	0.43
2:B:300:GLU:OE1	2:B:300:GLU:O	2.36	0.43
2:B:311:LYS:NZ	5:B:1079:HOH:O	2.50	0.43
1:A:17:ASP:CG	1:A:18:GLY:N	2.76	0.43
1:A:130:PHE:HE1	1:A:144:TYR:HB2	1.77	0.43
1:A:315:HIS:CD2	5:A:1029:HOH:O	2.71	0.43
2:B:92:LEU:HB2	2:B:158:ALA:HB1	1.99	0.43
2:B:142:ILE:H	2:B:142:ILE:HG12	1.58	0.43
2:B:209:LEU:HB3	2:B:214:LEU:HB2	2.00	0.43
2:B:269:GLN:HB3	2:B:346:PHE:CD2	2.53	0.43
1:A:50:ILE:HD12	1:A:50:ILE:H	1.83	0.43
1:A:54:ASN:N	1:A:55:PRO:CD	2.81	0.43
1:A:363:ASN:HD22	1:A:366:LYS:H	1.67	0.43
2:B:329:ILE:HD11	2:B:389:PHE:HD2	1.83	0.43
1:A:23:GLN:O	1:A:23:GLN:NE2	2.44	0.43
1:A:253:THR:OG1	1:A:290:THR:C	2.61	0.43
1:A:482:ILE:HD11	1:A:502:ALA:HB1	2.01	0.43
2:B:164:MET:C	2:B:166:LYS:H	2.26	0.43
2:B:425:LEU:O	2:B:425:LEU:CD2	2.66	0.43
1:A:165:THR:HG22	1:A:166:LYS:N	2.32	0.43
1:A:312:GLU:H	1:A:312:GLU:HG2	1.59	0.43
1:A:398:TRP:O	1:A:399:GLU:C	2.61	0.43
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.00	0.43
2:B:164:MET:O	2:B:167:ILE:N	2.51	0.43
2:B:426:TRP:CD1	2:B:427:TYR:N	2.86	0.43
1:A:246:LEU:O	1:A:247:PRO:C	2.61	0.43
1:A:325:LEU:CD1	1:A:383:TRP:CE3	3.02	0.43
1:A:394:GLN:O	1:A:395:LYS:C	2.61	0.43
1:A:395:LYS:HA	1:A:414:TRP:CZ2	2.45	0.43
2:B:274:ILE:HD12	2:B:274:ILE:N	2.33	0.43
2:B:316:GLY:HA2	2:B:318:TYR:HE1	1.84	0.43
1:A:63:ILE:C	1:A:63:ILE:HD12	2.44	0.43
1:A:497:THR:HG22	1:A:499:SER:HB3	2.01	0.43
1:A:193:LEU:O	1:A:194:GLU:C	2.62	0.43
2:B:231:GLY:O	2:B:233:GLU:HG3	2.19	0.43
2:B:277:ARG:HD3	2:B:277:ARG:N	2.27	0.43
1:A:261:VAL:CG2	1:A:279:LEU:HD22	2.48	0.42
1:A:264:LEU:CD1	1:A:279:LEU:HD13	2.49	0.42
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.51	0.42
2:B:203:GLU:OE2	2:B:207:GLN:HG2	2.19	0.42
2:B:220:LYS:CB	2:B:221:HIS:CD2	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:H	1:A:142:ILE:CD1	2.29	0.42
1:A:200:THR:CG2	1:A:201:LYS:N	2.82	0.42
1:A:279:LEU:HB2	1:A:302:GLU:OE2	2.18	0.42
1:A:398:TRP:NE1	1:A:402:TRP:HD1	2.18	0.42
1:A:478:GLU:CD	1:A:499:SER:HB2	2.44	0.42
2:B:43:LYS:C	2:B:45:GLY:H	2.26	0.42
2:B:349:LEU:HD12	2:B:383:TRP:CE2	2.53	0.42
1:A:107:THR:HG1	1:A:198:HIS:CD2	2.37	0.42
1:A:193:LEU:O	1:A:198:HIS:HB2	2.19	0.42
1:A:477:THR:O	1:A:480:GLN:N	2.53	0.42
2:B:44:GLU:C	2:B:46:LYS:N	2.77	0.42
2:B:44:GLU:C	2:B:46:LYS:H	2.25	0.42
2:B:218:ASP:O	2:B:220:LYS:N	2.51	0.42
1:A:218:ASP:C	1:A:221:HIS:HB2	2.43	0.42
1:A:319:TYR:HD1	1:A:325:LEU:HD21	1.84	0.42
1:A:433:PRO:HG3	2:B:255:ASN:ND2	2.34	0.42
1:A:434:ILE:HG13	1:A:530:LYS:HD3	2.01	0.42
2:B:17:ASP:O	2:B:18:GLY:C	2.62	0.42
2:B:183:TYR:HE1	2:B:380:ILE:HG13	1.83	0.42
2:B:345:PRO:HB2	2:B:346:PHE:CD1	2.51	0.42
1:A:85:GLN:O	1:A:154:LYS:CE	2.67	0.42
1:A:126:LYS:HG3	1:A:127:TYR:CD2	2.55	0.42
1:A:433:PRO:CG	2:B:255:ASN:ND2	2.82	0.42
1:A:541:GLY:O	1:A:545:ASN:HB3	2.19	0.42
2:B:34:LEU:HD21	2:B:61:PHE:O	2.20	0.42
2:B:53:GLU:O	2:B:55:PRO:HD3	2.20	0.42
2:B:171:PHE:CD1	2:B:171:PHE:C	2.98	0.42
2:B:334:GLN:CD	2:B:334:GLN:H	2.28	0.42
1:A:139:THR:CG2	1:A:140:PRO:CD	2.92	0.42
1:A:253:THR:HG22	1:A:256:ASP:CG	2.45	0.42
1:A:369:THR:O	1:A:373:GLN:N	2.45	0.42
2:B:23:GLN:HG3	2:B:133:PRO:HG3	1.95	0.42
2:B:64:LYS:HG3	2:B:71:TRP:CE3	2.55	0.42
2:B:96:HIS:CE1	2:B:384:GLY:N	2.88	0.42
2:B:156:SER:N	2:B:157:PRO:CD	2.82	0.42
1:A:390:LYS:HA	1:A:415:GLU:O	2.20	0.42
2:B:49:LYS:HE3	2:B:144:TYR:CZ	2.55	0.42
2:B:85:GLN:HG3	2:B:154:LYS:HD2	2.01	0.42
2:B:257:ILE:HG23	2:B:258:GLN:N	2.35	0.42
2:B:366:LYS:CG	2:B:405:TYR:CD2	3.01	0.42
1:A:47:ILE:HB	1:A:145:GLN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:C	1:A:212:TRP:H	2.27	0.42
1:A:341:ILE:HG12	1:A:383:TRP:CH2	2.55	0.42
2:B:171:PHE:CE2	2:B:205:LEU:CA	3.03	0.42
2:B:257:ILE:CD1	2:B:261:VAL:HG23	2.50	0.42
1:A:73:LYS:HE3	1:A:130:PHE:CE2	2.55	0.42
1:A:98:ALA:HB1	1:A:350:LYS:HB2	2.02	0.42
1:A:120:LEU:HD13	1:A:150:PRO:HD2	2.01	0.42
1:A:331:LYS:HG3	1:A:337:TRP:CZ2	2.55	0.42
1:A:485:ALA:C	1:A:487:GLN:N	2.76	0.42
1:A:492:GLU:CD	1:A:530:LYS:HD2	2.45	0.42
2:B:7:THR:HG22	2:B:119:PRO:HB2	2.01	0.42
2:B:60:VAL:O	2:B:60:VAL:CG2	2.67	0.42
2:B:358:ARG:CG	2:B:359:GLY:N	2.63	0.42
2:B:386:THR:HA	2:B:387:PRO:HD3	1.78	0.42
1:A:122:GLU:HA	1:A:125:ARG:NE	2.34	0.42
1:A:136:ASN:C	1:A:138:GLU:N	2.76	0.42
1:A:233:GLU:N	1:A:240:THR:O	2.44	0.42
1:A:311:LYS:NZ	5:A:1040:HOH:O	2.49	0.42
1:A:442:VAL:HG22	1:A:443:ASP:N	2.35	0.42
1:A:456:GLY:HA2	1:A:484:LEU:CD2	2.50	0.42
2:B:34:LEU:HD21	2:B:62:ALA:HB2	2.01	0.42
2:B:278:GLN:HG3	2:B:278:GLN:O	2.19	0.42
2:B:320:ASP:O	2:B:343:GLN:NE2	2.51	0.42
2:B:345:PRO:C	2:B:346:PHE:CD1	2.97	0.42
1:A:543:GLY:O	2:B:284:ARG:O	2.37	0.41
2:B:17:ASP:C	2:B:18:GLY:O	2.63	0.41
2:B:253:THR:HB	2:B:291:GLU:O	2.20	0.41
1:A:96:HIS:HD1	1:A:98:ALA:N	2.13	0.41
1:A:126:LYS:H	1:A:126:LYS:HG2	1.71	0.41
1:A:344:GLU:HA	1:A:345:PRO:HD2	1.58	0.41
1:A:370:GLU:O	1:A:373:GLN:HB3	2.20	0.41
1:A:441:TYR:HB2	1:A:458:VAL:O	2.21	0.41
2:B:370:GLU:C	2:B:372:VAL:N	2.77	0.41
1:A:434:ILE:CD1	1:A:494:ASN:HD21	2.33	0.41
2:B:92:LEU:CB	2:B:158:ALA:HB1	2.50	0.41
2:B:195:ILE:CG2	2:B:196:GLY:N	2.64	0.41
2:B:375:ILE:CG2	2:B:389:PHE:HE2	2.33	0.41
1:A:499:SER:OG	1:A:499:SER:O	2.36	0.41
2:B:269:GLN:HG2	2:B:346:PHE:CG	2.56	0.41
2:B:385:LYS:NZ	2:B:385:LYS:CB	2.83	0.41
1:A:183:TYR:CD2	1:A:229:TRP:CD1	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:HIS:CD2	1:A:315:HIS:H	2.38	0.41
2:B:192:ASP:C	2:B:193:LEU:HD23	2.45	0.41
2:B:244:ILE:HD13	2:B:244:ILE:N	2.30	0.41
2:B:372:VAL:O	2:B:374:LYS:N	2.53	0.41
1:A:48:SER:O	1:A:144:TYR:HA	2.21	0.41
1:A:168:LEU:HD13	1:A:180:ILE:HG21	2.02	0.41
1:A:183:TYR:CD2	1:A:229:TRP:HD1	2.39	0.41
1:A:278:GLN:HG3	1:A:298:GLU:HB3	2.03	0.41
1:A:354:TYR:CD2	1:A:354:TYR:C	2.98	0.41
1:A:435:VAL:HG13	2:B:290:THR:OG1	2.20	0.41
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.56	0.41
2:B:275:LYS:HA	2:B:277:ARG:CZ	2.50	0.41
2:B:328:GLU:OE1	2:B:342:TYR:OH	2.30	0.41
1:A:32:LYS:O	1:A:36:GLU:CG	2.69	0.41
1:A:164:MET:CE	1:A:187:LEU:HD22	2.50	0.41
1:A:224:GLU:N	1:A:225:PRO:HD3	2.34	0.41
1:A:367:GLN:O	1:A:368:LEU:C	2.64	0.41
1:A:483:TYR:CB	1:A:521:ILE:HG12	2.43	0.41
1:A:503:LEU:HD21	1:A:535:TRP:HB2	1.98	0.41
2:B:8:VAL:O	2:B:9:PRO:C	2.63	0.41
2:B:36:GLU:O	2:B:37:ILE:C	2.62	0.41
1:A:309:ILE:O	1:A:312:GLU:CG	2.68	0.41
1:A:339:TYR:CG	1:A:375:ILE:HD11	2.56	0.41
2:B:50:ILE:HG13	2:B:143:ARG:HB3	2.03	0.41
2:B:72:ARG:HH22	2:B:409:THR:CG2	2.34	0.41
2:B:78:ARG:CZ	2:B:411:ILE:HG21	2.51	0.41
2:B:91:GLN:NE2	2:B:91:GLN:O	2.48	0.41
2:B:149:LEU:HD12	2:B:156:SER:O	2.20	0.41
2:B:269:GLN:HG2	2:B:346:PHE:CD2	2.56	0.41
2:B:283:LEU:O	2:B:285:GLY:O	2.39	0.41
1:A:107:THR:O	1:A:189:VAL:N	2.33	0.41
1:A:162:SER:CB	2:B:52:PRO:HG3	2.51	0.41
1:A:219:LYS:HA	5:A:1088:HOH:O	2.21	0.41
1:A:253:THR:OG1	1:A:290:THR:CA	2.68	0.41
1:A:275:LYS:O	1:A:276:VAL:CG2	2.68	0.41
1:A:276:VAL:O	1:A:277:ARG:C	2.64	0.41
1:A:277:ARG:HA	1:A:277:ARG:HD2	1.92	0.41
1:A:472:THR:OG1	1:A:476:LYS:HB3	2.21	0.41
2:B:38:CYS:HA	2:B:41:MET:HG3	2.02	0.41
2:B:216:THR:C	2:B:218:ASP:N	2.78	0.41
2:B:217:PRO:C	2:B:219:LYS:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:LEU:CD1	2:B:264:LEU:HD11	2.50	0.41
2:B:261:VAL:HG21	2:B:283:LEU:CD1	2.50	0.41
2:B:276:VAL:O	2:B:276:VAL:HG12	2.21	0.41
2:B:295:LEU:HD23	2:B:295:LEU:N	2.36	0.41
2:B:375:ILE:HG21	2:B:389:PHE:HE2	1.84	0.41
1:A:21:VAL:HG12	1:A:22:LYS:N	2.36	0.41
1:A:163:SER:O	1:A:164:MET:C	2.62	0.41
1:A:261:VAL:HG13	1:A:276:VAL:HG11	2.01	0.41
1:A:356:ARG:NE	1:A:358:ARG:CG	2.79	0.41
1:A:443:ASP:HB2	1:A:548:VAL:CG2	2.50	0.41
2:B:23:GLN:HG3	2:B:24:TRP:O	2.20	0.41
2:B:306:ASN:HD22	2:B:306:ASN:HA	1.64	0.41
2:B:371:ALA:O	2:B:375:ILE:HB	2.21	0.41
1:A:23:GLN:CD	1:A:23:GLN:N	2.68	0.40
1:A:142:ILE:N	1:A:142:ILE:CD1	2.84	0.40
1:A:257:ILE:O	1:A:261:VAL:HG23	2.21	0.40
1:A:326:ILE:HG22	1:A:327:ALA:N	2.36	0.40
1:A:485:ALA:O	1:A:487:GLN:N	2.54	0.40
2:B:66:LYS:HB3	2:B:67:ASP:H	1.62	0.40
2:B:183:TYR:HD1	2:B:380:ILE:CG2	2.23	0.40
1:A:158:ALA:O	1:A:159:ILE:C	2.63	0.40
1:A:175:ASN:C	1:A:177:ASP:N	2.79	0.40
1:A:406:TRP:C	1:A:406:TRP:CD2	2.99	0.40
1:A:450:THR:HG22	1:A:452:LEU:CB	2.52	0.40
2:B:164:MET:O	2:B:165:THR:C	2.64	0.40
2:B:198:HIS:CD2	2:B:199:ARG:N	2.89	0.40
1:A:2:ILE:CG2	1:A:3:SER:H	2.25	0.40
2:B:100:LEU:C	2:B:102:LYS:H	2.28	0.40
2:B:156:SER:HB2	2:B:157:PRO:CD	2.51	0.40
2:B:253:THR:HG22	2:B:292:VAL:HG22	2.03	0.40
2:B:372:VAL:O	2:B:373:GLN:C	2.64	0.40
1:A:193:LEU:CB	1:A:197:GLN:HB3	2.46	0.40
1:A:303:LEU:O	1:A:307:ARG:HG2	2.21	0.40
1:A:481:ALA:O	1:A:484:LEU:N	2.54	0.40
2:B:171:PHE:CD1	2:B:171:PHE:O	2.74	0.40
2:B:232:TYR:CE2	2:B:234:LEU:HD21	2.48	0.40
1:A:104:LYS:CG	1:A:192:ASP:HA	2.52	0.40
1:A:111:VAL:O	1:A:112:GLY:C	2.64	0.40
1:A:135:ILE:HG22	1:A:136:ASN:N	2.37	0.40
1:A:540:LYS:C	1:A:542:ILE:H	2.30	0.40
2:B:125:ARG:HD3	2:B:147:ASN:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ARG:HD3	2:B:147:ASN:HA	2.03	0.40
2:B:137:ASN:C	2:B:139:THR:H	2.29	0.40
2:B:181:TYR:O	2:B:188:TYR:N	2.51	0.40
2:B:187:LEU:HD23	2:B:187:LEU:HA	1.90	0.40
2:B:372:VAL:C	2:B:374:LYS:N	2.76	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%)	404 (74%)	92 (17%)	54 (10%)	0	1
2	B	425/430 (99%)	277 (65%)	94 (22%)	54 (13%)	0	0
All	All	975/990 (98%)	681 (70%)	186 (19%)	108 (11%)	0	1

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	25	PRO
1	A	52	PRO
1	A	65	LYS
1	A	112	GLY
1	A	153	TRP
1	A	162	SER
1	A	163	SER
1	A	273	GLY
1	A	359	GLY
1	A	538	ALA
2	B	66	LYS
2	B	68	SER

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Mol	Chain	Res	Type
2	B	71	TRP
2	B	77	PHE
2	B	116	PHE
2	B	126	LYS
2	B	161	GLN
2	B	176	PRO
2	B	177	ASP
2	B	195	ILE
2	B	218	ASP
2	B	242	GLN
2	B	267	ALA
2	B	284	ARG
2	B	297	GLU
2	B	362	THR
2	B	365	VAL
2	B	404	GLU
2	B	421	PRO
1	A	98	ALA
1	A	122	GLU
1	A	164	MET
1	A	195	ILE
1	A	223	LYS
1	A	230	MET
1	A	276	VAL
1	A	277	ARG
1	A	399	GLU
1	A	491	LEU
1	A	546	GLU
2	B	18	GLY
2	B	85	GLN
2	B	112	GLY
2	B	154	LYS
2	B	162	SER
2	B	165	THR
2	B	174	GLN
2	B	196	GLY
2	B	202	ILE
2	B	228	LEU
2	B	232	TYR
2	B	239	TRP
2	B	250	ASP
2	B	345	PRO

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Mol	Chain	Res	Type
1	A	2	ILE
1	A	64	LYS
1	A	66	LYS
1	A	78	ARG
1	A	102	LYS
1	A	156	SER
1	A	158	ALA
1	A	222	GLN
1	A	272	PRO
1	A	311	LYS
1	A	324	ASP
1	A	398	TRP
1	A	539	HIS
2	B	125	ARG
2	B	173	LYS
2	B	199	ARG
2	B	249	LYS
2	B	294	PRO
1	A	14	PRO
1	A	27	THR
1	A	104	LYS
1	A	176	PRO
1	A	254	VAL
1	A	465	LYS
1	A	482	ILE
2	B	122	GLU
2	B	170	PRO
2	B	251	SER
2	B	276	VAL
1	A	184	MET
1	A	194	GLU
1	A	345	PRO
1	A	392	PRO
1	A	542	ILE
2	B	184	MET
2	B	222	GLN
2	B	236	PRO
2	B	33	ALA
2	B	141	GLY
1	A	159	ILE
1	A	543	GLY
1	A	24	TRP

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Mol	Chain	Res	Type
1	A	54	ASN
1	A	135	ILE
1	A	236	PRO
2	B	111	VAL
2	B	155	GLY
1	A	419	THR
2	B	241	VAL
2	B	245	VAL
2	B	225	PRO
2	B	412	PRO
2	B	423	VAL

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	494/500 (99%)	443 (90%)	51 (10%)	7	23
2	B	389/392 (99%)	335 (86%)	54 (14%)	3	11
All	All	883/892 (99%)	778 (88%)	105 (12%)	5	16

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	23	GLN
1	A	25	PRO
1	A	36	GLU
1	A	50	ILE
1	A	56	TYR
1	A	64	LYS
1	A	66	LYS
1	A	74	LEU
1	A	86	ASP
1	A	120	LEU
1	A	126	LYS

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Mol	Chain	Res	Type
1	A	130	PHE
1	A	131	THR
1	A	132	ILE
1	A	136	ASN
1	A	142	ILE
1	A	159	ILE
1	A	165	THR
1	A	177	ASP
1	A	188	TYR
1	A	195	ILE
1	A	245	VAL
1	A	253	THR
1	A	256	ASP
1	A	274	ILE
1	A	314	VAL
1	A	317	VAL
1	A	326	ILE
1	A	330	GLN
1	A	334	GLN
1	A	340	GLN
1	A	356	ARG
1	A	374	LYS
1	A	385	LYS
1	A	386	THR
1	A	395	LYS
1	A	397	THR
1	A	401	TRP
1	A	402	TRP
1	A	411	ILE
1	A	413	GLU
1	A	439	THR
1	A	449	GLU
1	A	457	TYR
1	A	516	GLU
1	A	521	ILE
1	A	522	ILE
1	A	533	LEU
1	A	548	VAL
1	A	551	LEU
2	B	31	ILE
2	B	41	MET
2	B	50	ILE

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Mol	Chain	Res	Type
2	B	58	THR
2	B	60	VAL
2	B	63	ILE
2	B	67	ASP
2	B	73	LYS
2	B	74	LEU
2	B	86	ASP
2	B	91	GLN
2	B	110	ASP
2	B	131	THR
2	B	135	ILE
2	B	142	ILE
2	B	148	VAL
2	B	149	LEU
2	B	161	GLN
2	B	169	GLU
2	B	175	ASN
2	B	183	TYR
2	B	186	ASP
2	B	189	VAL
2	B	198	HIS
2	B	205	LEU
2	B	208	HIS
2	B	215	THR
2	B	221	HIS
2	B	224	GLU
2	B	232	TYR
2	B	239	TRP
2	B	244	ILE
2	B	252	TRP
2	B	257	ILE
2	B	277	ARG
2	B	305	GLU
2	B	308	GLU
2	B	310	LEU
2	B	313	PRO
2	B	322	SER
2	B	332	GLN
2	B	340	GLN
2	B	342	TYR
2	B	349	LEU
2	B	358	ARG

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Mol	Chain	Res	Type
2	B	362	THR
2	B	372	VAL
2	B	375	ILE
2	B	383	TRP
2	B	385	LYS
2	B	393	ILE
2	B	409	THR
2	B	425	LEU
2	B	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	136	ASN
1	A	161	GLN
1	A	182	GLN
1	A	197	GLN
1	A	208	HIS
1	A	235	HIS
1	A	258	GLN
1	A	315	HIS
1	A	330	GLN
1	A	343	GLN
1	A	363	ASN
1	A	418	ASN
1	A	471	ASN
1	A	487	GLN
1	A	494	ASN
1	A	500	GLN
1	A	507	GLN
1	A	509	GLN
1	A	519	ASN
2	B	23	GLN
2	B	91	GLN
2	B	136	ASN
2	B	137	ASN
2	B	151	GLN
2	B	174	GLN
2	B	208	HIS
2	B	221	HIS
2	B	255	ASN

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Mol	Chain	Res	Type
2	B	258	GLN
2	B	278	GLN
2	B	306	ASN
2	B	330	GLN
2	B	336	GLN
2	B	340	GLN
2	B	348	ASN
2	B	394	GLN
2	B	407	GLN

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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	IET	A	701	-	24,24,24	5.14	14 (58%)	29,32,32	2.41	7 (24%)

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	IET	A	701	-	-	6/12/14/14	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	IET	C7-C8	-17.97	1.39	1.51
4	A	701	IET	C6-CL6	-9.50	1.51	1.73
4	A	701	IET	C2-CL2	-9.46	1.51	1.73
4	A	701	IET	C2-C1	4.32	1.46	1.39
4	A	701	IET	C16-C11	4.00	1.46	1.39
4	A	701	IET	C8-N3	3.98	1.35	1.27
4	A	701	IET	C16-C15	3.92	1.45	1.38
4	A	701	IET	C7-C1	3.28	1.58	1.51
4	A	701	IET	C6-C1	2.82	1.44	1.39
4	A	701	IET	C9-N1	-2.70	1.34	1.39
4	A	701	IET	C3-C2	2.54	1.44	1.38
4	A	701	IET	C4-C3	2.44	1.43	1.38
4	A	701	IET	C13-C12	2.12	1.42	1.38
4	A	701	IET	C9-S2	2.09	1.72	1.68

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	IET	C8-N1-C9	-7.23	121.42	128.72
4	A	701	IET	C1-C7-C8	5.97	124.82	113.64
4	A	701	IET	N5-C9-N1	5.24	123.15	115.31
4	A	701	IET	C7-C1-C6	-3.97	116.63	121.97
4	A	701	IET	C7-C1-C2	3.28	126.39	121.97
4	A	701	IET	S2-C9-N5	-2.70	116.50	124.33
4	A	701	IET	C1-C2-CL2	2.25	123.56	119.60

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	IET	C7-C8-N1-C9
4	A	701	IET	N5-C9-N1-C8
4	A	701	IET	S2-C9-N1-C8
4	A	701	IET	C2-C1-C7-C8

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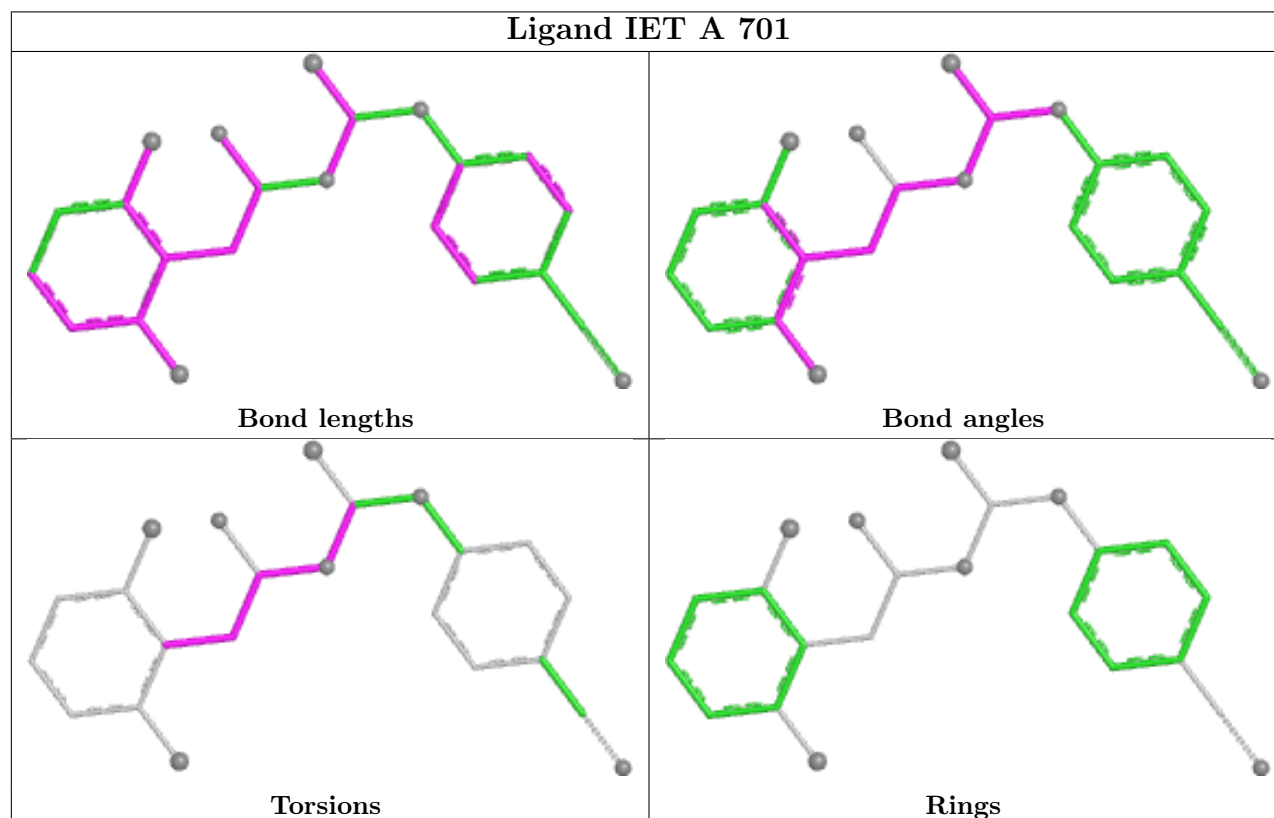
Mol	Chain	Res	Type	Atoms
4	A	701	IET	C1-C7-C8-N1
4	A	701	IET	C6-C1-C7-C8

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	IET	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	552/560 (98%)	-0.07	8 (1%) 73 65	37, 82, 109, 111	5 (0%)
2	B	427/430 (99%)	-0.16	3 (0%) 84 79	19, 69, 110, 111	4 (0%)
All	All	979/990 (98%)	-0.11	11 (1%) 78 71	19, 77, 110, 111	9 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	GLY	4.8
1	A	449	GLU	4.3
2	B	231	GLY	4.1
1	A	59	PRO	3.6
1	A	319	TYR	2.6
1	A	439	THR	2.3
2	B	266	TRP	2.3
2	B	427	TYR	2.3
1	A	552	VAL	2.1
1	A	543	GLY	2.1
1	A	544	GLY	2.1

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](#)

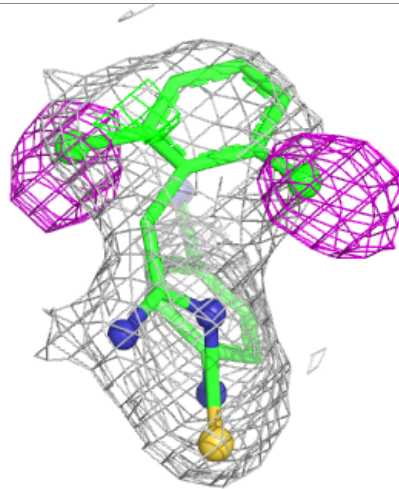
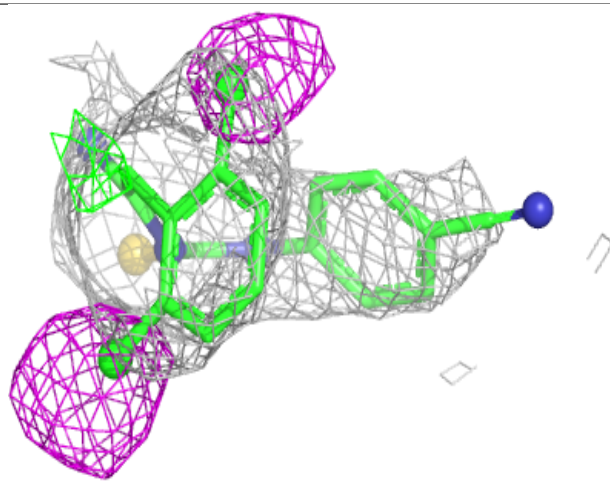
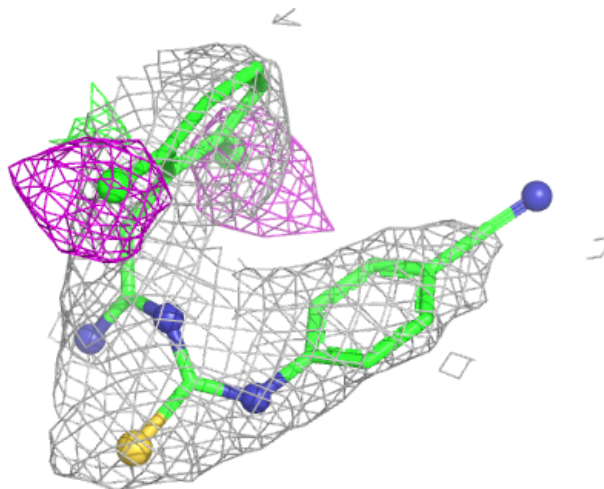
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	IET	A	701	23/23	0.80	0.13	63,78,84,92	0
3	MG	A	601	1/1	0.85	0.08	79,79,79,79	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 IET A 701:

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.