



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:46 pm GMT

PDB ID : 2JLE  
Title : NOVEL INDAZOLE NNRTIS CREATED USING MOLECULAR TEMPLATE HYBRIDIZATION BASED ON CRYSTALLOGRAPHIC OVERLAYS  
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Deposited on : 2008-09-08  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

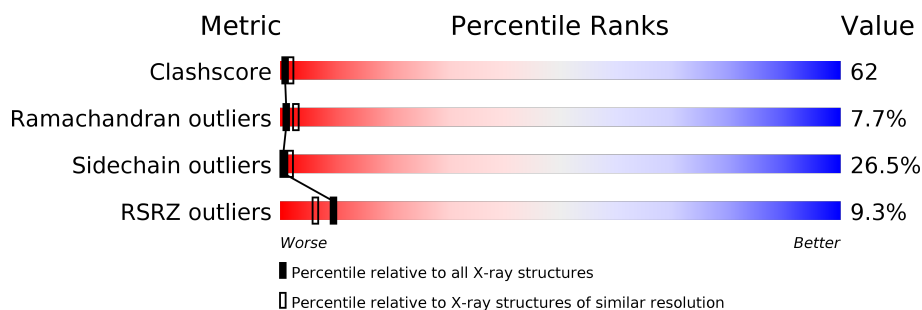
# 1 Overall quality at a glance

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))
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	566	
1	B	566	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8120 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.

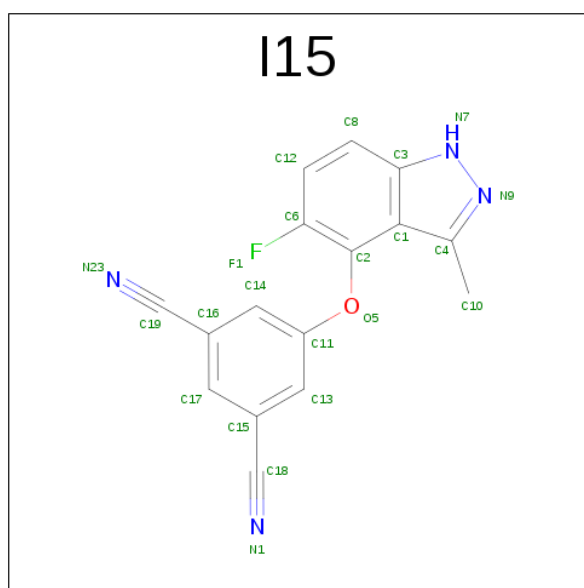
- Molecule 1 is a protein called REVERSE TRANSCRIPTASE/RNASEH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4445	2875	742	820	8			
1	B	416	Total	C	N	O	S	0	0	1
			3414	2218	569	620	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	LYS	ARG	CONFLICT	UNP Q72547
B	103	LYS	ARG	CONFLICT	UNP Q72547
A	350	LYS	ARG	CONFLICT	UNP Q72547
B	350	LYS	ARG	CONFLICT	UNP Q72547

- Molecule 2 is 5-[(5-FLUORO-3-METHYL-1H-INDAZOL-4-YL)OXY]BENZENE-1,3-DICARBONITRILE (three-letter code: I15) (formula: C<sub>16</sub>H<sub>9</sub>FN<sub>4</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			22	16	1	4	1		

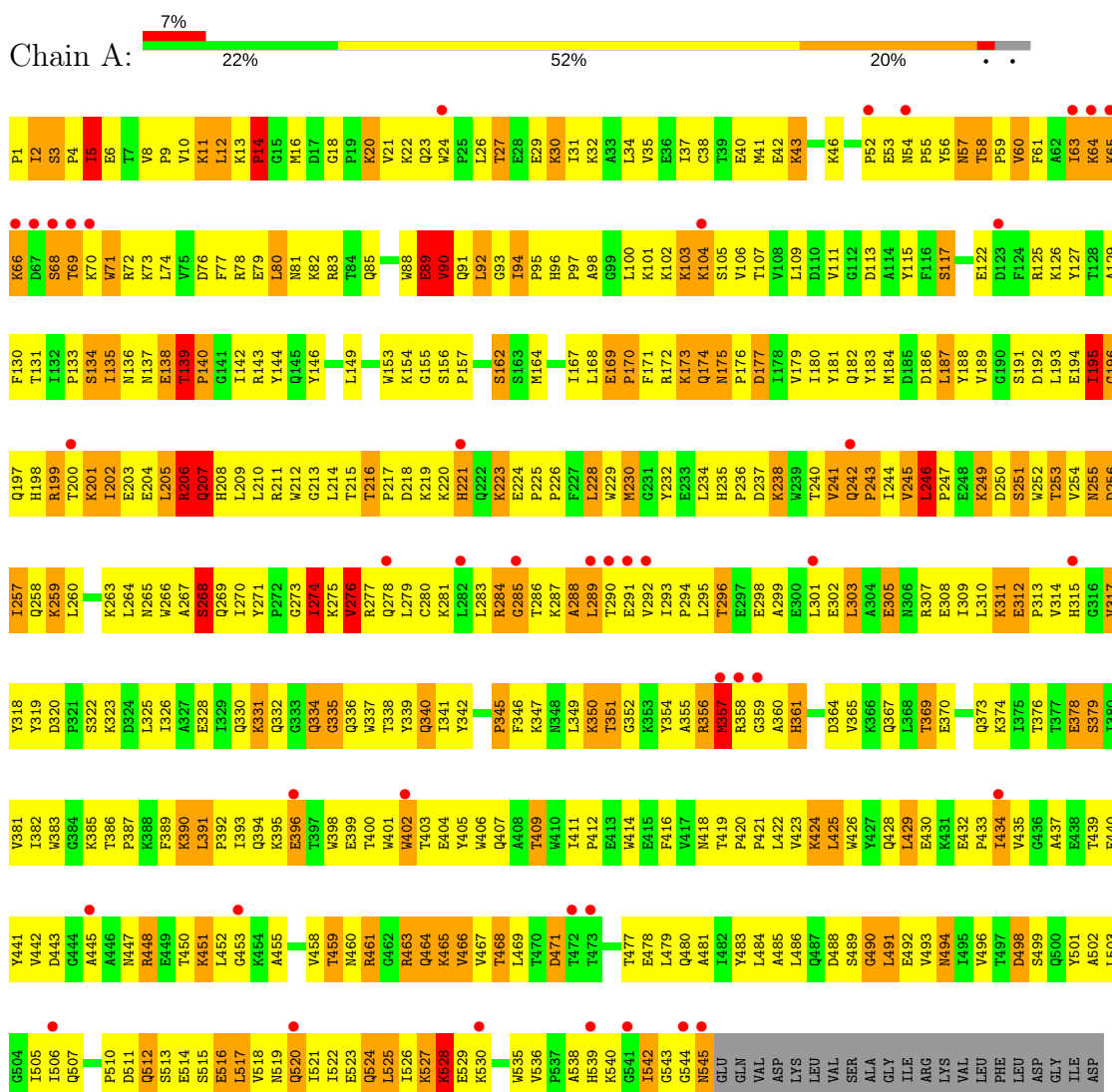
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	0
			152	152		
3	B	87	Total	O	0	0
			87	87		

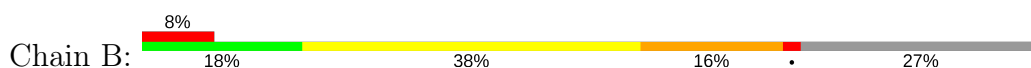
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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/RNASEH



#### • Molecule 1: REVERSE TRANSCRIPTASE/RNASEH



ASP	ILE	ALA	Y318	1257	D192	A129	K65	PR0
GLN	ASN	ASN	Y319	Q258	L193	I132	K66	ILE
ALA	ARG	GLU	D320	K259	E194	P133	S3	Y
GLN	THR	THR	P321	L260	I195	S68	P4	Y
ASP	LYS	LYS	S322	V261	G196	T69	I5	Y
GLN	LEU	LEU	D324		Q197	I135	E6	Y
SER	GLY	LEU	P387	L264	H198	H136	T7	Y
GLU	LYS	LYS	L325	W265	R199	M137	V8	Y
GLU	LYS	LYS	L326	W266	T200	K73	Y	Y
SER	ALA	ALA	A327	A267	K201	R72	V10	Y
GLU	GLY	GLY	E328	S268	I202	T139	K11	Y
LEU	TYR	TYR	K331	Q269	G141	D76	L12	Y
VAL	VAL	VAL	Q332	I270	I142	F77	K13	Y
ASN	THR	THR	Q333	Y271	R143	R78	P14	Y
GLN	ASN	ASN	G334	P272	Y144	E79	G15	Y
ILE	ARG	ARG	Q335	G273	Q145	L80	M16	Y
ILE	GLY	GLY	G336	I274	V148	N81	D17	Y
GLU	ARG	ARG	Q336	K275	L209	K82	G18	Y
GLN	GLN	GLN	Y337	V276	L210	R83	P19	Y
LYS	LYS	LYS	T338	R277	P150	T84	K20	Y
VAL	VAL	VAL	Y339	Q278	Q151	Q85	V21	Y
LYS	VAL	VAL	Q340	L279	G152	F87	K22	Y
THR	THR	THR	Y341	C280	W153	N87	L26	Y
LEU	LEU	LEU	Y342	K281	K154	N88	T27	Y
LYS	THR	THR	Q343	L282	G155	E89	T27	Y
ASP	ASP	ASP	E344	L283	S156	V90	E28	Y
TYR	THR	THR	P345	R284	P157	Q91	E29	Y
LEU	THR	THR	F346	G285	A158	L92	K30	Y
ALA	ASN	ASN	K347	T286	I159	G93	I31	Y
GLN	GLN	GLN	N348	K287	F160	I94	K32	Y
LYS	LYS	LYS	I349	A288	Q161	P95	A33	Y
THR	THR	THR	K350	L289	S162	H96	L34	Y
ALA	GLU	GLU	T351	T290	M164	P97	V35	Y
LEU	LEU	LEU	G352	E291	T165	L100	E36	Y
GLN	GLN	GLN	K353	V292	PR0	K101	I37	Y
LYS	LYS	LYS	Y354	I293	PHE	K102	C38	Y
ALA	ALA	ALA	A355	P294	LEU	R103	T39	Y
L421	L422	L423	R356	L295	L167	E40	E40	Y
L423	K424	K425	K357	T296	L168	M41	M41	Y
L425	L426	L427	R358	E297	P170	E42	E42	Y
W426	Y427	Y428	G359	E298	F171	K43	K43	Y
Q428	Q429	L429	A360	A299	R172	E44	E44	Y
E430	LYS	LYS	H361	E300	K173	G45	G45	Y
LYS	LEU	LEU	T362	L301	Q174	I47	I47	Y
LEU	GLU	GLU	K363	E302	M175	D113	D113	Y
GLU	GLU	GLU	D364	Q303	I178	A114	A114	Y
VAL	VAL	VAL	V365	A304	P243	Y115	Y115	Y
SER	PRO	PRO	K366	E305	V179	F116	F116	Y
ASN	ASN	ASN	Q367	N306	I180	S117	G51	Y
ILE	ILE	ILE	L368	R307	Y181	V118	P52	Y
VAL	VAL	VAL	T369	E308	Q182	P119	E53	Y
ARG	THR	THR	E370	I309	Y183	L120	N54	Y
LYS	ASP	ASP	A371	L310	M184	D121	P55	Y
VAL	VAL	VAL	THR	K311	E122	E123	T58	Y
LEU	GLN	GLN	PHE	E312	D185	F124	P59	Y
TYR	TYR	TYR	T375	P313	L187	R125	I62	Y
ALA	VAL	VAL	T376	V314	Y188	Y127	I63	Y
LEU	LEU	LEU	T377	H315	V189	T128	A62	Y
ASP	GLY	GLY	S379	G316	G190	I63	I63	Y
ILE	ILE	ILE		D256	S191	K64	K64	Y

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.20Å 154.60Å 155.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.13 – 2.90 29.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (14.13-2.90) 90.4 (29.94-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.90Å)	Xtriage
Refinement program	BUSTER/TNT	Depositor
R, $R_{free}$	0.261 , 0.351 0.276 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	66.3	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 84.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.58$ , $\langle L^2 \rangle = 0.44$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8120	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: I15

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	0.90	3/4562 (0.1%)	1.08	8/6199 (0.1%)
1	B	0.90	0/3510	1.07	8/4772 (0.2%)
All	All	0.90	3/8072 (0.0%)	1.08	16/10971 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	GLU	CG-CD	6.18	1.61	1.51
1	A	516	GLU	CB-CG	5.39	1.62	1.52
1	A	432	GLU	CG-CD	5.20	1.59	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	420	PRO	C-N-CD	-9.69	99.27	120.60
1	A	139	THR	C-N-CD	-9.58	99.53	120.60
1	B	312	GLU	C-N-CD	-9.18	100.40	120.60
1	B	344	GLU	C-N-CD	-7.69	103.68	120.60
1	B	132	ILE	C-N-CD	-7.13	104.90	120.60
1	A	357	MET	N-CA-C	-6.21	94.23	111.00
1	A	349	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	216	THR	C-N-CD	-5.78	107.87	120.60
1	A	246	LEU	CA-CB-CG	5.73	128.49	115.30
1	A	346	PHE	CB-CA-C	5.66	121.71	110.40
1	B	286	THR	N-CA-C	-5.31	96.67	111.00
1	B	103	LYS	CD-CE-NZ	-5.28	99.55	111.70
1	B	312	GLU	C-N-CA	5.21	143.88	122.00
1	B	320	ASP	C-N-CD	-5.19	109.18	120.60
1	A	425	LEU	CA-CB-CG	-5.09	103.58	115.30
1	A	429	LEU	CB-CG-CD1	-5.09	102.34	111.00



There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4445	0	4493	620	0
1	B	3414	0	3443	399	0
2	A	22	0	9	1	0
3	A	152	0	0	25	0
3	B	87	0	0	10	0
All	All	8120	0	7945	989	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 62.

All (989) 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:104:LYS:HB3	1:A:192:ASP:HA	1.20	1.18
1:B:103:LYS:HE3	1:B:179:VAL:HG21	1.24	1.15
1:A:64:LYS:HE3	1:A:69:THR:HA	1.22	1.10
1:A:174:GLN:HA	1:A:174:GLN:HE21	1.14	1.07
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.33	1.06
1:B:84:THR:HG21	1:B:153:TRP:HE1	1.20	1.05
1:A:52:PRO:HD2	1:A:53:GLU:HG2	1.38	1.03
1:B:241:VAL:HG23	1:B:243:PRO:HD3	1.36	1.03
1:B:260:LEU:HG	1:B:264:LEU:HD12	1.42	1.02
1:A:288:ALA:CB	1:A:291:GLU:HB2	1.90	1.01
1:A:102:LYS:HE2	1:A:320:ASP:HB2	1.41	1.01
1:A:538:ALA:HA	1:A:545:ASN:HD21	1.23	1.00
1:B:194:GLU:HG3	1:B:197:GLN:HB2	1.42	1.00
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.25	0.99
1:A:64:LYS:HB3	1:A:65:LYS:HA	1.45	0.98
1:A:101:LYS:HD3	1:A:103:LYS:HE2	1.47	0.97
1:A:94:ILE:HD12	1:A:95:PRO:HD2	1.46	0.96
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:HD12	1:A:267:ALA:HB2	1.47	0.95
1:A:540:LYS:HB3	1:A:542:ILE:HD12	1.49	0.94
1:A:257:ILE:HG22	1:A:283:LEU:HD11	1.49	0.94
1:A:381:VAL:HG12	1:A:382:ILE:N	1.82	0.93
1:B:103:LYS:HE3	1:B:179:VAL:CG2	1.98	0.93
1:B:209:LEU:HD22	1:B:214:LEU:HD12	1.49	0.93
1:A:241:VAL:HG22	1:A:266:TRP:NE1	1.85	0.92
1:A:96:HIS:HD2	1:A:98:ALA:H	1.08	0.92
1:B:175:ASN:HD21	1:B:201:LYS:HE2	1.34	0.92
1:A:258:GLN:HG3	1:A:283:LEU:CD2	2.01	0.91
1:A:252:TRP:HD1	1:A:295:LEU:HD11	1.33	0.91
1:A:76:ASP:OD1	1:A:78:ARG:HG3	1.69	0.90
1:A:435:VAL:HA	1:B:290:THR:HG21	1.53	0.90
1:A:241:VAL:HG22	1:A:266:TRP:CD1	2.07	0.90
1:B:246:LEU:HD21	1:B:310:LEU:HD11	1.52	0.89
1:A:311:LYS:HE3	1:A:311:LYS:HA	1.51	0.89
1:B:84:THR:HG21	1:B:153:TRP:NE1	1.86	0.89
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.54	0.89
1:A:88:TRP:HD1	1:A:90:VAL:HG13	1.37	0.89
1:B:241:VAL:CG2	1:B:243:PRO:HD3	2.02	0.89
1:B:365:VAL:O	1:B:369:THR:HG23	1.73	0.88
1:A:356:ARG:HD2	1:A:359:GLY:HA3	1.56	0.88
1:A:172:ARG:HH12	1:A:182:GLN:HE21	1.22	0.88
1:A:174:GLN:HA	1:A:174:GLN:NE2	1.86	0.87
1:A:252:TRP:CD1	1:A:295:LEU:HD11	2.08	0.87
1:A:335:GLY:HA2	1:A:367:GLN:NE2	1.89	0.87
1:A:334:GLN:HE22	1:A:336:GLN:HE21	1.23	0.87
1:B:118:VAL:HG12	1:B:149:LEU:HG	1.55	0.87
1:A:293:ILE:CG1	1:A:294:PRO:HD2	2.05	0.87
1:A:64:LYS:CE	1:A:69:THR:HA	2.03	0.87
1:B:28:GLU:HB2	1:B:135:ILE:HD11	1.52	0.87
1:A:172:ARG:HH12	1:A:182:GLN:NE2	1.73	0.86
1:B:215:THR:HG22	1:B:217:PRO:CD	2.06	0.86
1:A:252:TRP:HB3	1:A:257:ILE:CD1	2.05	0.86
1:A:424:LYS:HE2	1:A:426:TRP:CZ2	2.10	0.86
1:A:224:GLU:HB2	1:A:225:PRO:HD2	1.57	0.86
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.40	0.86
1:A:5:ILE:HD13	1:A:167:ILE:HG13	1.55	0.86
1:B:163:SER:O	1:B:167:ILE:HG13	1.74	0.86
1:A:189:VAL:HG11	1:A:202:ILE:HD11	1.58	0.86
1:B:284:ARG:NH2	1:B:284:ARG:HB3	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LYS:CB	1:A:192:ASP:HA	2.04	0.85
1:B:13:LYS:HB2	1:B:16:MET:HE3	1.59	0.85
1:B:257:ILE:HG22	1:B:283:LEU:HD11	1.58	0.85
1:A:335:GLY:HA3	1:A:356:ARG:CG	2.07	0.84
1:B:103:LYS:HG2	1:B:191:SER:N	1.92	0.84
1:A:335:GLY:HA3	1:A:356:ARG:HG2	1.59	0.84
1:A:96:HIS:CD2	1:A:98:ALA:H	1.94	0.84
1:B:258:GLN:HG3	1:B:283:LEU:HD22	1.60	0.84
1:B:341:ILE:HD11	1:B:375:ILE:HG23	1.60	0.84
1:A:357:MET:CE	1:A:360:ALA:HB3	2.08	0.83
1:A:252:TRP:HB3	1:A:257:ILE:HD11	1.58	0.83
1:A:395:LYS:HD3	1:A:414:TRP:CZ3	2.13	0.83
1:B:260:LEU:HG	1:B:264:LEU:CD1	2.08	0.83
1:B:84:THR:HG22	1:B:88:TRP:HD1	1.43	0.83
1:A:293:ILE:HG13	1:A:294:PRO:HD2	1.61	0.83
1:A:402:TRP:CD1	1:A:403:THR:HG23	2.13	0.82
1:A:125:ARG:HG2	1:A:146:TYR:O	1.78	0.82
1:A:27:THR:CG2	1:A:29:GLU:HB3	2.08	0.82
1:B:366:LYS:HG2	1:B:405:TYR:CD2	2.15	0.82
1:A:242:GLN:HG3	1:A:243:PRO:HD2	1.60	0.82
1:B:37:ILE:O	1:B:41:MET:HG3	1.80	0.82
1:B:215:THR:HG22	1:B:217:PRO:HD3	1.61	0.81
1:B:76:ASP:OD1	1:B:78:ARG:HG3	1.80	0.81
1:A:238:LYS:HE3	1:A:315:HIS:CG	2.15	0.81
1:B:28:GLU:CB	1:B:135:ILE:HD11	2.09	0.81
1:B:254:VAL:HB	1:B:289:LEU:HA	1.63	0.81
1:A:434:ILE:HG13	1:A:494:ASN:HD21	1.44	0.81
1:A:451:LYS:NZ	1:A:451:LYS:HB3	1.95	0.81
1:A:538:ALA:HA	1:A:545:ASN:ND2	1.94	0.81
1:A:395:LYS:HD3	1:A:414:TRP:CH2	2.15	0.81
1:A:516:GLU:O	1:A:520:GLN:HG2	1.80	0.81
1:A:258:GLN:HG3	1:A:283:LEU:HD21	1.63	0.80
1:A:424:LYS:HE2	1:A:426:TRP:CH2	2.15	0.80
1:B:81:ASN:ND2	1:B:154:LYS:HD2	1.97	0.80
1:B:175:ASN:ND2	1:B:201:LYS:HE2	1.96	0.80
1:A:486:LEU:HD22	1:A:528:LYS:HD2	1.63	0.80
1:A:350:LYS:HE3	1:A:378:GLU:OE2	1.81	0.79
1:A:396:GLU:H	1:A:396:GLU:CD	1.85	0.79
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.64	0.79
1:B:249:LYS:HD3	1:B:250:ASP:N	1.96	0.79
1:B:3:SER:N	1:B:4:PRO:HD2	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:VAL:O	1:B:280:CYS:HB2	1.82	0.79
1:B:358:ARG:HB3	1:B:358:ARG:CZ	2.11	0.79
1:B:246:LEU:HD21	1:B:310:LEU:CD1	2.11	0.79
1:A:325:LEU:C	1:A:326:ILE:HD13	2.04	0.78
1:A:197:GLN:O	1:A:201:LYS:HB2	1.84	0.78
1:A:211:ARG:HD2	3:A:2070:HOH:O	1.84	0.78
1:A:167:ILE:HG21	1:A:209:LEU:HD23	1.65	0.78
1:B:276:VAL:HA	1:B:302:GLU:OE2	1.84	0.77
1:A:29:GLU:HG2	1:A:71:TRP:HH2	1.49	0.77
1:B:284:ARG:HB3	1:B:284:ARG:HH21	1.48	0.77
1:B:356:ARG:NH1	1:B:358:ARG:NH2	2.33	0.77
1:A:540:LYS:HB3	1:A:542:ILE:CD1	2.15	0.77
1:A:31:ILE:HD13	1:A:133:PRO:O	1.84	0.77
1:A:177:ASP:HB2	3:A:2059:HOH:O	1.85	0.77
1:B:278:GLN:HB2	1:B:302:GLU:OE1	1.85	0.77
1:A:21:VAL:HG12	1:A:59:PRO:HD3	1.67	0.77
1:A:538:ALA:CA	1:A:545:ASN:HD21	1.98	0.76
1:A:195:ILE:HG22	1:A:199:ARG:HD2	1.67	0.76
1:A:64:LYS:CB	1:A:65:LYS:HA	2.16	0.76
1:B:64:LYS:HE3	1:B:69:THR:OG1	1.85	0.76
1:A:206:ARG:HH21	1:A:218:ASP:N	1.83	0.76
1:B:91:GLN:C	1:B:92:LEU:HD23	2.06	0.76
1:A:545:ASN:HA	3:A:2139:HOH:O	1.86	0.76
1:A:228:LEU:HD13	1:A:242:GLN:HE21	1.50	0.76
1:A:419:THR:O	1:A:419:THR:HG23	1.86	0.76
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.82	0.75
1:B:249:LYS:HA	1:B:252:TRP:CZ2	2.20	0.75
1:A:311:LYS:HA	1:A:311:LYS:CE	2.14	0.75
1:A:516:GLU:HA	1:A:519:ASN:HB2	1.68	0.75
1:B:260:LEU:O	1:B:264:LEU:HD12	1.87	0.75
1:A:29:GLU:HG2	1:A:71:TRP:CH2	2.21	0.74
1:B:27:THR:OG1	1:B:30:LYS:HG3	1.86	0.74
1:A:524:GLN:HA	1:A:524:GLN:NE2	2.02	0.74
1:B:40:GLU:O	1:B:44:GLU:HG3	1.86	0.74
1:A:228:LEU:HD13	1:A:242:GLN:NE2	2.02	0.74
1:B:94:ILE:HD12	1:B:94:ILE:N	2.02	0.74
1:A:458:VAL:HG23	1:B:286:THR:CG2	2.17	0.74
1:B:21:VAL:CG2	1:B:79:GLU:HG3	2.18	0.74
1:A:394:GLN:HB3	1:A:396:GLU:OE1	1.86	0.74
1:A:258:GLN:HG3	1:A:283:LEU:HD22	1.69	0.74
1:A:31:ILE:O	1:A:35:VAL:HG23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:HD3	1:A:103:LYS:CE	2.17	0.74
1:B:189:VAL:HB	1:B:202:ILE:HD11	1.70	0.73
1:B:255:ASN:O	1:B:259:LYS:HG3	1.88	0.73
1:B:253:THR:O	1:B:257:ILE:HG13	1.87	0.73
1:A:433:PRO:HG3	1:B:255:ASN:ND2	2.04	0.73
1:A:448:ARG:HG3	1:A:448:ARG:HH11	1.54	0.73
1:B:231:GLY:HA3	1:B:232:TYR:C	2.09	0.73
1:B:66:LYS:HG3	1:B:407:GLN:OE1	1.88	0.73
1:A:247:PRO:HG2	3:A:2088:HOH:O	1.89	0.73
1:A:296:THR:CG2	1:A:299:ALA:H	2.02	0.73
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.71	0.72
1:A:173:LYS:HE3	1:A:174:GLN:HG2	1.70	0.72
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.24	0.72
1:A:510:PRO:HG3	3:A:2141:HOH:O	1.90	0.72
1:A:511:ASP:OD1	1:A:512:GLN:HG3	1.88	0.72
1:A:485:ALA:O	1:A:489:SER:HB3	1.89	0.72
1:A:88:TRP:CD1	1:A:90:VAL:HG13	2.24	0.72
1:B:312:GLU:OE1	1:B:313:PRO:HD2	1.89	0.72
1:A:109:LEU:HD13	1:A:216:THR:HG21	1.72	0.71
1:B:20:LYS:HE3	1:B:55:PRO:HB2	1.72	0.71
1:A:271:TYR:CD1	1:A:310:LEU:HD23	2.24	0.71
1:B:345:PRO:O	1:B:346:PHE:HB2	1.89	0.71
1:A:406:TRP:HZ3	1:B:418:ASN:HA	1.56	0.71
1:A:491:LEU:HD23	1:A:491:LEU:H	1.55	0.71
1:B:371:ALA:O	1:B:375:ILE:HD12	1.90	0.71
1:B:162:SER:O	1:B:166:LYS:HD2	1.90	0.70
1:B:134:SER:HB3	1:B:139:THR:HB	1.73	0.70
1:B:66:LYS:HA	1:B:407:GLN:NE2	2.05	0.70
1:A:402:TRP:HD1	1:A:403:THR:HG23	1.57	0.70
1:A:524:GLN:O	1:A:526:ILE:N	2.25	0.70
1:B:269:GLN:HG2	1:B:346:PHE:CE2	2.26	0.70
1:B:331:LYS:HE3	1:B:364:ASP:OD2	1.89	0.70
1:A:288:ALA:HB3	1:A:291:GLU:CB	2.17	0.70
1:B:85:GLN:HA	1:B:88:TRP:NE1	2.06	0.70
1:A:220:LYS:HB3	1:A:221:HIS:CD2	2.26	0.70
1:A:189:VAL:HG21	1:A:205:LEU:HD23	1.72	0.70
1:A:494:ASN:HD22	1:A:494:ASN:N	1.88	0.70
1:B:284:ARG:O	1:B:284:ARG:HG2	1.91	0.70
1:B:40:GLU:HG3	3:B:2015:HOH:O	1.90	0.70
1:B:248:GLU:HA	1:B:307:ARG:HH22	1.56	0.70
1:A:27:THR:HG22	1:A:29:GLU:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ALA:O	1:A:356:ARG:O	2.10	0.69
1:A:434:ILE:HG13	1:A:494:ASN:ND2	2.07	0.69
1:A:461:ARG:HH11	1:A:461:ARG:CG	2.05	0.69
1:A:542:ILE:O	1:A:545:ASN:HB3	1.91	0.69
1:A:53:GLU:O	1:A:55:PRO:HD3	1.93	0.69
1:B:319:TYR:OH	1:B:385:LYS:HE3	1.92	0.69
1:A:536:VAL:HG21	1:A:545:ASN:HB2	1.75	0.69
1:B:72:ARG:NH2	1:B:151:GLN:HE22	1.91	0.69
1:A:245:VAL:O	1:A:247:PRO:HD3	1.92	0.69
1:B:92:LEU:HD23	1:B:92:LEU:N	2.08	0.69
1:A:334:GLN:NE2	1:A:336:GLN:HE21	1.90	0.69
1:A:58:THR:HG22	1:A:76:ASP:O	1.92	0.69
1:A:5:ILE:HD13	1:A:167:ILE:CG1	2.23	0.68
1:A:277:ARG:NH2	1:A:334:GLN:HG3	2.07	0.68
1:A:464:GLN:HG3	1:A:465:LYS:N	2.08	0.68
1:A:61:PHE:HB2	3:A:2025:HOH:O	1.91	0.68
1:B:354:TYR:HE1	1:B:357:MET:HE1	1.58	0.68
1:B:182:GLN:HB2	1:B:187:LEU:HD23	1.74	0.68
1:B:72:ARG:HG2	1:B:73:LYS:N	2.09	0.68
1:B:231:GLY:HA3	1:B:232:TYR:O	1.94	0.68
1:A:1:PRO:O	1:A:2:ILE:HG13	1.94	0.68
1:B:395:LYS:HG2	1:B:416:PHE:CE2	2.28	0.68
1:A:172:ARG:NH1	1:A:182:GLN:HE21	1.92	0.67
1:A:260:LEU:O	1:A:264:LEU:HB2	1.94	0.67
1:A:26:LEU:HD12	1:A:133:PRO:CD	2.24	0.67
1:A:274:ILE:HD12	1:A:309:ILE:HG21	1.75	0.67
1:A:326:ILE:N	1:A:326:ILE:HD13	2.07	0.67
1:A:216:THR:HG22	1:A:217:PRO:N	2.10	0.67
1:B:139:THR:HG22	1:B:140:PRO:O	1.94	0.67
1:A:357:MET:HE1	1:A:360:ALA:HB3	1.76	0.67
1:B:313:PRO:O	1:B:315:HIS:N	2.27	0.67
1:B:21:VAL:HB	1:B:59:PRO:HD3	1.77	0.67
1:B:241:VAL:HG23	1:B:243:PRO:CD	2.20	0.66
1:A:189:VAL:CG1	1:A:202:ILE:HD11	2.24	0.66
1:A:175:ASN:H	1:A:176:PRO:HD3	1.60	0.66
1:A:23:GLN:HE22	1:A:60:VAL:H	1.42	0.66
1:A:206:ARG:O	1:A:209:LEU:N	2.27	0.66
1:A:175:ASN:N	1:A:176:PRO:HD3	2.08	0.66
1:A:216:THR:HG23	1:A:217:PRO:HD2	1.78	0.66
1:A:288:ALA:HB1	1:A:291:GLU:HB2	1.78	0.66
1:A:273:GLY:O	1:A:332:GLN:NE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LYS:HE3	1:A:69:THR:CA	2.13	0.66
1:B:175:ASN:HB2	1:B:178:ILE:HG13	1.78	0.66
1:A:257:ILE:CG2	1:A:283:LEU:HD11	2.25	0.66
1:A:491:LEU:HD23	1:A:491:LEU:N	2.10	0.66
1:A:27:THR:HB	1:A:30:LYS:HD2	1.77	0.65
1:A:543:GLY:HA3	1:B:285:GLY:H	1.61	0.65
1:B:84:THR:CG2	1:B:153:TRP:HE1	2.04	0.65
1:A:101:LYS:CD	1:A:103:LYS:HE2	2.24	0.65
1:A:390:LYS:C	1:A:391:LEU:HD23	2.16	0.65
1:A:407:GLN:NE2	1:B:418:ASN:OD1	2.29	0.65
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.95	0.65
1:A:357:MET:HE2	1:A:360:ALA:HB3	1.77	0.65
1:A:96:HIS:HD2	1:A:98:ALA:N	1.89	0.65
1:B:295:LEU:HD12	1:B:295:LEU:H	1.62	0.65
1:B:114:ALA:HB1	1:B:160:PHE:CZ	2.32	0.65
1:B:341:ILE:HD11	1:B:375:ILE:CG2	2.27	0.65
1:A:381:VAL:CG1	1:A:382:ILE:N	2.57	0.64
1:A:458:VAL:HG23	1:B:286:THR:HG21	1.78	0.64
1:B:84:THR:HG22	1:B:88:TRP:CD1	2.28	0.64
1:A:278:GLN:HG2	1:A:298:GLU:HB3	1.78	0.64
1:A:486:LEU:HB3	1:A:524:GLN:HG3	1.79	0.64
1:B:214:LEU:HD23	1:B:214:LEU:N	2.12	0.64
1:A:199:ARG:O	1:A:219:LYS:NZ	2.30	0.64
1:A:275:LYS:HE3	1:A:305:GLU:OE1	1.97	0.64
1:B:278:GLN:N	1:B:302:GLU:OE1	2.30	0.64
1:A:356:ARG:HH11	1:A:512:GLN:NE2	1.96	0.64
1:A:335:GLY:CA	1:A:367:GLN:HE22	2.06	0.64
1:A:230:MET:HE3	3:A:2079:HOH:O	1.97	0.64
1:A:11:LYS:HG3	1:A:12:LEU:N	2.12	0.63
1:B:142:ILE:HG22	1:B:144:TYR:CE1	2.34	0.63
1:A:52:PRO:CD	1:A:53:GLU:H	2.11	0.63
1:A:172:ARG:NH1	1:A:182:GLN:NE2	2.46	0.63
1:A:29:GLU:CG	1:A:71:TRP:HH2	2.11	0.63
1:B:103:LYS:HG2	1:B:190:GLY:C	2.19	0.63
1:B:28:GLU:OE2	1:B:32:LYS:NZ	2.29	0.63
1:A:228:LEU:HB3	1:A:242:GLN:HE22	1.63	0.63
1:A:293:ILE:HG12	1:A:294:PRO:HD2	1.80	0.63
1:B:122:GLU:CD	1:B:122:GLU:H	2.02	0.63
1:B:279:LEU:HG	1:B:302:GLU:OE2	1.99	0.63
1:A:189:VAL:HG21	1:A:205:LEU:CD2	2.28	0.63
1:A:271:TYR:CE1	1:A:310:LEU:HD23	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:HD3	3:A:2016:HOH:O	1.97	0.63
1:A:334:GLN:O	1:A:334:GLN:NE2	2.27	0.63
1:A:543:GLY:N	1:B:283:LEU:O	2.27	0.63
1:B:13:LYS:CB	1:B:16:MET:HE3	2.28	0.63
1:B:94:ILE:HD12	1:B:94:ILE:H	1.64	0.63
1:B:12:LEU:HD11	1:B:127:TYR:CE1	2.34	0.63
1:B:360:ALA:CB	1:B:366:LYS:HZ3	2.11	0.63
1:B:21:VAL:HG21	1:B:79:GLU:HG3	1.80	0.62
1:A:107:THR:HG21	1:A:202:ILE:HG13	1.81	0.62
1:B:114:ALA:HB2	1:B:214:LEU:HD13	1.81	0.62
1:A:97:PRO:HG2	1:A:232:TYR:CE2	2.34	0.62
1:A:503:LEU:HD23	1:B:422:LEU:HD11	1.80	0.62
1:B:319:TYR:O	1:B:321:PRO:HD3	1.99	0.62
1:A:105:SER:HB2	1:A:198:HIS:CD2	2.34	0.62
1:A:13:LYS:O	1:A:16:MET:HB2	2.00	0.62
1:A:206:ARG:HH21	1:A:217:PRO:C	2.02	0.62
1:B:344:GLU:O	1:B:347:LYS:HB2	1.99	0.62
1:A:360:ALA:HB2	1:A:514:GLU:OE2	2.00	0.62
1:B:279:LEU:HA	1:B:282:LEU:CD1	2.29	0.62
1:B:274:ILE:C	1:B:275:LYS:HG2	2.20	0.62
1:A:460:ASN:ND2	1:B:288:ALA:HB2	2.14	0.62
1:A:162:SER:OG	1:B:52:PRO:HG3	2.00	0.62
1:B:85:GLN:HG3	1:B:85:GLN:O	1.98	0.62
1:A:252:TRP:HB3	1:A:257:ILE:HD12	1.81	0.62
1:A:253:THR:HA	1:A:292:VAL:HA	1.82	0.62
1:A:254:VAL:CG2	1:A:291:GLU:HB3	2.30	0.62
1:B:308:GLU:O	1:B:311:LYS:HD3	2.00	0.62
1:B:34:LEU:HD22	1:B:73:LYS:HG2	1.81	0.62
1:B:366:LYS:O	1:B:370:GLU:HG2	2.00	0.62
1:B:114:ALA:HB1	1:B:160:PHE:CE2	2.35	0.61
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.35	0.61
1:A:434:ILE:HD13	1:A:530:LYS:CB	2.25	0.61
1:B:20:LYS:HG2	1:B:55:PRO:O	2.00	0.61
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.32	0.61
1:B:210:LEU:HD12	1:B:210:LEU:O	1.99	0.61
1:A:1:PRO:O	1:A:46:LYS:NZ	2.33	0.61
1:B:203:GLU:O	1:B:206:ARG:HB2	2.01	0.61
1:A:303:LEU:O	1:A:303:LEU:HD12	2.01	0.61
1:B:215:THR:HG22	1:B:217:PRO:HD2	1.81	0.61
1:A:312:GLU:N	1:A:312:GLU:OE2	2.27	0.61
1:B:13:LYS:HB2	1:B:16:MET:CE	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:PRO:HG2	1:B:389:PHE:CZ	2.36	0.61
1:B:324:ASP:O	1:B:343:GLN:HG2	2.01	0.60
1:A:101:LYS:HE2	1:A:103:LYS:HZ1	1.66	0.60
1:A:93:GLY:O	1:B:137:ASN:ND2	2.34	0.60
1:B:118:VAL:CG1	1:B:149:LEU:HG	2.30	0.60
1:A:335:GLY:CA	1:A:356:ARG:HG2	2.30	0.60
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.36	0.60
1:B:115:TYR:HB3	1:B:149:LEU:HB2	1.83	0.60
1:B:259:LYS:NZ	3:B:2060:HOH:O	2.25	0.60
1:B:374:LYS:O	1:B:378:GLU:HG3	2.01	0.60
1:B:425:LEU:O	1:B:428:GLN:HB3	2.01	0.60
1:A:180:ILE:HG12	1:A:189:VAL:HG22	1.84	0.60
1:B:379:SER:HB2	1:B:385:LYS:O	2.02	0.60
1:B:241:VAL:HG23	1:B:242:GLN:N	2.16	0.60
1:B:258:GLN:HG3	1:B:283:LEU:CD2	2.31	0.60
1:A:194:GLU:O	1:A:196:GLY:N	2.34	0.60
1:A:228:LEU:HB3	1:A:242:GLN:NE2	2.17	0.60
1:A:103:LYS:NZ	1:A:192:ASP:OD2	2.30	0.60
1:B:92:LEU:HB2	1:B:158:ALA:HB1	1.82	0.60
1:A:238:LYS:HE3	1:A:315:HIS:CD2	2.37	0.59
1:B:278:GLN:HG3	1:B:298:GLU:C	2.23	0.59
1:A:242:GLN:CG	1:A:243:PRO:HD2	2.30	0.59
1:A:296:THR:HG22	1:A:299:ALA:H	1.65	0.59
1:A:369:THR:O	1:A:373:GLN:HB2	2.02	0.59
1:A:167:ILE:CG2	1:A:209:LEU:HD23	2.33	0.59
1:A:206:ARG:NH2	1:A:218:ASP:OD1	2.35	0.59
1:A:252:TRP:CB	1:A:257:ILE:HD11	2.30	0.59
1:A:398:TRP:CH2	1:A:409:THR:HG23	2.37	0.59
1:B:376:THR:CG2	1:B:386:THR:HG22	2.32	0.59
1:A:241:VAL:CG2	1:A:266:TRP:CD1	2.85	0.59
1:B:254:VAL:HG23	1:B:291:GLU:O	2.02	0.59
1:B:248:GLU:HA	1:B:307:ARG:NH2	2.17	0.59
1:B:295:LEU:HD22	1:B:300:GLU:CD	2.23	0.59
1:A:543:GLY:HA3	1:B:285:GLY:N	2.17	0.59
1:A:20:LYS:NZ	1:A:55:PRO:HB2	2.18	0.59
1:A:206:ARG:NH2	1:A:218:ASP:HA	2.18	0.58
1:A:30:LYS:HD3	3:A:2011:HOH:O	2.03	0.58
1:A:460:ASN:HA	1:B:286:THR:O	2.02	0.58
1:A:527:LYS:O	1:A:528:LYS:O	2.21	0.58
1:B:351:THR:OG1	1:B:351:THR:O	2.20	0.58
1:A:254:VAL:HG23	1:A:291:GLU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:HD11	1:A:501:TYR:CE2	2.39	0.58
1:B:216:THR:H	1:B:217:PRO:CD	2.16	0.58
1:B:387:PRO:HG2	1:B:389:PHE:CE1	2.38	0.58
1:B:78:ARG:NH1	1:B:412:PRO:O	2.36	0.58
1:B:34:LEU:CD2	1:B:73:LYS:HG2	2.33	0.58
1:A:189:VAL:HG11	1:A:202:ILE:CD1	2.33	0.58
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.84	0.58
1:A:265:ASN:HA	1:A:268:SER:HB3	1.85	0.58
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.32	0.58
1:A:155:GLY:HA2	3:A:2053:HOH:O	2.04	0.58
1:A:172:ARG:NH2	1:A:180:ILE:O	2.37	0.58
1:B:272:PRO:O	1:B:274:ILE:N	2.37	0.58
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.32	0.58
1:B:103:LYS:HD3	1:B:190:GLY:HA3	1.86	0.58
1:B:278:GLN:NE2	1:B:298:GLU:HB2	2.18	0.58
1:B:30:LYS:HB3	1:B:62:ALA:HB3	1.84	0.58
1:B:50:ILE:CG2	1:B:145:GLN:HB3	2.33	0.58
1:A:221:HIS:CD2	1:A:221:HIS:N	2.71	0.57
1:A:285:GLY:HA2	1:A:286:THR:OG1	2.03	0.57
1:B:295:LEU:HD13	1:B:300:GLU:OE2	2.04	0.57
1:A:320:ASP:OD2	1:A:323:LYS:HE3	2.03	0.57
1:B:249:LYS:HA	1:B:252:TRP:HZ2	1.67	0.57
1:B:335:GLY:HA3	1:B:356:ARG:HB3	1.85	0.57
1:B:72:ARG:HH21	1:B:151:GLN:NE2	2.02	0.57
1:A:295:LEU:HD12	1:A:295:LEU:H	1.69	0.57
1:A:493:VAL:C	1:A:494:ASN:HD22	2.08	0.57
1:B:422:LEU:HB3	1:B:426:TRP:CZ2	2.39	0.57
1:A:296:THR:HG23	1:A:299:ALA:H	1.69	0.57
1:A:411:ILE:HG21	1:A:414:TRP:CD1	2.39	0.57
1:B:356:ARG:HH12	1:B:358:ARG:NH2	1.98	0.57
1:B:50:ILE:HG23	1:B:145:GLN:HB3	1.85	0.57
1:A:358:ARG:O	1:A:358:ARG:HD3	2.05	0.57
1:B:266:TRP:CZ3	1:B:427:TYR:CZ	2.93	0.57
1:B:363:ASN:HB3	1:B:366:LYS:HB2	1.86	0.57
1:B:323:LYS:NZ	3:B:2068:HOH:O	2.36	0.57
1:A:448:ARG:CG	1:A:448:ARG:HH11	2.16	0.57
1:B:274:ILE:O	1:B:275:LYS:HE2	2.04	0.57
1:A:479:LEU:HD11	1:A:501:TYR:HE2	1.69	0.57
1:A:284:ARG:O	1:A:284:ARG:HG3	2.05	0.57
1:B:68:SER:O	1:B:68:SER:OG	2.21	0.57
1:A:379:SER:HB3	1:A:383:TRP:HE3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:SER:HB2	1:B:157:PRO:HD3	1.87	0.56
1:A:89:GLU:O	1:A:91:GLN:N	2.38	0.56
1:B:276:VAL:HG22	1:B:276:VAL:O	2.05	0.56
1:A:460:ASN:HD22	1:B:288:ALA:HB2	1.70	0.56
1:B:331:LYS:O	1:B:424:LYS:HD2	2.04	0.56
1:B:63:ILE:HD12	1:B:407:GLN:HA	1.86	0.56
1:A:195:ILE:HG22	1:A:199:ARG:CD	2.34	0.56
1:A:92:LEU:HD12	1:A:92:LEU:O	2.04	0.56
1:A:518:VAL:O	1:A:522:ILE:HD12	2.05	0.56
1:B:156:SER:HB2	1:B:157:PRO:CD	2.36	0.56
1:B:246:LEU:HB3	1:B:260:LEU:HD11	1.88	0.56
1:B:295:LEU:HD22	1:B:300:GLU:OE2	2.05	0.56
1:A:206:ARG:HH21	1:A:218:ASP:CA	2.19	0.56
1:A:52:PRO:HD2	1:A:53:GLU:CG	2.26	0.56
1:A:20:LYS:HE2	1:A:56:TYR:CE1	2.40	0.56
1:A:164:MET:CE	1:A:187:LEU:HD22	2.36	0.56
1:A:320:ASP:OD1	1:A:322:SER:OG	2.24	0.56
1:A:228:LEU:HD23	1:A:228:LEU:N	2.19	0.56
1:A:398:TRP:CZ2	1:A:409:THR:HG23	2.40	0.56
1:A:433:PRO:CG	1:B:255:ASN:ND2	2.68	0.56
1:A:40:GLU:OE2	1:A:43:LYS:HD3	2.06	0.56
1:A:228:LEU:CB	1:A:242:GLN:HE22	2.18	0.56
1:A:258:GLN:CG	1:A:283:LEU:HD22	2.36	0.56
1:B:243:PRO:HA	1:B:310:LEU:O	2.06	0.56
1:A:486:LEU:HD13	1:A:524:GLN:HB3	1.89	0.55
1:B:420:PRO:HB2	1:B:423:VAL:HG23	1.88	0.55
1:A:210:LEU:C	1:A:212:TRP:H	2.07	0.55
1:B:125:ARG:O	1:B:145:GLN:HG3	2.06	0.55
1:B:395:LYS:HD3	1:B:399:GLU:CD	2.27	0.55
1:B:41:MET:CE	1:B:47:ILE:HG23	2.36	0.55
1:A:275:LYS:HG2	1:A:332:GLN:HE22	1.71	0.55
1:A:434:ILE:HB	1:A:437:ALA:HB3	1.89	0.55
1:A:96:HIS:CE1	1:A:269:GLN:HE21	2.24	0.55
1:B:298:GLU:HA	1:B:301:LEU:HD22	1.89	0.55
1:B:27:THR:O	1:B:31:ILE:HG13	2.07	0.55
1:B:356:ARG:HH12	1:B:358:ARG:HH21	1.53	0.55
1:A:228:LEU:CA	1:A:242:GLN:HE22	2.20	0.55
1:A:61:PHE:CE2	1:A:63:ILE:HD12	2.42	0.55
1:B:155:GLY:O	1:B:158:ALA:HB3	2.05	0.55
1:A:296:THR:HG22	1:A:299:ALA:HB2	1.89	0.55
1:B:81:ASN:OD1	1:B:153:TRP:HD1	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:O	1:A:194:GLU:HB3	2.06	0.55
1:A:358:ARG:HE	1:A:358:ARG:HA	1.72	0.55
1:B:257:ILE:O	1:B:261:VAL:HG23	2.06	0.55
1:B:328:GLU:OE2	1:B:342:TYR:OH	2.25	0.55
1:A:88:TRP:HB2	1:B:54:ASN:O	2.07	0.55
1:A:271:TYR:CZ	1:A:314:VAL:HG23	2.42	0.55
1:B:266:TRP:O	1:B:269:GLN:HB2	2.07	0.55
1:A:5:ILE:CD1	1:A:167:ILE:HG13	2.32	0.54
1:A:191:SER:OG	1:A:193:LEU:HB2	2.08	0.54
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.43	0.54
1:B:292:VAL:HG12	1:B:293:ILE:N	2.22	0.54
1:B:46:LYS:HD3	1:B:116:PHE:HB3	1.89	0.54
1:A:295:LEU:HD13	3:A:2099:HOH:O	2.06	0.54
1:A:113:ASP:O	1:A:117:SER:OG	2.25	0.54
1:A:23:GLN:NE2	1:A:59:PRO:HA	2.23	0.54
1:A:27:THR:O	1:A:31:ILE:HG13	2.07	0.54
1:A:351:THR:HG23	1:A:352:GLY:H	1.71	0.54
1:B:216:THR:H	1:B:217:PRO:HD3	1.73	0.54
1:B:282:LEU:H	1:B:282:LEU:HD12	1.73	0.54
1:A:331:LYS:HB2	1:A:337:TRP:CZ3	2.43	0.54
1:A:376:THR:HG23	1:A:386:THR:HG22	1.88	0.54
1:B:169:GLU:O	1:B:173:LYS:HB2	2.08	0.54
1:B:425:LEU:O	1:B:425:LEU:HD22	2.08	0.54
1:A:205:LEU:O	1:A:208:HIS:HB3	2.08	0.54
1:A:402:TRP:CZ3	1:B:364:ASP:HB2	2.43	0.54
1:A:513:SER:CB	1:A:518:VAL:HG11	2.37	0.54
1:A:521:ILE:HG22	1:A:525:LEU:HD12	1.89	0.54
1:A:426:TRP:O	1:A:526:ILE:HG23	2.08	0.54
1:B:122:GLU:HB3	3:B:2038:HOH:O	2.08	0.54
1:A:480:GLN:O	1:A:483:TYR:HB3	2.08	0.54
1:B:175:ASN:CB	1:B:178:ILE:HG13	2.38	0.54
1:A:364:ASP:CB	1:A:423:VAL:HG13	2.37	0.54
1:A:471:ASP:HB3	3:A:2135:HOH:O	2.08	0.54
1:A:312:GLU:O	1:A:312:GLU:OE2	2.27	0.53
1:A:502:ALA:O	1:A:506:ILE:HG13	2.09	0.53
1:B:104:LYS:HD2	1:B:192:ASP:OD1	2.08	0.53
1:B:245:VAL:HG21	1:B:429:LEU:CD2	2.38	0.53
1:B:70:LYS:O	1:B:70:LYS:HG3	2.09	0.53
1:A:253:THR:HG23	1:A:256:ASP:OD1	2.08	0.53
1:A:278:GLN:HG2	1:A:298:GLU:CB	2.38	0.53
1:A:402:TRP:CD1	1:A:403:THR:CG2	2.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LEU:HD12	1:B:127:TYR:CZ	2.43	0.53
1:A:93:GLY:C	1:B:137:ASN:HD22	2.12	0.53
1:A:10:VAL:HG11	1:A:153:TRP:CH2	2.43	0.53
1:A:206:ARG:O	1:A:208:HIS:N	2.41	0.53
1:A:216:THR:CG2	1:A:217:PRO:N	2.72	0.53
1:A:65:LYS:N	3:A:2026:HOH:O	2.40	0.53
1:A:419:THR:CG2	1:A:419:THR:O	2.55	0.53
1:B:72:ARG:NH2	1:B:151:GLN:NE2	2.56	0.53
1:A:156:SER:N	1:A:157:PRO:CD	2.71	0.53
1:A:223:LYS:HG2	3:A:2041:HOH:O	2.08	0.53
1:A:254:VAL:HG23	1:A:291:GLU:HB3	1.91	0.53
1:B:161:GLN:O	1:B:165:THR:HG22	2.08	0.53
1:B:246:LEU:HD12	1:B:307:ARG:HG2	1.91	0.53
1:B:260:LEU:HD23	1:B:279:LEU:HD13	1.91	0.53
1:A:406:TRP:HZ3	1:B:418:ASN:CA	2.20	0.52
1:B:266:TRP:CH2	1:B:427:TYR:CE2	2.97	0.52
1:A:169:GLU:O	1:A:171:PHE:N	2.42	0.52
1:A:308:GLU:O	1:A:311:LYS:HB2	2.09	0.52
1:A:238:LYS:HE3	1:A:315:HIS:ND1	2.24	0.52
1:A:27:THR:HB	1:A:30:LYS:CD	2.40	0.52
1:A:92:LEU:C	1:A:92:LEU:HD12	2.28	0.52
1:B:33:ALA:O	1:B:37:ILE:HD12	2.08	0.52
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.89	0.52
1:A:351:THR:HG23	1:A:352:GLY:N	2.24	0.52
1:A:489:SER:HB2	1:A:493:VAL:HB	1.90	0.52
1:A:538:ALA:CB	1:A:545:ASN:HD21	2.22	0.52
1:B:13:LYS:HG3	1:B:83:ARG:O	2.09	0.52
1:A:255:ASN:O	1:A:258:GLN:N	2.40	0.52
1:A:351:THR:CG2	1:A:352:GLY:N	2.72	0.52
1:A:511:ASP:C	1:A:512:GLN:HG3	2.29	0.52
1:B:363:ASN:CG	1:B:366:LYS:HB2	2.30	0.52
1:B:66:LYS:HB2	1:B:407:GLN:HB3	1.91	0.52
1:A:451:LYS:NZ	1:A:451:LYS:CB	2.70	0.52
1:A:536:VAL:O	1:A:536:VAL:HG23	2.09	0.52
1:B:278:GLN:O	1:B:281:LYS:HB2	2.09	0.52
1:A:94:ILE:CD1	1:A:95:PRO:HD2	2.30	0.52
1:B:118:VAL:HG11	1:B:149:LEU:HD11	1.91	0.52
1:B:390:LYS:HG2	1:B:417:VAL:HG11	1.92	0.52
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.46	0.51
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.46	0.51
1:B:101:LYS:HG2	3:B:2081:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:PRO:HD2	1:B:422:LEU:H	1.75	0.51
1:A:115:TYR:HB3	1:A:149:LEU:HB2	1.92	0.51
1:A:210:LEU:C	1:A:212:TRP:N	2.63	0.51
1:A:208:HIS:O	1:A:212:TRP:HD1	1.93	0.51
1:A:56:TYR:O	1:A:57:ASN:HB2	2.10	0.51
1:B:91:GLN:HB3	1:B:92:LEU:HD23	1.92	0.51
1:B:379:SER:OG	1:B:387:PRO:HD3	2.09	0.51
1:A:198:HIS:C	1:A:200:THR:H	2.12	0.51
1:A:224:GLU:HB2	1:A:225:PRO:CD	2.36	0.51
1:A:335:GLY:HA2	1:A:367:GLN:CD	2.31	0.51
1:B:193:LEU:HB3	1:B:197:GLN:HB3	1.92	0.51
1:A:493:VAL:HG22	1:A:494:ASN:O	2.11	0.51
1:A:523:GLU:O	1:A:524:GLN:O	2.29	0.51
1:B:183:TYR:HE2	1:B:184:MET:HE3	1.76	0.51
1:B:314:VAL:HG11	1:B:317:VAL:HG11	1.93	0.51
1:A:111:VAL:HG11	1:A:214:LEU:HD22	1.91	0.51
1:A:71:TRP:N	1:A:71:TRP:CD1	2.79	0.51
1:B:97:PRO:HG3	1:B:181:TYR:HB2	1.92	0.51
1:A:134:SER:O	1:A:137:ASN:N	2.39	0.51
1:A:188:TYR:HH	1:A:229:TRP:HE1	1.58	0.51
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.32	0.51
1:A:420:PRO:HA	1:A:421:PRO:C	2.31	0.51
1:A:521:ILE:HG22	1:A:525:LEU:CD1	2.40	0.51
1:A:521:ILE:O	1:A:525:LEU:HD12	2.10	0.51
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.93	0.51
1:A:402:TRP:HE3	1:A:409:THR:HG22	1.74	0.51
1:A:63:ILE:O	1:A:71:TRP:HB3	2.11	0.51
1:B:150:PRO:HG2	1:B:153:TRP:HB3	1.92	0.51
1:B:85:GLN:HA	1:B:88:TRP:CE2	2.46	0.51
1:B:22:LYS:O	1:B:59:PRO:HG3	2.11	0.51
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.46	0.51
1:A:406:TRP:CD1	1:A:406:TRP:N	2.75	0.51
1:B:72:ARG:HH21	1:B:151:GLN:HE22	1.59	0.51
1:B:312:GLU:OE1	1:B:312:GLU:HA	2.11	0.51
1:A:228:LEU:CD2	1:A:228:LEU:N	2.74	0.50
1:A:434:ILE:HB	1:A:437:ALA:CB	2.42	0.50
1:A:503:LEU:HD11	1:A:507:GLN:NE2	2.26	0.50
1:B:175:ASN:HD21	1:B:201:LYS:CE	2.17	0.50
1:B:319:TYR:CD1	1:B:383:TRP:CD1	2.99	0.50
1:A:129:ALA:HA	1:A:144:TYR:O	2.11	0.50
1:A:171:PHE:CE2	1:A:205:LEU:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:HG23	1:A:271:TYR:HD2	1.76	0.50
1:A:361:HIS:ND1	1:A:505:ILE:HD13	2.26	0.50
1:B:332:GLN:HB2	1:B:336:GLN:HB2	1.93	0.50
1:B:38:CYS:SG	1:B:132:ILE:HD11	2.50	0.50
1:A:157:PRO:HD2	3:A:2053:HOH:O	2.11	0.50
1:A:405:TYR:CE1	1:A:406:TRP:NE1	2.79	0.50
1:A:11:LYS:O	1:A:85:GLN:HG2	2.12	0.50
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.47	0.50
1:A:209:LEU:O	1:A:212:TRP:HB2	2.12	0.50
1:A:20:LYS:HZ3	1:A:55:PRO:HB2	1.76	0.50
1:A:341:ILE:N	1:A:350:LYS:O	2.35	0.50
1:A:391:LEU:N	1:A:391:LEU:HD23	2.27	0.50
1:B:354:TYR:HE1	1:B:357:MET:CE	2.22	0.50
1:A:20:LYS:HE2	1:A:56:TYR:CD1	2.47	0.50
1:A:451:LYS:HZ3	1:A:451:LYS:HB3	1.73	0.50
1:A:494:ASN:N	1:A:494:ASN:ND2	2.60	0.50
1:B:272:PRO:C	1:B:274:ILE:H	2.15	0.50
1:A:138:GLU:HG2	3:A:2048:HOH:O	2.10	0.50
1:A:398:TRP:CH2	1:A:409:THR:CG2	2.95	0.50
1:A:240:THR:HG23	1:A:241:VAL:O	2.12	0.50
1:A:257:ILE:HG22	1:A:283:LEU:CD1	2.33	0.50
1:B:360:ALA:CB	1:B:366:LYS:NZ	2.75	0.50
1:A:188:TYR:OH	1:A:229:TRP:NE1	2.42	0.49
1:A:228:LEU:CB	1:A:242:GLN:NE2	2.75	0.49
1:A:469:LEU:HD13	1:A:477:THR:HG22	1.93	0.49
1:A:393:ILE:O	1:A:416:PHE:HD1	1.95	0.49
1:B:209:LEU:CD2	1:B:214:LEU:HD12	2.31	0.49
1:A:136:ASN:H	1:A:138:GLU:HG3	1.77	0.49
1:A:271:TYR:CE1	1:A:314:VAL:CG2	2.95	0.49
1:A:238:LYS:HE3	1:A:315:HIS:CE1	2.48	0.49
1:A:328:GLU:OE2	1:A:342:TYR:OH	2.24	0.49
1:A:498:ASP:CB	1:A:538:ALA:HB2	2.42	0.49
1:A:334:GLN:N	1:A:334:GLN:NE2	2.60	0.49
1:B:168:LEU:HD13	1:B:180:ILE:HG21	1.94	0.49
1:A:396:GLU:HA	1:A:399:GLU:HG2	1.95	0.49
1:A:503:LEU:HD11	1:A:507:GLN:HE22	1.77	0.49
1:A:52:PRO:CD	1:A:53:GLU:N	2.74	0.49
1:B:12:LEU:CD1	1:B:127:TYR:CZ	2.96	0.49
1:B:339:TYR:O	1:B:351:THR:HA	2.12	0.49
1:A:296:THR:HG23	1:A:298:GLU:N	2.27	0.49
1:B:212:TRP:CD1	1:B:212:TRP:N	2.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASN:CA	1:A:268:SER:HB3	2.43	0.49
1:A:41:MET:SD	1:A:73:LYS:NZ	2.86	0.49
1:B:178:ILE:HD11	1:B:201:LYS:HG2	1.95	0.49
1:A:249:LYS:CB	1:A:249:LYS:NZ	2.75	0.49
1:A:1:PRO:O	1:A:2:ILE:CG1	2.61	0.49
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.12	0.49
1:B:245:VAL:HG21	1:B:429:LEU:HD22	1.95	0.49
1:B:247:PRO:O	1:B:307:ARG:NH2	2.46	0.49
1:B:266:TRP:CH2	1:B:427:TYR:OH	2.63	0.49
1:A:241:VAL:HG11	1:A:267:ALA:HA	1.94	0.49
1:A:296:THR:HG22	1:A:299:ALA:CB	2.43	0.49
1:B:93:GLY:O	1:B:95:PRO:HD3	2.13	0.49
1:B:116:PHE:HD2	3:B:2034:HOH:O	1.94	0.48
1:B:28:GLU:HB2	1:B:135:ILE:CD1	2.33	0.48
1:A:194:GLU:C	1:A:196:GLY:H	2.17	0.48
1:A:246:LEU:HD21	1:A:310:LEU:HD13	1.95	0.48
1:A:27:THR:HG22	1:A:30:LYS:H	1.78	0.48
1:A:308:GLU:HA	1:A:311:LYS:HD2	1.95	0.48
1:A:358:ARG:HA	1:A:358:ARG:NE	2.28	0.48
1:A:360:ALA:O	1:A:361:HIS:HB2	2.13	0.48
1:A:434:ILE:CG1	1:A:494:ASN:HD21	2.22	0.48
1:A:79:GLU:CG	1:A:83:ARG:HH11	2.26	0.48
1:B:360:ALA:HB2	1:B:366:LYS:NZ	2.28	0.48
1:A:486:LEU:HD13	1:A:524:GLN:CB	2.43	0.48
1:B:44:GLU:HB2	1:B:46:LYS:HG3	1.95	0.48
1:A:529:GLU:HG3	1:A:529:GLU:O	2.12	0.48
1:B:22:LYS:HD3	3:B:2007:HOH:O	2.14	0.48
1:B:41:MET:HE2	1:B:47:ILE:HG23	1.95	0.48
1:B:111:VAL:HG23	1:B:111:VAL:O	2.13	0.48
1:B:172:ARG:HH11	1:B:172:ARG:HG3	1.77	0.48
1:B:242:GLN:O	1:B:242:GLN:OE1	2.31	0.48
1:B:402:TRP:O	1:B:406:TRP:HB2	2.14	0.48
1:A:168:LEU:HD11	1:A:187:LEU:HD21	1.95	0.48
1:A:175:ASN:HD21	1:A:201:LYS:HE3	1.79	0.48
1:A:52:PRO:HD2	1:A:53:GLU:H	1.79	0.48
1:B:103:LYS:HG2	1:B:190:GLY:CA	2.43	0.48
1:A:206:ARG:NH1	1:A:206:ARG:HG2	2.29	0.48
1:A:398:TRP:CE2	1:A:411:ILE:CD1	2.96	0.48
1:A:195:ILE:HB	1:A:199:ARG:HD3	1.95	0.48
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.49	0.48
1:B:317:VAL:HG21	1:B:348:ASN:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:C	1:A:196:GLY:N	2.67	0.48
1:A:402:TRP:CD1	1:A:403:THR:N	2.82	0.48
1:B:118:VAL:HG12	1:B:149:LEU:CG	2.38	0.48
1:B:183:TYR:CE2	1:B:184:MET:HE3	2.49	0.48
1:A:101:LYS:HE2	1:A:103:LYS:NZ	2.29	0.47
1:A:270:ILE:HA	1:A:351:THR:HB	1.96	0.47
1:A:14:PRO:C	1:A:16:MET:H	2.17	0.47
1:B:209:LEU:HD22	1:B:214:LEU:CD1	2.32	0.47
1:B:361:HIS:HB2	3:B:2076:HOH:O	2.14	0.47
3:A:2140:HOH:O	1:B:422:LEU:HB2	2.14	0.47
1:A:228:LEU:CD1	1:A:242:GLN:NE2	2.75	0.47
1:A:490:GLY:O	1:A:492:GLU:N	2.47	0.47
1:A:479:LEU:HB2	1:A:517:LEU:HD13	1.95	0.47
1:B:18:GLY:HA3	1:B:127:TYR:CD1	2.50	0.47
1:B:314:VAL:HG11	1:B:317:VAL:CG1	2.44	0.47
1:A:183:TYR:O	1:A:186:ASP:HB2	2.14	0.47
1:A:448:ARG:HG2	1:A:448:ARG:H	1.55	0.47
1:A:181:TYR:CD1	1:B:138:GLU:HB3	2.49	0.47
1:B:7:THR:O	1:B:9:PRO:HD3	2.14	0.47
1:A:209:LEU:O	1:A:212:TRP:N	2.46	0.47
1:A:23:GLN:HE22	1:A:60:VAL:N	2.10	0.47
1:A:276:VAL:HG13	1:A:276:VAL:O	2.14	0.47
1:A:339:TYR:OH	1:A:378:GLU:OE1	2.30	0.47
1:A:4:PRO:HG2	1:A:212:TRP:CE3	2.50	0.47
1:A:79:GLU:O	1:A:82:LYS:N	2.47	0.47
1:B:30:LYS:O	1:B:34:LEU:HG	2.14	0.47
1:A:77:PHE:CD1	1:A:80:LEU:HD23	2.49	0.47
1:B:299:ALA:O	1:B:303:LEU:HB2	2.15	0.47
1:A:206:ARG:NH2	1:A:218:ASP:CA	2.76	0.47
1:A:224:GLU:CB	1:A:225:PRO:CD	2.92	0.47
1:B:366:LYS:O	1:B:370:GLU:CG	2.63	0.47
1:A:195:ILE:HB	1:A:199:ARG:CD	2.45	0.47
1:A:218:ASP:HB2	1:A:221:HIS:HD2	1.80	0.47
1:A:265:ASN:C	1:A:268:SER:HB3	2.35	0.47
1:A:365:VAL:HG11	1:A:401:TRP:CE3	2.50	0.47
1:B:120:LEU:O	1:B:125:ARG:NH2	2.36	0.47
1:A:460:ASN:CB	1:B:286:THR:O	2.63	0.47
1:B:363:ASN:CB	1:B:366:LYS:HB2	2.44	0.47
1:B:84:THR:HG21	1:B:153:TRP:CE2	2.48	0.47
1:A:175:ASN:H	1:A:176:PRO:CD	2.28	0.47
1:A:350:LYS:CG	1:A:351:THR:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TRP:O	1:A:90:VAL:N	2.46	0.47
1:A:89:GLU:OE1	1:A:89:GLU:O	2.33	0.47
1:B:278:GLN:HG3	1:B:299:ALA:N	2.30	0.47
1:B:360:ALA:HB1	3:B:2078:HOH:O	2.14	0.47
1:A:461:ARG:CG	1:A:461:ARG:NH1	2.72	0.46
1:B:148:VAL:O	1:B:149:LEU:C	2.54	0.46
1:B:323:LYS:O	1:B:385:LYS:NZ	2.47	0.46
1:B:269:GLN:CG	1:B:346:PHE:CE2	2.97	0.46
1:A:100:LEU:HD21	2:A:1546:I15:N1	2.30	0.46
1:A:26:LEU:HD12	1:A:133:PRO:HD2	1.96	0.46
1:A:459:THR:HG23	1:A:463:ARG:HB2	1.98	0.46
1:B:391:LEU:HD12	1:B:414:TRP:HB2	1.97	0.46
1:A:197:GLN:HE21	1:A:201:LYS:NZ	2.13	0.46
1:A:216:THR:CG2	1:A:217:PRO:HD2	2.43	0.46
1:A:486:LEU:CD2	1:A:528:LYS:HD2	2.38	0.46
1:A:93:GLY:C	1:B:137:ASN:ND2	2.68	0.46
1:B:266:TRP:HZ3	1:B:427:TYR:CZ	2.34	0.46
1:B:50:ILE:HD12	1:B:54:ASN:ND2	2.30	0.46
1:A:277:ARG:HH11	1:A:277:ARG:HG2	1.80	0.46
1:A:296:THR:CG2	1:A:299:ALA:N	2.77	0.46
1:B:295:LEU:HD22	1:B:300:GLU:OE1	2.16	0.46
1:B:356:ARG:HD2	1:B:358:ARG:HA	1.98	0.46
1:B:266:TRP:CD2	1:B:426:TRP:CD1	3.04	0.46
1:A:167:ILE:CD1	1:A:214:LEU:HD12	2.45	0.46
1:A:249:LYS:HG2	1:A:251:SER:O	2.16	0.46
1:A:317:VAL:HG13	1:A:318:TYR:N	2.30	0.46
1:A:486:LEU:HA	1:A:486:LEU:HD23	1.62	0.46
1:A:536:VAL:HG11	1:A:542:ILE:HG21	1.97	0.46
1:B:183:TYR:CE2	1:B:184:MET:CE	2.99	0.46
1:A:406:TRP:CZ3	1:B:418:ASN:HA	2.45	0.46
1:A:201:LYS:O	1:A:204:GLU:HB3	2.16	0.46
1:A:278:GLN:HB2	1:A:302:GLU:OE1	2.16	0.46
1:A:27:THR:HG22	1:A:30:LYS:HG2	1.97	0.46
1:B:35:VAL:CG1	1:B:36:GLU:N	2.78	0.46
1:A:125:ARG:CG	1:A:146:TYR:O	2.58	0.46
1:A:521:ILE:CG2	1:A:525:LEU:HD11	2.46	0.46
1:A:416:PHE:CE2	1:A:418:ASN:HB2	2.51	0.46
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.16	0.45
1:A:173:LYS:HE2	1:A:173:LYS:HB3	1.20	0.45
1:A:180:ILE:HG22	1:A:187:LEU:CD1	2.46	0.45
1:A:270:ILE:HG23	1:A:271:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TRP:NE1	1:A:367:GLN:NE2	2.58	0.45
1:A:411:ILE:CG2	1:A:414:TRP:CD1	2.98	0.45
1:A:434:ILE:HG21	1:A:492:GLU:HB3	1.97	0.45
1:A:23:GLN:HG2	1:A:57:ASN:HD21	1.81	0.45
1:B:195:ILE:O	1:B:199:ARG:HG2	2.16	0.45
1:B:242:GLN:HB2	1:B:429:LEU:HD11	1.98	0.45
1:B:26:LEU:HA	1:B:26:LEU:HD23	1.49	0.45
1:B:247:PRO:C	1:B:307:ARG:HH12	2.20	0.45
1:A:135:ILE:HB	1:A:138:GLU:OE2	2.15	0.45
1:A:277:ARG:NH1	1:A:277:ARG:HG2	2.31	0.45
1:A:317:VAL:CG1	1:A:318:TYR:N	2.79	0.45
1:A:335:GLY:HA3	1:A:356:ARG:CD	2.45	0.45
1:A:379:SER:HA	1:A:383:TRP:CE3	2.52	0.45
1:A:447:ASN:O	1:A:451:LYS:N	2.46	0.45
1:A:440:PHE:CD1	1:A:493:VAL:CG2	2.99	0.45
1:A:479:LEU:CD1	1:A:501:TYR:HE2	2.29	0.45
1:B:47:ILE:HB	1:B:145:GLN:O	2.17	0.45
1:B:249:LYS:HA	1:B:252:TRP:CE2	2.51	0.45
1:B:295:LEU:HB2	1:B:300:GLU:OE2	2.17	0.45
1:B:5:ILE:HD12	1:B:6:GLU:OE1	2.17	0.45
1:B:58:THR:CG2	1:B:75:VAL:HG12	2.46	0.45
1:A:264:LEU:HA	1:A:264:LEU:HD23	1.84	0.45
1:A:288:ALA:HB3	1:A:291:GLU:OE1	2.17	0.45
1:A:357:MET:C	1:A:359:GLY:N	2.68	0.45
1:A:38:CYS:HB3	1:A:144:TYR:CZ	2.52	0.45
1:B:312:GLU:HA	1:B:313:PRO:HD2	1.11	0.45
1:B:266:TRP:HZ3	1:B:427:TYR:HH	1.55	0.45
1:B:245:VAL:CG2	1:B:429:LEU:CD2	2.94	0.45
1:A:244:ILE:HG12	3:A:2083:HOH:O	2.16	0.45
1:A:71:TRP:H	1:A:71:TRP:HD1	1.64	0.45
1:B:46:LYS:O	1:B:148:VAL:HG22	2.17	0.45
1:B:292:VAL:CG1	1:B:293:ILE:N	2.79	0.45
1:A:226:PRO:HA	1:A:234:LEU:O	2.17	0.45
1:B:216:THR:N	1:B:217:PRO:CD	2.78	0.45
1:B:35:VAL:HG12	1:B:36:GLU:N	2.32	0.45
1:A:167:ILE:HD13	1:A:214:LEU:HD12	1.98	0.45
1:A:529:GLU:O	1:A:530:LYS:HG2	2.16	0.45
1:A:52:PRO:CD	1:A:53:GLU:HG2	2.28	0.45
1:A:105:SER:CB	1:A:198:HIS:CD2	2.98	0.45
1:A:207:GLN:HG3	3:A:2068:HOH:O	2.17	0.45
1:A:103:LYS:HD3	1:A:103:LYS:HA	1.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:CZ3	1:A:407:GLN:NE2	2.86	0.44
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.76	0.44
1:B:249:LYS:O	1:B:250:ASP:HB2	2.16	0.44
1:B:92:LEU:N	1:B:92:LEU:CD2	2.79	0.44
1:A:63:ILE:HG12	1:A:65:LYS:NZ	2.33	0.44
1:A:391:LEU:C	1:A:393:ILE:H	2.20	0.44
1:A:401:TRP:CD1	1:A:425:LEU:HD11	2.53	0.44
1:A:441:TYR:CG	1:A:544:GLY:HA3	2.52	0.44
1:A:169:GLU:HG2	1:A:170:PRO:N	2.33	0.44
1:A:253:THR:OG1	1:A:289:LEU:O	2.24	0.44
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.49	0.44
1:A:364:ASP:HB2	1:A:423:VAL:HG13	1.99	0.44
1:A:513:SER:CB	1:A:518:VAL:CG1	2.96	0.44
1:B:298:GLU:HG3	1:B:298:GLU:H	1.48	0.44
1:B:20:LYS:CE	1:B:55:PRO:HB2	2.45	0.44
1:B:58:THR:CG2	1:B:75:VAL:CG1	2.96	0.44
1:A:206:ARG:HH11	1:A:206:ARG:CG	2.31	0.44
1:A:210:LEU:O	1:A:212:TRP:N	2.51	0.44
1:A:296:THR:HG22	1:A:299:ALA:N	2.33	0.44
1:A:391:LEU:HA	1:A:392:PRO:HD3	1.78	0.44
1:B:261:VAL:HA	1:B:276:VAL:HG21	1.98	0.44
1:A:201:LYS:HD2	1:A:201:LYS:HA	1.59	0.44
1:A:273:GLY:HA3	1:A:309:ILE:CD1	2.48	0.44
1:B:388:LYS:HE2	1:B:388:LYS:HB3	1.47	0.44
1:A:10:VAL:HG11	1:A:153:TRP:HH2	1.83	0.44
1:A:136:ASN:HB2	1:A:138:GLU:CG	2.47	0.44
1:A:416:PHE:CE1	1:A:422:LEU:HD13	2.52	0.44
1:A:54:ASN:HA	1:A:55:PRO:HD2	1.68	0.44
1:A:64:LYS:HA	1:A:71:TRP:HB3	2.00	0.44
1:B:36:GLU:O	1:B:38:CYS:N	2.50	0.44
1:B:5:ILE:HD13	1:B:5:ILE:HA	1.69	0.44
1:A:153:TRP:CD1	1:A:154:LYS:N	2.86	0.44
1:A:180:ILE:HG22	1:A:187:LEU:HD11	1.99	0.44
1:A:237:ASP:HB2	3:A:2033:HOH:O	2.18	0.44
1:A:30:LYS:HG2	1:A:30:LYS:H	1.50	0.44
1:A:445:ALA:O	1:A:453:GLY:HA3	2.17	0.44
1:A:79:GLU:O	1:A:81:ASN:N	2.51	0.44
1:B:246:LEU:HB3	1:B:260:LEU:CD1	2.48	0.44
1:A:102:LYS:HB3	1:A:318:TYR:HB2	2.00	0.43
1:A:131:THR:OG1	1:A:143:ARG:HG2	2.18	0.43
1:A:450:THR:O	1:A:451:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ILE:CG2	1:A:525:LEU:CD1	2.95	0.43
1:B:326:ILE:HG12	1:B:388:LYS:CE	2.48	0.43
1:B:78:ARG:O	1:B:82:LYS:HG3	2.18	0.43
1:A:136:ASN:HB2	3:A:2048:HOH:O	2.18	0.43
1:A:171:PHE:O	1:A:175:ASN:HB2	2.17	0.43
1:A:27:THR:HB	1:A:30:LYS:CG	2.48	0.43
1:A:398:TRP:CZ2	1:A:411:ILE:HG13	2.52	0.43
1:A:441:TYR:HB3	1:A:544:GLY:HA3	2.00	0.43
1:B:246:LEU:HD12	1:B:307:ARG:CG	2.48	0.43
1:B:341:ILE:HG21	1:B:383:TRP:CZ3	2.52	0.43
1:B:393:ILE:HG12	1:B:394:GLN:H	1.83	0.43
1:B:94:ILE:CD1	1:B:94:ILE:N	2.73	0.43
1:A:328:GLU:O	1:A:339:TYR:HA	2.18	0.43
1:A:334:GLN:HB2	3:A:2107:HOH:O	2.18	0.43
1:A:379:SER:HB3	1:A:383:TRP:CE3	2.53	0.43
1:B:118:VAL:HG11	1:B:149:LEU:CD1	2.48	0.43
1:B:13:LYS:CB	1:B:16:MET:CE	2.95	0.43
1:B:214:LEU:N	1:B:214:LEU:CD2	2.79	0.43
1:A:357:MET:C	1:A:359:GLY:H	2.21	0.43
1:A:467:VAL:HG13	1:A:468:THR:N	2.33	0.43
1:B:157:PRO:HG3	1:B:184:MET:O	2.18	0.43
1:B:281:LYS:O	1:B:283:LEU:N	2.51	0.43
1:B:376:THR:HG23	1:B:386:THR:HG22	1.99	0.43
1:A:167:ILE:CD1	1:A:214:LEU:CD1	2.96	0.43
1:A:455:ALA:O	1:A:467:VAL:N	2.52	0.43
1:B:391:LEU:O	1:B:393:ILE:N	2.52	0.43
1:A:139:THR:HA	1:A:140:PRO:HD3	1.85	0.43
1:A:164:MET:HE3	1:A:187:LEU:HD22	2.01	0.43
1:A:278:GLN:CG	1:A:298:GLU:CB	2.96	0.43
1:A:441:TYR:HB3	1:A:544:GLY:CA	2.49	0.43
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.33	0.43
1:B:243:PRO:C	1:B:245:VAL:N	2.72	0.43
1:B:333:GLY:O	1:B:334:GLN:HB2	2.19	0.43
1:A:277:ARG:NH2	1:A:334:GLN:CG	2.80	0.43
1:A:356:ARG:HB3	1:A:359:GLY:H	1.82	0.43
1:A:448:ARG:NH1	1:A:448:ARG:CG	2.77	0.43
1:A:450:THR:O	1:A:451:LYS:CB	2.67	0.43
1:A:8:VAL:HA	1:A:9:PRO:HD2	1.46	0.43
1:B:249:LYS:HD3	1:B:250:ASP:H	1.80	0.43
1:B:356:ARG:HH11	1:B:358:ARG:NH2	2.10	0.43
1:B:367:GLN:HA	1:B:370:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ALA:HB3	1:B:366:LYS:HZ3	1.84	0.43
1:A:542:ILE:HA	1:B:283:LEU:O	2.19	0.43
1:B:241:VAL:CG2	1:B:242:GLN:N	2.78	0.43
1:A:254:VAL:HG21	1:A:291:GLU:HB3	1.99	0.43
1:A:273:GLY:HA3	1:A:309:ILE:HD13	2.00	0.43
1:A:406:TRP:CZ3	1:A:407:GLN:CD	2.93	0.43
1:B:132:ILE:O	1:B:133:PRO:O	2.36	0.43
1:B:175:ASN:N	1:B:175:ASN:OD1	2.51	0.43
1:B:274:ILE:CG2	1:B:275:LYS:N	2.82	0.43
1:A:102:LYS:HE2	1:A:320:ASP:CB	2.30	0.42
1:A:195:ILE:CB	1:A:199:ARG:CD	2.97	0.42
1:A:376:THR:HG23	1:A:386:THR:CG2	2.49	0.42
1:A:433:PRO:CG	1:B:255:ASN:HD22	2.31	0.42
1:A:538:ALA:O	1:A:539:HIS:HB2	2.19	0.42
1:A:406:TRP:CZ3	1:B:419:THR:N	2.87	0.42
1:A:183:TYR:CE1	1:A:230:MET:SD	3.12	0.42
1:A:540:LYS:CB	1:A:542:ILE:CD1	2.92	0.42
1:B:346:PHE:HD1	1:B:346:PHE:HA	1.72	0.42
1:B:358:ARG:HB2	3:B:2076:HOH:O	2.19	0.42
1:B:51:GLY:HA3	1:B:53:GLU:OE1	2.19	0.42
1:A:136:ASN:C	1:A:138:GLU:N	2.72	0.42
1:A:206:ARG:HH11	1:A:206:ARG:HG2	1.83	0.42
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.78	0.42
1:B:244:ILE:O	1:B:245:VAL:HG22	2.18	0.42
1:B:350:LYS:HB2	1:B:383:TRP:HH2	1.83	0.42
1:A:246:LEU:HD21	1:A:310:LEU:CD1	2.50	0.42
1:A:255:ASN:O	1:A:258:GLN:HB2	2.19	0.42
1:A:263:LYS:HA	1:A:263:LYS:HD3	1.87	0.42
1:A:328:GLU:OE2	1:A:342:TYR:CE2	2.72	0.42
1:A:356:ARG:HB3	1:A:359:GLY:N	2.34	0.42
1:B:175:ASN:ND2	1:B:201:LYS:CE	2.75	0.42
1:B:243:PRO:HB2	1:B:245:VAL:HG13	2.01	0.42
1:B:421:PRO:CD	1:B:422:LEU:H	2.31	0.42
1:A:153:TRP:CG	1:A:154:LYS:N	2.87	0.42
1:A:424:LYS:HE2	1:A:426:TRP:CE2	2.50	0.42
1:A:467:VAL:CG1	1:A:468:THR:N	2.82	0.42
1:A:3:SER:OG	1:A:5:ILE:HB	2.19	0.42
1:B:58:THR:HG21	1:B:75:VAL:HG12	2.00	0.42
1:A:101:LYS:CD	1:A:103:LYS:CE	2.93	0.42
1:A:240:THR:OG1	1:A:241:VAL:N	2.52	0.42
1:A:279:LEU:HG	1:A:302:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:TYR:CB	1:A:544:GLY:HA3	2.49	0.42
1:A:3:SER:HA	1:A:4:PRO:HD2	1.81	0.42
1:A:379:SER:OG	1:A:387:PRO:HD3	2.19	0.42
1:B:50:ILE:HD11	1:B:129:ALA:HB1	2.02	0.42
1:A:3:SER:HA	1:A:213:GLY:HA3	2.01	0.42
1:A:357:MET:HG2	1:A:357:MET:O	2.20	0.42
1:A:68:SER:C	1:A:70:LYS:H	2.23	0.42
1:B:172:ARG:NH1	1:B:172:ARG:HG3	2.35	0.42
1:A:277:ARG:CZ	1:A:334:GLN:CG	2.97	0.42
1:A:2:ILE:O	1:A:3:SER:C	2.57	0.42
1:A:334:GLN:O	1:A:336:GLN:HG3	2.20	0.42
1:A:356:ARG:NH1	1:A:512:GLN:NE2	2.66	0.42
1:B:271:TYR:HA	1:B:272:PRO:HD2	1.91	0.42
1:A:268:SER:O	1:A:351:THR:HG22	2.18	0.42
1:A:391:LEU:HB2	1:A:393:ILE:HG22	2.01	0.42
1:A:398:TRP:CZ2	1:A:409:THR:CG2	3.03	0.42
1:B:111:VAL:HG11	1:B:187:LEU:HG	2.02	0.42
1:A:249:LYS:NZ	1:A:249:LYS:HB2	2.18	0.41
1:A:253:THR:OG1	1:A:256:ASP:OD1	2.38	0.41
1:B:287:LYS:HD3	1:B:293:ILE:HD11	2.02	0.41
1:B:369:THR:HG22	1:B:398:TRP:CZ3	2.54	0.41
1:B:382:ILE:HG22	1:B:382:ILE:O	2.18	0.41
1:B:425:LEU:HD23	1:B:425:LEU:HA	1.34	0.41
1:B:266:TRP:HH2	1:B:427:TYR:HH	1.61	0.41
1:A:130:PHE:N	1:A:130:PHE:CD2	2.88	0.41
1:A:202:ILE:HD12	1:A:202:ILE:HA	1.81	0.41
1:A:256:ASP:HA	1:A:259:LYS:HG3	2.01	0.41
1:A:271:TYR:HB3	1:A:274:ILE:CD1	2.50	0.41
1:A:452:LEU:HD23	3:A:2126:HOH:O	2.20	0.41
1:A:501:TYR:O	1:A:505:ILE:HG13	2.20	0.41
1:B:205:LEU:HD12	1:B:205:LEU:O	2.19	0.41
1:B:419:THR:HA	1:B:420:PRO:HD2	1.94	0.41
1:B:297:GLU:HA	1:B:300:GLU:HG3	2.01	0.41
1:B:34:LEU:HA	1:B:34:LEU:HD23	1.84	0.41
1:B:331:LYS:CE	1:B:364:ASP:OD2	2.63	0.41
1:A:195:ILE:CG2	1:A:199:ARG:CD	2.98	0.41
1:A:107:THR:HG21	1:A:202:ILE:HG21	2.02	0.41
1:A:4:PRO:HD2	1:A:212:TRP:C	2.40	0.41
1:B:242:GLN:O	1:B:242:GLN:CG	2.68	0.41
1:B:266:TRP:CH2	1:B:427:TYR:CZ	3.07	0.41
1:B:50:ILE:HD12	1:B:54:ASN:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ASP:HA	1:B:90:VAL:HG23	2.02	0.41
1:A:334:GLN:O	1:A:336:GLN:N	2.53	0.41
1:B:180:ILE:HD13	1:B:189:VAL:HG22	2.02	0.41
1:B:21:VAL:HG21	1:B:79:GLU:CG	2.50	0.41
1:B:270:ILE:HD13	1:B:270:ILE:HG21	1.85	0.41
1:A:136:ASN:HB2	1:A:138:GLU:HG3	2.02	0.41
1:A:257:ILE:CG2	1:A:283:LEU:CD1	2.97	0.41
1:A:37:ILE:CG2	1:A:41:MET:HE1	2.50	0.41
1:A:393:ILE:O	1:A:416:PHE:CD1	2.73	0.41
1:A:433:PRO:CD	1:B:255:ASN:ND2	2.83	0.41
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.51	0.41
1:A:430:GLU:CD	1:A:530:LYS:HD2	2.41	0.41
1:B:132:ILE:HA	1:B:133:PRO:HD2	1.65	0.41
1:B:328:GLU:HG2	1:B:390:LYS:HD2	2.03	0.41
1:A:443:ASP:O	1:A:481:ALA:HB2	2.20	0.41
1:A:542:ILE:HB	1:A:545:ASN:HB3	2.02	0.41
1:A:284:ARG:O	1:A:285:GLY:O	2.38	0.41
1:A:491:LEU:HD13	3:A:2149:HOH:O	2.21	0.41
1:B:287:LYS:CD	1:B:293:ILE:HD11	2.51	0.41
1:B:359:GLY:C	1:B:361:HIS:H	2.24	0.41
1:B:363:ASN:HB3	1:B:366:LYS:CB	2.50	0.41
1:A:183:TYR:HE1	1:A:230:MET:SD	2.44	0.41
1:A:268:SER:O	1:A:351:THR:CG2	2.69	0.41
1:A:450:THR:HB	1:A:452:LEU:CD1	2.51	0.41
1:A:513:SER:HB3	1:A:518:VAL:HG12	2.03	0.41
1:A:361:HIS:CD2	1:A:513:SER:OG	2.74	0.41
1:A:540:LYS:CB	1:A:542:ILE:HD12	2.35	0.41
1:B:339:TYR:OH	1:B:378:GLU:OE1	2.39	0.41
1:A:238:LYS:HD2	3:A:2082:HOH:O	2.21	0.41
1:A:37:ILE:CG2	1:A:41:MET:CE	2.99	0.41
1:A:440:PHE:HD1	1:A:493:VAL:HG23	1.86	0.41
1:A:448:ARG:CZ	1:A:448:ARG:HB3	2.51	0.41
1:A:491:LEU:CD2	1:A:491:LEU:H	2.25	0.41
1:B:119:PRO:HA	1:B:148:VAL:HA	2.02	0.41
1:B:160:PHE:CD2	1:B:164:MET:HE2	2.56	0.41
1:B:264:LEU:CD2	1:B:306:ASN:ND2	2.83	0.41
1:B:81:ASN:HD22	1:B:154:LYS:HD2	1.82	0.41
1:B:100:LEU:HD22	1:B:181:TYR:HB3	2.03	0.41
1:B:403:THR:C	1:B:405:TYR:N	2.74	0.41
1:B:88:TRP:CZ3	1:B:89:GLU:HB2	2.56	0.41
1:A:340:GLN:HE21	1:A:340:GLN:HB3	1.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:THR:O	1:A:409:THR:HG22	2.21	0.40
1:B:103:LYS:CD	1:B:190:GLY:HA3	2.50	0.40
1:B:51:GLY:C	1:B:53:GLU:N	2.74	0.40
1:A:216:THR:CG2	1:A:217:PRO:CD	2.99	0.40
1:A:354:TYR:OH	1:A:370:GLU:OE1	2.37	0.40
1:A:405:TYR:O	1:B:331:LYS:HD3	2.20	0.40
1:A:493:VAL:HG22	1:A:494:ASN:N	2.36	0.40
1:A:79:GLU:HG3	1:A:83:ARG:HH11	1.85	0.40
1:B:356:ARG:HD2	1:B:358:ARG:CA	2.52	0.40
1:A:136:ASN:H	1:A:138:GLU:CG	2.34	0.40
1:A:164:MET:HG3	1:A:164:MET:O	2.20	0.40
1:A:180:ILE:CG2	1:A:187:LEU:CD1	2.99	0.40
1:A:34:LEU:HD22	1:A:73:LYS:HG3	2.04	0.40
1:B:153:TRP:CZ2	1:B:155:GLY:HA3	2.56	0.40
1:B:171:PHE:HB2	1:B:208:HIS:CD2	2.57	0.40
1:A:460:ASN:CA	1:B:286:THR:O	2.68	0.40
1:B:376:THR:CG2	1:B:386:THR:CG2	2.98	0.40
1:A:395:LYS:CD	1:A:414:TRP:CH2	2.96	0.40
1:B:161:GLN:HB2	1:B:161:GLN:HE21	1.72	0.40
1:B:207:GLN:HB3	1:B:211:ARG:NH1	2.36	0.40
1:B:320:ASP:CG	1:B:322:SER:HG	2.25	0.40
1:B:5:ILE:HG22	1:B:5:ILE:O	2.22	0.40
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.56	0.40
1:A:139:THR:CB	1:A:140:PRO:CD	2.96	0.40
1:A:181:TYR:HB2	1:A:188:TYR:HB2	2.04	0.40
1:B:210:LEU:HD12	1:B:210:LEU:HA	1.71	0.40
1:B:332:GLN:NE2	1:B:428:GLN:HA	2.37	0.40
1:B:339:TYR:CD1	1:B:375:ILE:HG12	2.56	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	543/566 (96%)	415 (76%)	86 (16%)	42 (8%)	1	3
1	B	412/566 (73%)	338 (82%)	42 (10%)	32 (8%)	1	3
All	All	955/1132 (84%)	753 (79%)	128 (13%)	74 (8%)	1	3

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	14	PRO
1	A	90	VAL
1	A	135	ILE
1	A	139	THR
1	A	169	GLU
1	A	175	ASN
1	A	251	SER
1	A	287	LYS
1	A	356	ARG
1	A	491	LEU
1	A	524	GLN
1	A	525	LEU
1	A	528	LYS
1	A	542	ILE
1	B	4	PRO
1	B	133	PRO
1	B	232	TYR
1	B	249	LYS
1	B	250	ASP
1	B	313	PRO
1	B	315	HIS
1	A	195	ILE
1	A	196	GLY
1	A	206	ARG
1	A	207	GLN
1	A	243	PRO
1	A	255	ASN
1	A	274	ILE
1	A	285	GLY
1	A	361	HIS
1	A	412	PRO
1	B	241	VAL
1	B	272	PRO
1	B	273	GLY

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Mol	Chain	Res	Type
1	B	282	LEU
1	B	310	LEU
1	B	314	VAL
1	B	345	PRO
1	A	80	LEU
1	A	256	ASP
1	A	335	GLY
1	A	345	PRO
1	B	6	GLU
1	B	9	PRO
1	B	160	PHE
1	B	216	THR
1	B	358	ARG
1	A	3	SER
1	A	140	PRO
1	A	268	SER
1	B	69	THR
1	B	71	TRP
1	B	286	THR
1	B	346	PHE
1	B	350	LYS
1	A	5	ILE
1	A	66	LYS
1	A	303	LEU
1	B	65	LYS
1	B	85	GLN
1	B	119	PRO
1	B	245	VAL
1	B	297	GLU
1	A	57	ASN
1	A	89	GLU
1	A	288	ALA
1	A	490	GLY
1	B	149	LEU
1	B	392	PRO
1	A	170	PRO
1	A	466	VAL
1	B	18	GLY
1	A	276	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	487/505 (96%)	356 (73%)	131 (27%)	0	2
1	B	375/505 (74%)	278 (74%)	97 (26%)	0	2
All	All	862/1010 (85%)	634 (74%)	228 (26%)	0	2

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU
1	A	11	LYS
1	A	12	LEU
1	A	14	PRO
1	A	20	LYS
1	A	22	LYS
1	A	24	TRP
1	A	27	THR
1	A	30	LYS
1	A	42	GLU
1	A	43	LYS
1	A	58	THR
1	A	60	VAL
1	A	63	ILE
1	A	64	LYS
1	A	65	LYS
1	A	66	LYS
1	A	68	SER
1	A	69	THR
1	A	71	TRP
1	A	72	ARG
1	A	74	LEU
1	A	89	GLU
1	A	90	VAL
1	A	92	LEU
1	A	94	ILE

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Mol	Chain	Res	Type
1	A	103	LYS
1	A	104	LYS
1	A	106	VAL
1	A	117	SER
1	A	126	LYS
1	A	134	SER
1	A	138	GLU
1	A	139	THR
1	A	142	ILE
1	A	162	SER
1	A	173	LYS
1	A	174	GLN
1	A	177	ASP
1	A	179	VAL
1	A	184	MET
1	A	187	LEU
1	A	195	ILE
1	A	199	ARG
1	A	201	LYS
1	A	202	ILE
1	A	203	GLU
1	A	205	LEU
1	A	206	ARG
1	A	207	GLN
1	A	215	THR
1	A	221	HIS
1	A	223	LYS
1	A	228	LEU
1	A	230	MET
1	A	238	LYS
1	A	241	VAL
1	A	242	GLN
1	A	245	VAL
1	A	246	LEU
1	A	249	LYS
1	A	250	ASP
1	A	253	THR
1	A	257	ILE
1	A	259	LYS
1	A	268	SER
1	A	274	ILE
1	A	276	VAL

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Mol	Chain	Res	Type
1	A	280	CYS
1	A	281	LYS
1	A	284	ARG
1	A	289	LEU
1	A	290	THR
1	A	296	THR
1	A	301	LEU
1	A	305	GLU
1	A	307	ARG
1	A	311	LYS
1	A	312	GLU
1	A	313	PRO
1	A	317	VAL
1	A	331	LYS
1	A	334	GLN
1	A	338	THR
1	A	340	GLN
1	A	345	PRO
1	A	347	LYS
1	A	350	LYS
1	A	351	THR
1	A	357	MET
1	A	369	THR
1	A	374	LYS
1	A	378	GLU
1	A	379	SER
1	A	390	LYS
1	A	391	LEU
1	A	396	GLU
1	A	400	THR
1	A	402	TRP
1	A	404	GLU
1	A	409	THR
1	A	424	LYS
1	A	428	GLN
1	A	429	LEU
1	A	434	ILE
1	A	439	THR
1	A	448	ARG
1	A	451	LYS
1	A	459	THR
1	A	461	ARG

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Mol	Chain	Res	Type
1	A	463	ARG
1	A	464	GLN
1	A	465	LYS
1	A	466	VAL
1	A	468	THR
1	A	471	ASP
1	A	478	GLU
1	A	484	LEU
1	A	488	ASP
1	A	494	ASN
1	A	496	VAL
1	A	498	ASP
1	A	499	SER
1	A	512	GLN
1	A	515	SER
1	A	517	LEU
1	A	520	GLN
1	A	527	LYS
1	A	528	LYS
1	A	545	ASN
1	B	5	ILE
1	B	11	LYS
1	B	16	MET
1	B	22	LYS
1	B	35	VAL
1	B	40	GLU
1	B	42	GLU
1	B	48	SER
1	B	54	ASN
1	B	58	THR
1	B	63	ILE
1	B	65	LYS
1	B	67	ASP
1	B	68	SER
1	B	69	THR
1	B	73	LYS
1	B	83	ARG
1	B	85	GLN
1	B	86	ASP
1	B	90	VAL
1	B	94	ILE
1	B	101	LYS

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Mol	Chain	Res	Type
1	B	103	LYS
1	B	109	LEU
1	B	113	ASP
1	B	117	SER
1	B	118	VAL
1	B	125	ARG
1	B	126	LYS
1	B	134	SER
1	B	138	GLU
1	B	165	THR
1	B	166	LYS
1	B	169	GLU
1	B	172	ARG
1	B	174	GLN
1	B	175	ASN
1	B	178	ILE
1	B	182	GLN
1	B	194	GLU
1	B	201	LYS
1	B	203	GLU
1	B	206	ARG
1	B	211	ARG
1	B	214	LEU
1	B	215	THR
1	B	216	THR
1	B	233	GLU
1	B	240	THR
1	B	242	GLN
1	B	246	LEU
1	B	249	LYS
1	B	250	ASP
1	B	268	SER
1	B	269	GLN
1	B	275	LYS
1	B	277	ARG
1	B	278	GLN
1	B	279	LEU
1	B	280	CYS
1	B	282	LEU
1	B	284	ARG
1	B	286	THR
1	B	289	LEU

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Mol	Chain	Res	Type
1	B	290	THR
1	B	291	GLU
1	B	295	LEU
1	B	298	GLU
1	B	301	LEU
1	B	305	GLU
1	B	307	ARG
1	B	308	GLU
1	B	311	LYS
1	B	317	VAL
1	B	325	LEU
1	B	338	THR
1	B	344	GLU
1	B	346	PHE
1	B	350	LYS
1	B	353	LYS
1	B	354	TYR
1	B	356	ARG
1	B	358	ARG
1	B	362	THR
1	B	364	ASP
1	B	366	LYS
1	B	369	THR
1	B	370	GLU
1	B	385	LYS
1	B	388	LYS
1	B	392	PRO
1	B	393	ILE
1	B	395	LYS
1	B	413	GLU
1	B	424	LYS
1	B	425	LEU
1	B	428	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	96	HIS
1	A	137	ASN
1	A	161	GLN
1	A	174	GLN

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Mol	Chain	Res	Type
1	A	182	GLN
1	A	197	GLN
1	A	221	HIS
1	A	222	GLN
1	A	242	GLN
1	A	269	GLN
1	A	332	GLN
1	A	334	GLN
1	A	361	HIS
1	A	367	GLN
1	A	475	GLN
1	A	480	GLN
1	A	494	ASN
1	A	507	GLN
1	A	512	GLN
1	A	524	GLN
1	A	545	ASN
1	B	91	GLN
1	B	137	ASN
1	B	147	ASN
1	B	151	GLN
1	B	161	GLN
1	B	182	GLN
1	B	208	HIS
1	B	255	ASN
1	B	278	GLN
1	B	315	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	I15	A	1546	-	21,24,24	2.41	7 (33%)	25,34,34	2.11	10 (40%)

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
2	I15	A	1546	-	-	0/8/8/8	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1546	I15	C10-C4	-7.26	1.45	1.50
2	A	1546	I15	C8-C3	-2.85	1.36	1.41
2	A	1546	I15	C13-C15	-2.78	1.34	1.39
2	A	1546	I15	C4-N9	2.51	1.37	1.33
2	A	1546	I15	C12-C6	3.14	1.44	1.37
2	A	1546	I15	C8-C12	3.34	1.43	1.36
2	A	1546	I15	F1-C6	3.36	1.43	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1546	I15	C12-C6-C2	-3.36	115.23	122.81
2	A	1546	I15	C16-C14-C11	-3.26	115.21	119.24
2	A	1546	I15	C13-C15-C18	-2.17	116.90	119.53
2	A	1546	I15	C15-C13-C11	2.27	122.06	119.24
2	A	1546	I15	C11-O5-C2	2.35	122.50	118.54
2	A	1546	I15	C17-C15-C18	2.44	122.50	119.53
2	A	1546	I15	F1-C6-C12	2.59	124.26	118.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1546	I15	C17-C16-C14	2.64	124.24	119.75
2	A	1546	I15	C10-C4-N9	3.20	126.67	119.65
2	A	1546	I15	C8-C3-N7	5.16	138.65	130.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1546	I15	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	545/566 (96%)	0.40	42 (7%)	14 10	34, 59, 86, 107	0
1	B	416/566 (73%)	0.58	47 (11%)	6 4	36, 58, 95, 119	0
All	All	961/1132 (84%)	0.48	89 (9%)	9 6	34, 59, 90, 119	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	357	MET	8.9
1	B	284	ARG	5.8
1	A	285	GLY	4.8
1	A	291	GLU	4.6
1	A	290	THR	4.5
1	B	4	PRO	4.4
1	A	359	GLY	4.4
1	B	15	GLY	4.3
1	B	14	PRO	4.1
1	B	361	HIS	4.1
1	A	65	LYS	4.0
1	B	251	SER	4.0
1	B	296	THR	3.8
1	A	54	ASN	3.8
1	A	66	LYS	3.8
1	B	39	THR	3.7
1	A	67	ASP	3.6
1	B	3	SER	3.6
1	B	362	THR	3.6
1	B	217	PRO	3.5
1	A	453	GLY	3.4
1	B	70	LYS	3.4
1	B	69	THR	3.3
1	B	232	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	16	MET	3.3
1	B	7	THR	3.2
1	B	278	GLN	3.2
1	A	68	SER	3.2
1	B	13	LYS	3.2
1	A	64	LYS	3.2
1	A	292	VAL	3.1
1	B	5	ILE	3.1
1	A	282	LEU	3.1
1	A	278	GLN	3.1
1	B	40	GLU	3.1
1	B	359	GLY	3.1
1	A	221	HIS	3.0
1	B	230	MET	3.0
1	B	356	ARG	3.0
1	B	184	MET	3.0
1	A	104	LYS	3.0
1	A	402	TRP	2.9
1	B	360	ALA	2.9
1	B	301	LEU	2.8
1	A	539	HIS	2.8
1	B	43	LYS	2.8
1	A	289	LEU	2.7
1	B	355	ALA	2.7
1	A	69	THR	2.7
1	B	335	GLY	2.7
1	B	6	GLU	2.6
1	A	541	GLY	2.6
1	B	298	GLU	2.6
1	B	88	TRP	2.5
1	B	231	GLY	2.5
1	A	472	THR	2.5
1	B	336	GLN	2.5
1	B	186	ASP	2.5
1	A	70	LYS	2.5
1	A	473	THR	2.4
1	A	358	ARG	2.4
1	A	530	LYS	2.4
1	A	242	GLN	2.4
1	B	358	ARG	2.4
1	A	545	ASN	2.3
1	A	357	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	297	GLU	2.3
1	A	200	THR	2.3
1	B	173	LYS	2.3
1	A	24	TRP	2.3
1	A	520	GLN	2.3
1	A	544	GLY	2.3
1	B	152	GLY	2.2
1	A	52	PRO	2.2
1	B	67	ASP	2.2
1	B	123	ASP	2.2
1	B	295	LEU	2.2
1	A	123	ASP	2.1
1	A	63	ILE	2.1
1	A	506	ILE	2.1
1	B	65	LYS	2.1
1	B	183	TYR	2.1
1	B	299	ALA	2.1
1	A	396	GLU	2.1
1	B	92	LEU	2.0
1	A	434	ILE	2.0
1	A	445	ALA	2.0
1	A	315	HIS	2.0
1	A	301	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	I15	A	1546	22/22	0.95	0.21	-0.51	42,51,55,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.