



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:59 AM GMT

PDB ID : 2JLE
Title : NOVEL INDAZOLE NNRTIS CREATED USING MOLECULAR TEMPLATE HYBRIDIZATION BASED ON CRYSTALLOGRAPHIC OVERLAYS
Authors : Jones, L.H.; Allan, G.; Barba, O.; Burt, C.; Corbau, R.; Dupont, T.; Irving, S.; Mowbray, C.E.; Phillips, C.; Swain, N.A.; Webster, R.; Westby, M.
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

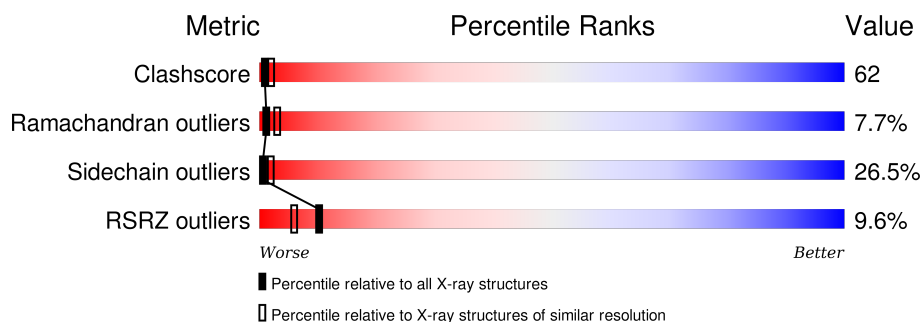
1 Overall quality at a glance

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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 ≥ 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	<div> <div>7%</div> <div>22%</div> <div>52%</div> <div>20%</div> <div>• •</div> </div>
1	B	566	<div> <div>9%</div> <div>18%</div> <div>38%</div> <div>16%</div> <div>•</div> <div>27%</div> </div>

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.

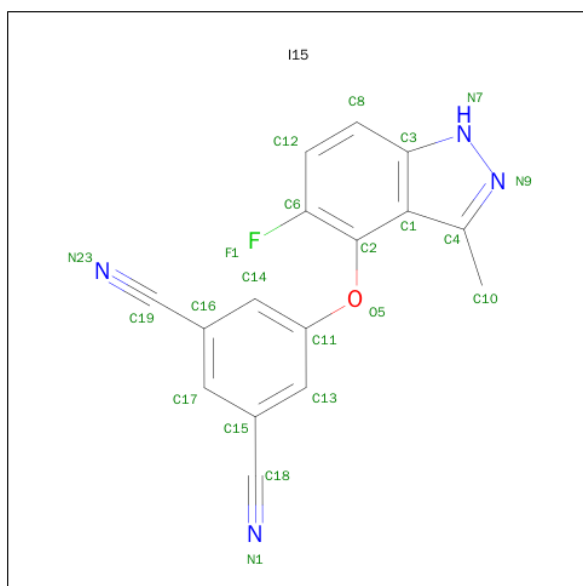
- Molecule 1 is a protein called REVERSE TRANSCRIPTASE/RNASEH.

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: C₁₆H₉FN₄O).



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

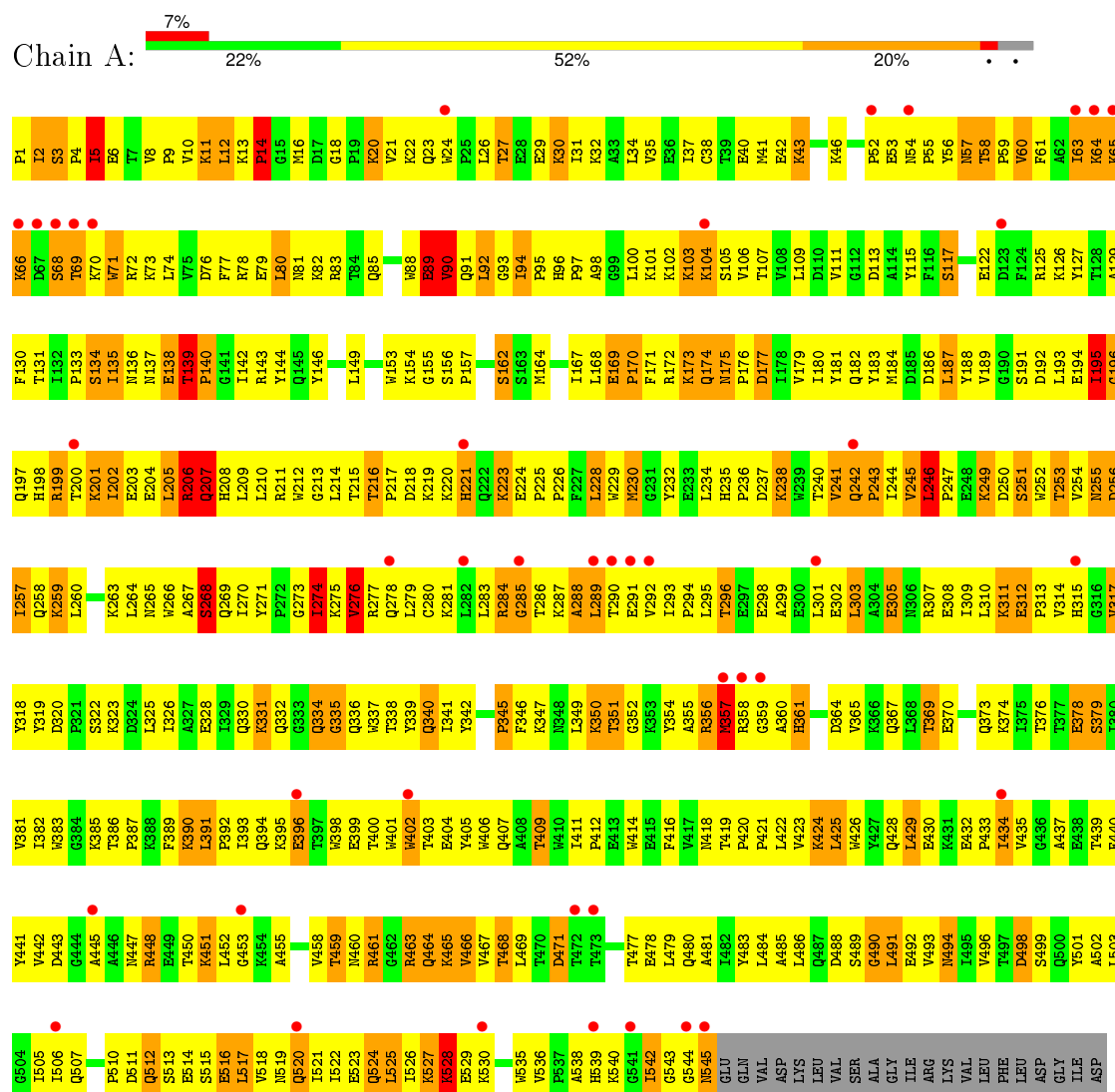
- Molecule 3 is water.

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

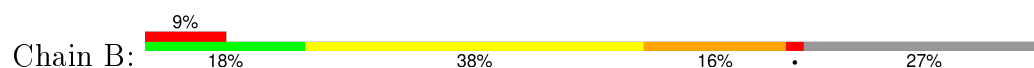
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



LEU	ASP	GLY	ILE	ASP	VAL	E378	G316	V255	D192	A129	K65	PR0
ASP	GLY	GLY	ASP	ASP	ASP	S379	V317	D256	L193	I132	K66	ILR
ILE	ALA	ALA	GLY	GLY	GLY	I382	Y318	L257	E194	P133	D67	S3
GLN	ALA	ALA	ILE	ALA	ALA	V383	Y319	Q258	I195	P133	S68	P4
ALA	GLN	ALA	GLN	ASN	ASN	D384	P321	D259	G196	S134	T69	I5
GLN	ALA	ARG	ALA	ASN	ASN	K385	S322	L260	Q197	I135	E6	E6
GLN	GLU	ARG	ARG	ASN	ASN	T386	K323	V261	H198	H136	T7	T7
PRO	THR	GLU	THR	THR	THR	D387	K324	L264	A199	N137	V8	V8
ASP	LEU	THR	THR	THR	THR	K388	L325	D265	T200	E138	P9	P9
GLN	LEU	THR	THR	THR	THR	F389	L326	D266	I202	T139	L74	K11
SER	GLY	THR	THR	THR	THR	K390	A327	A267	I204	P140	V75	K11
GLY	LYS	THR	THR	THR	THR	L391	E328	S268	E203	G141	D76	L12
ALA	ALA	THR	THR	THR	THR	P392	K331	Q269	E204	I142	F77	K13
GLU	GLY	THR	THR	THR	THR	L393	Q332	I270	L205	A143	K78	P14
LEU	TYR	THR	THR	THR	THR	Q394	Q333	I271	R206	Y144	E79	G15
VAL	VAL	THR	THR	THR	THR	K395	G334	P272	Q207	Q145	L80	M16
GLN	ASN	THR	THR	THR	THR	E398	G335	D273	E208	V148	N81	G18
ASN	ASN	THR	THR	THR	THR	H399	Q336	I274	L210	I149	K83	P19
ILE	ARG	THR	THR	THR	THR	E399	F337	K275	R211	P150	T84	K20
GLY	ARG	THR	THR	THR	THR	W402	T338	V276	W212	Q151	K85	V21
GLU	ARG	THR	THR	THR	THR	T403	Y339	K277	G213	G152	D86	K22
GLN	GLN	THR	THR	THR	THR	E404	Q340	L279	L214	W153	F87	L26
LEU	LYS	THR	THR	THR	THR	Y405	I341	C280	T215	K154	N88	T27
ILE	VAL	THR	THR	THR	THR	W406	Y342	C281	T216	G155	P89	T27
LYS	VAL	THR	THR	THR	THR	Q407	Q343	K281	P217	S156	V90	E28
LYS	THR	THR	THR	THR	THR	W410	E344	L282	ASP	P157	Q91	E29
GLU	LEU	THR	THR	THR	THR	I411	F345	R284	LYS	A158	L92	K30
LYS	LYS	THR	THR	THR	THR	P412	P346	Q285	HIS	I159	G93	K31
VAL	VAL	THR	THR	THR	THR	E413	K347	T286	LYS	Q161	I94	I32
ALA	ASN	THR	THR	THR	THR	W414	I348	K287	GLN	P95	P35	A33
TRP	GLN	THR	THR	THR	THR	E415	L349	A288	GLU	S162	N86	L34
VAL	LYS	THR	THR	THR	THR	F416	K350	L289	PR0	M164	P97	V35
PRO	PRO	THR	THR	THR	THR	V417	T351	T290	PHE	K166	L100	I37
ALA	ALA	THR	THR	THR	THR	N418	G352	E291	LEU	I167	K101	C38
HIS	LYS	THR	THR	THR	THR	T419	Y354	I293	TRP	L168	K102	T39
LYS	GLN	THR	THR	THR	THR	P420	A355	P294	R230	E169	E40	E40
GLY	ALA	THR	THR	THR	THR	P421	R356	L295	G231	P170	M41	E42
ILE	ILE	THR	THR	THR	THR	L422	M357	T296	Y232	F171	K43	E44
GLY	TYR	THR	THR	THR	THR	V423	R358	E297	E233	R172	G45	G45
GLY	LEU	THR	THR	THR	THR	K424	G359	E298	E237	K173	I47	I47
ASN	ALA	THR	THR	THR	THR	L425	A360	A299	D237	Q174	S48	S48
GLU	GLN	THR	THR	THR	THR	W426	R361	E300	L178	M175	I50	I50
GLN	ASP	THR	THR	THR	THR	Q428	N363	E302	V241	I178	F16	F16
ASP	SER	THR	THR	THR	THR	L429	D364	L303	Q242	V179	S17	G51
LYS	GLY	THR	THR	THR	THR	E430	V365	A304	P243	I180	V18	P52
LEU	LEU	THR	THR	THR	THR	LYS	K366	E305	I244	Y181	P19	E53
VAL	GLU	THR	THR	THR	THR	GLU	Q367	N306	V245	Q182	L120	N54
SER	VAL	THR	THR	THR	THR	PRO	L368	R307	L246	Y183	E122	P55
ALA	ALA	THR	THR	THR	THR	ILE	T369	E308	P247	M184	D121	P55
GLY	ILE	THR	THR	THR	THR	VAL	E370	I309	E248	E122	F124	T58
ILE	VAL	THR	THR	THR	THR	GLY	A371	L310	K249	D185	D123	P59
ARG	THR	THR	THR	THR	THR	ALA	K374	K311	D250	D186	F124	T58
LYS	ASP	THR	THR	THR	THR	GLU	T376	E312	S251	I187	R125	P59
VAL	SER	THR	THR	THR	THR	THR	I375	P313	W252	V189	K126	A62
LEU	GLN	THR	THR	THR	THR	PHE	T376	V314	T253	G190	I63	A62
PHE	PHE	THR	THR	THR	THR	TYR	T377	R315	V254	S191	T128	K64

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.20 Å 154.60 Å 155.00 Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.90 Å)	Xtriage
Refinement program	BUSTER/TNT	Depositor
R, R_{free}	0.261 , 0.351 0.270 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 84.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.44$	Xtriage
Outliers	3 of 30525 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8120	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:B:103:LYS:HE3	1:B:179:VAL:CG2	1.98	0.93
1:A:381:VAL:HG12	1:A:382:ILE:N	1.82	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:252:TRP:HD1	1:A:295:LEU:HD11	1.33	0.91
1:A:258:GLN:HG3	1:A:283:LEU:CD2	2.01	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:B:241:VAL:CG2	1:B:243:PRO:HD3	2.02	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: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:64:LYS:CE	1:A:69:THR:HA	2.03	0.87
1:A:293:ILE:CG1	1:A:294:PRO:HD2	2.05	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: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:461:ARG:HG3	1:A:461:ARG:HH11	1.40	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:B:103:LYS:HG2	1:B:191:SER:N	1.92	0.84
1:A:335:GLY:HA3	1:A:356:ARG:CG	2.07	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:84:THR:HG22	1:B:88:TRP:HD1	1.43	0.83
1:B:260:LEU:HG	1:B:264:LEU:CD1	2.08	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:27:THR:CG2	1:A:29:GLU:HB3	2.08	0.82
1:A:125:ARG:HG2	1:A:146:TYR:O	1.78	0.82
1:B:366:LYS:HG2	1:B:405:TYR:CD2	2.15	0.82
1:B:37:ILE:O	1:B:41:MET:HG3	1.80	0.82
1:A:242:GLN:HG3	1:A:243:PRO:HD2	1.60	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:B:28:GLU:CB	1:B:135:ILE:HD11	2.09	0.81
1:A:238:LYS:HE3	1:A:315:HIS:CG	2.15	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:B:3:SER:N	1:B:4:PRO:HD2	1.96	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

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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:B:91:GLN:C	1:B:92:LEU:HD23	2.06	0.76
1:A:206:ARG:HH21	1:A:218:ASP:N	1.83	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:B:40:GLU:O	1:B:44:GLU:HG3	1.86	0.74
1:A:524:GLN:HA	1:A:524:GLN:NE2	2.02	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:31:ILE:O	1:A:35:VAL:HG23	1.87	0.74
1:A:258:GLN:HG3	1:A:283:LEU:HD22	1.69	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:253:THR:O	1:B:257:ILE:HG13	1.87	0.73
1:B:255:ASN:O	1:B:259:LYS:HG3	1.88	0.73
1:A:433:PRO:HG3	1:B:255:ASN:ND2	2.04	0.73
1:B:66:LYS:HG3	1:B:407:GLN:OE1	1.88	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:A:296:THR:CG2	1:A:299:ALA:H	2.02	0.73
1:A:247:PRO:HG2	3:A:2088:HOH:O	1.89	0.73
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:122:GLU:HA	1:A:125:ARG:HD2	1.71	0.72
1:A:511:ASP:OD1	1:A:512:GLN:HG3	1.88	0.72
1:A:510:PRO:HG3	3:A:2141:HOH:O	1.90	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:66:LYS:HA	1:B:407:GLN:NE2	2.05	0.70
1:B:134:SER:HB3	1:B:139:THR:HB	1.73	0.70
1:A:524:GLN:O	1:A:526:ILE:N	2.25	0.70
1:A:402:TRP:HD1	1:A:403:THR:HG23	1.57	0.70
1:B:331:LYS:HE3	1:B:364:ASP:OD2	1.89	0.70
1:B:269:GLN:HG2	1:B:346:PHE:CE2	2.26	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:494:ASN:HD22	1:A:494:ASN:N	1.88	0.70
1:A:189:VAL:HG21	1:A:205:LEU:HD23	1.72	0.70
1:B:40:GLU:HG3	3:B:2015:HOH:O	1.90	0.70
1:B:284:ARG:O	1:B:284:ARG:HG2	1.91	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:53:GLU:O	1:A:55:PRO:HD3	1.93	0.69
1:A:542:ILE:O	1:A:545:ASN:HB3	1.91	0.69
1:A:461:ARG:HH11	1:A:461:ARG:CG	2.05	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:B:92:LEU:HD23	1:B:92:LEU:N	2.08	0.69
1:A:245:VAL:O	1:A:247:PRO:HD3	1.92	0.69
1:A:58:THR:HG22	1:A:76:ASP:O	1.92	0.69
1:A:334:GLN:NE2	1:A:336:GLN:HE21	1.90	0.69
1:A:5:ILE:HD13	1:A:167:ILE:CG1	2.23	0.68
1:A:61:PHE:HB2	3:A:2025:HOH:O	1.91	0.68
1:A:277:ARG:NH2	1:A:334:GLN:HG3	2.07	0.68
1:B:354:TYR:HE1	1:B:357:MET:HE1	1.58	0.68
1:A:464:GLN:HG3	1:A:465:LYS:N	2.08	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:26:LEU:HD12	1:A:133:PRO:CD	2.24	0.67
1:A:172:ARG:NH1	1:A:182:GLN:HE21	1.92	0.67
1:A:274:ILE:HD12	1:A:309:ILE:HG21	1.75	0.67
1:A:260:LEU:O	1:A:264:LEU:HB2	1.94	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:23:GLN:HE22	1:A:60:VAL:H	1.42	0.66
1:A:175:ASN:H	1:A:176:PRO:HD3	1.60	0.66
1:A:206:ARG:O	1:A:209:LEU:N	2.27	0.66
1:A:288:ALA:HB1	1:A:291:GLU:HB2	1.78	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: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:B:84:THR:CG2	1:B:153:TRP:HE1	2.04	0.65
1:A:543:GLY:HA3	1:B:285:GLY:H	1.61	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:B:84:THR:HG22	1:B:88:TRP:CD1	2.28	0.64
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:A:278:GLN:HG2	1:A:298:GLU:HB3	1.78	0.64
1:B:214:LEU:HD23	1:B:214:LEU:N	2.12	0.64
1:A:486:LEU:HB3	1:A:524:GLN:HG3	1.79	0.64
1:A:199:ARG:O	1:A:219:LYS:NZ	2.30	0.64
1:B:278:GLN:N	1:B:302:GLU:OE1	2.30	0.64
1:A:275:LYS:HE3	1:A:305:GLU:OE1	1.97	0.64
1:A:335:GLY:CA	1:A:367:GLN:HE22	2.06	0.64
1:A:356:ARG:HH11	1:A:512:GLN:NE2	1.96	0.64
1:A:230:MET:HE3	3:A:2079:HOH:O	1.97	0.64
1:B:142:ILE:HG22	1:B:144:TYR:CE1	2.34	0.63
1:A:11:LYS:HG3	1:A:12:LEU:N	2.12	0.63
1:A:52:PRO:CD	1:A:53:GLU:H	2.11	0.63
1:B:103:LYS:HG2	1:B:190:GLY:C	2.19	0.63
1:A:29:GLU:CG	1:A:71:TRP:HH2	2.11	0.63
1:A:172:ARG:NH1	1:A:182:GLN:NE2	2.46	0.63
1:B:28:GLU:OE2	1:B:32:LYS:NZ	2.29	0.63
1:B:279:LEU:HG	1:B:302:GLU:OE2	1.99	0.63
1:A:293:ILE:HG12	1:A:294:PRO:HD2	1.80	0.63
1:A:228:LEU:HB3	1:A:242:GLN:HE22	1.63	0.63
1:B:122:GLU:CD	1:B:122:GLU:H	2.02	0.63
1:A:543:GLY:N	1:B:283:LEU:O	2.27	0.63
1:A:189:VAL:HG21	1:A:205:LEU:CD2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLN:O	1:A:334:GLN:NE2	2.27	0.63
1:A:271:TYR:CE1	1:A:310:LEU:HD23	2.33	0.63
1:A:32:LYS:HD3	3:A:2016:HOH:O	1.97	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:360:ALA:CB	1:B:366:LYS:HZ3	2.11	0.63
1:B:12:LEU:HD11	1:B:127:TYR:CE1	2.34	0.63
1:B:21:VAL:HG21	1:B:79:GLU:HG3	1.80	0.62
1:B:114:ALA:HB2	1:B:214:LEU:HD13	1.81	0.62
1:A:107:THR:HG21	1:A:202:ILE:HG13	1.81	0.62
1:A:97:PRO:HG2	1:A:232:TYR:CE2	2.34	0.62
1:B:319:TYR:O	1:B:321:PRO:HD3	1.99	0.62
1:A:503:LEU:HD23	1:B:422:LEU:HD11	1.80	0.62
1:A:206:ARG:HH21	1:A:217:PRO:C	2.02	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:B:344:GLU:O	1:B:347:LYS:HB2	1.99	0.62
1:B:279:LEU:HA	1:B:282:LEU:CD1	2.29	0.62
1:A:360:ALA:HB2	1:A:514:GLU:OE2	2.00	0.62
1:B:85:GLN:O	1:B:85:GLN:HG3	1.98	0.62
1:A:460:ASN:ND2	1:B:288:ALA:HB2	2.14	0.62
1:B:274:ILE:C	1:B:275:LYS:HG2	2.20	0.62
1:A:162:SER:OG	1:B:52:PRO:HG3	2.00	0.62
1:A:254:VAL:CG2	1:A:291:GLU:HB3	2.30	0.62
1:A:252:TRP:HB3	1:A:257:ILE:HD12	1.81	0.62
1:B:34:LEU:HD22	1:B:73:LYS:HG2	1.81	0.62
1:B:308:GLU:O	1:B:311:LYS:HD3	2.00	0.62
1:A:253:THR:HA	1:A:292:VAL:HA	1.82	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:434:ILE:HD13	1:A:530:LYS:CB	2.25	0.61
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.35	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:B:13:LYS:HB2	1:B:16:MET:CE	2.30	0.61
1:B:387:PRO:HG2	1:B:389:PHE:CZ	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLU:N	1:A:312:GLU:OE2	2.27	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:B:118:VAL:CG1	1:B:149:LEU:HG	2.30	0.60
1:A:93:GLY:O	1:B:137:ASN:ND2	2.34	0.60
1:A:335:GLY:CA	1:A:356:ARG:HG2	2.30	0.60
1:B:115:TYR:HB3	1:B:149:LEU:HB2	1.83	0.60
1:B:374:LYS:O	1:B:378:GLU:HG3	2.01	0.60
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.36	0.60
1:B:259:LYS:NZ	3:B:2060:HOH:O	2.25	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:228:LEU:HB3	1:A:242:GLN:NE2	2.17	0.60
1:A:194:GLU:O	1:A:196:GLY:N	2.34	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:B:278:GLN:HG3	1:B:298:GLU:C	2.23	0.59
1:A:238:LYS:HE3	1:A:315:HIS:CD2	2.37	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:252:TRP:CB	1:A:257:ILE:HD11	2.30	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: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:30:LYS:HD3	3:A:2011:HOH:O	2.03	0.58
1:A:206:ARG:NH2	1:A:218:ASP:HA	2.18	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:460:ASN:HA	1:B:286:THR:O	2.02	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:265:ASN:HA	1:A:268:SER:HB3	1.85	0.58
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.84	0.58
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.32	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:155:GLY:HA2	3:A:2053:HOH:O	2.04	0.58
1:B:103:LYS:HD3	1:B:190:GLY:HA3	1.86	0.58
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.32	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:B:295:LEU:HD13	1:B:300:GLU:OE2	2.04	0.57
1:A:285:GLY:HA2	1:A:286:THR:OG1	2.03	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:493:VAL:C	1:A:494:ASN:HD22	2.08	0.57
1:A:295:LEU:HD12	1:A:295:LEU:H	1.69	0.57
1:B:422:LEU:HB3	1:B:426:TRP:CZ2	2.39	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:A:296:THR:HG23	1:A:299:ALA:H	1.69	0.57
1:B:50:ILE:HG23	1:B:145:GLN:HB3	1.85	0.57
1:B:363:ASN:HB3	1:B:366:LYS:HB2	1.86	0.57
1:B:266:TRP:CZ3	1:B:427:TYR:CZ	2.93	0.57
1:A:358:ARG:O	1:A:358:ARG:HD3	2.05	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:B:276:VAL:HG22	1:B:276:VAL:O	2.05	0.56
1:B:331:LYS:O	1:B:424:LYS:HD2	2.04	0.56
1:A:460:ASN:HD22	1:B:288:ALA:HB2	1.70	0.56
1:B:63:ILE:HD12	1:B:407:GLN:HA	1.86	0.56
1:A:89:GLU:O	1:A:91:GLN:N	2.38	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:B:246:LEU:HB3	1:B:260:LEU:HD11	1.88	0.56
1:A:518:VAL:O	1:A:522:ILE:HD12	2.05	0.56
1:B:295:LEU:HD22	1:B:300:GLU:OE2	2.05	0.56
1:B:156:SER:HB2	1:B:157:PRO:CD	2.36	0.56
1:A:20:LYS:HE2	1:A:56:TYR:CE1	2.40	0.56
1:A:52:PRO:HD2	1:A:53:GLU:CG	2.26	0.56
1:A:206:ARG:HH21	1:A:218:ASP:CA	2.19	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:398:TRP:CZ2	1:A:409:THR:HG23	2.40	0.56
1:A:228:LEU:HD23	1:A:228:LEU:N	2.19	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:B:243:PRO:HA	1:B:310:LEU:O	2.06	0.56
1:A:258:GLN:CG	1:A:283:LEU:HD22	2.36	0.56
1:A:228:LEU:CB	1:A:242:GLN:HE22	2.18	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:B:125:ARG:O	1:B:145:GLN:HG3	2.06	0.55
1:B:41:MET:CE	1:B:47:ILE:HG23	2.36	0.55
1:A:210:LEU:C	1:A:212:TRP:H	2.07	0.55
1:B:395:LYS:HD3	1:B:399:GLU:CD	2.27	0.55
1:B:298:GLU:HA	1:B:301:LEU:HD22	1.89	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:A:275:LYS:HG2	1:A:332:GLN:HE22	1.71	0.55
1:B:356:ARG:HH12	1:B:358:ARG:HH21	1.53	0.55
1:B:27:THR:O	1:B:31:ILE:HG13	2.07	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:228:LEU:CA	1:A:242:GLN:HE22	2.20	0.55
1:B:81:ASN:OD1	1:B:153:TRP:HD1	1.90	0.55
1:A:296:THR:HG22	1:A:299:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ILE:O	1:B:261:VAL:HG23	2.06	0.55
1:A:88:TRP:HB2	1:B:54:ASN:O	2.07	0.55
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:328:GLU:OE2	1:B:342:TYR:OH	2.25	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:18:GLY:HA3	1:A:56:TYR:CE1	2.43	0.54
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:B:46:LYS:HD3	1:B:116:PHE:HB3	1.89	0.54
1:B:292:VAL:HG12	1:B:293:ILE:N	2.22	0.54
1:A:295:LEU:HD13	3:A:2099:HOH:O	2.06	0.54
1:A:27:THR:O	1:A:31:ILE:HG13	2.07	0.54
1:A:23:GLN:NE2	1:A:59:PRO:HA	2.23	0.54
1:A:351:THR:HG23	1:A:352:GLY:H	1.71	0.54
1:A:113:ASP:O	1:A:117:SER:OG	2.25	0.54
1:B:282:LEU:H	1:B:282:LEU:HD12	1.73	0.54
1:B:216:THR:H	1:B:217:PRO:HD3	1.73	0.54
1:A:331:LYS:HB2	1:A:337:TRP:CZ3	2.43	0.54
1:B:425:LEU:O	1:B:425:LEU:HD22	2.08	0.54
1:B:169:GLU:O	1:B:173:LYS:HB2	2.08	0.54
1:A:376:THR:HG23	1:A:386:THR:HG22	1.88	0.54
1:A:513:SER:CB	1:A:518:VAL:HG11	2.37	0.54
1:A:205:LEU:O	1:A:208:HIS:HB3	2.08	0.54
1:A:426:TRP:O	1:A:526:ILE:HG23	2.08	0.54
1:A:402:TRP:CZ3	1:B:364:ASP:HB2	2.43	0.54
1:B:122:GLU:HB3	3:B:2038:HOH:O	2.08	0.54
1:A:521:ILE:HG22	1:A:525:LEU:HD12	1.89	0.54
1:B:175:ASN:CB	1:B:178:ILE:HG13	2.38	0.54
1:A:480:GLN:O	1:A:483:TYR:HB3	2.08	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:B:245:VAL:HG21	1:B:429:LEU:CD2	2.38	0.53
1:A:312:GLU:O	1:A:312:GLU:OE2	2.27	0.53
1:B:70:LYS:O	1:B:70:LYS:HG3	2.09	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:A:402:TRP:CD1	1:A:403:THR:CG2	2.88	0.53
1:A:278:GLN:HG2	1:A:298:GLU:CB	2.38	0.53
1:B:12:LEU:HD12	1:B:127:TYR:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HG23	1:A:256:ASP:OD1	2.08	0.53
1:A:93:GLY:C	1:B:137:ASN:HD22	2.12	0.53
1:A:65:LYS:N	3:A:2026:HOH:O	2.40	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:10:VAL:HG11	1:A:153:TRP:CH2	2.43	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:260:LEU:HD23	1:B:279:LEU:HD13	1.91	0.53
1:B:246:LEU:HD12	1:B:307:ARG:HG2	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:308:GLU:O	1:A:311:LYS:HB2	2.09	0.52
1:A:169:GLU:O	1:A:171:PHE:N	2.42	0.52
1:A:27:THR:HB	1:A:30:LYS:CD	2.40	0.52
1:A:238:LYS:HE3	1:A:315:HIS:ND1	2.24	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:538:ALA:CB	1:A:545:ASN:HD21	2.22	0.52
1:A:489:SER:HB2	1:A:493:VAL:HB	1.90	0.52
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.89	0.52
1:B:13:LYS:HG3	1:B:83:ARG:O	2.09	0.52
1:A:351:THR:HG23	1:A:352:GLY:N	2.24	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:536:VAL:HG23	1:A:536:VAL:O	2.09	0.52
1:A:451:LYS:NZ	1:A:451:LYS:CB	2.70	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:18:GLY:HA3	1:A:56:TYR:CD1	2.46	0.51
1:B:421:PRO:HD2	1:B:422:LEU:H	1.75	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:A:441:TYR:CD2	1:A:544:GLY:HA3	2.46	0.51
1:B:91:GLN:HB3	1:B:92:LEU:HD23	1.92	0.51
1:A:56:TYR:O	1:A:57:ASN:HB2	2.10	0.51
1:A:208:HIS:O	1:A:212:TRP:HD1	1.93	0.51
1:A:210:LEU:C	1:A:212:TRP:N	2.63	0.51
1:A:115:TYR:HB3	1:A:149:LEU:HB2	1.92	0.51
1:B:379:SER:OG	1:B:387:PRO:HD3	2.09	0.51
1:B:193:LEU:HB3	1:B:197:GLN:HB3	1.92	0.51
1:A:335:GLY:HA2	1:A:367:GLN:CD	2.31	0.51
1:A:224:GLU:HB2	1:A:225:PRO:CD	2.36	0.51
1:A:198:HIS:C	1:A:200:THR:H	2.12	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:71:TRP:N	1:A:71:TRP:CD1	2.79	0.51
1:A:111:VAL:HG11	1:A:214:LEU:HD22	1.91	0.51
1:B:97:PRO:HG3	1:B:181:TYR:HB2	1.92	0.51
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.32	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:188:TYR:HH	1:A:229:TRP:HE1	1.58	0.51
1:A:134:SER:O	1:A:137:ASN:N	2.39	0.51
1:A:420:PRO:HA	1:A:421:PRO:C	2.31	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:A:402:TRP:HE3	1:A:409:THR:HG22	1.74	0.51
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.93	0.51
1:B:22:LYS:O	1:B:59:PRO:HG3	2.11	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:12:LEU:HD11	1:A:127:TYR:CE1	2.46	0.51
1:A:434:ILE:HB	1:A:437:ALA:CB	2.42	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:228:LEU:CD2	1:A:228:LEU:N	2.74	0.50
1:A:503:LEU:HD11	1:A:507:GLN:NE2	2.26	0.50
1:A:171:PHE:CE2	1:A:205:LEU:HA	2.46	0.50
1:A:129:ALA:HA	1:A:144:TYR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:HIS:ND1	1:A:505:ILE:HD13	2.26	0.50
1:A:270:ILE:HG23	1:A:271:TYR:HD2	1.76	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:20:LYS:HZ3	1:A:55:PRO:HB2	1.76	0.50
1:A:391:LEU:N	1:A:391:LEU:HD23	2.27	0.50
1:A:209:LEU:O	1:A:212:TRP:HB2	2.12	0.50
1:A:341:ILE:N	1:A:350:LYS:O	2.35	0.50
1:B:354:TYR:HE1	1:B:357:MET:CE	2.22	0.50
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.47	0.50
1:A:20:LYS:HE2	1:A:56:TYR:CD1	2.47	0.50
1:A:494:ASN:N	1:A:494:ASN:ND2	2.60	0.50
1:A:451:LYS:HZ3	1:A:451:LYS:HB3	1.73	0.50
1:B:272:PRO:C	1:B:274:ILE:H	2.15	0.50
1:A:398:TRP:CH2	1:A:409:THR:CG2	2.95	0.50
1:A:138:GLU:HG2	3:A:2048:HOH:O	2.10	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:228:LEU:CB	1:A:242:GLN:NE2	2.75	0.49
1:A:188:TYR:OH	1:A:229:TRP:NE1	2.42	0.49
1:A:469:LEU:HD13	1:A:477:THR:HG22	1.93	0.49
1:B:209:LEU:CD2	1:B:214:LEU:HD12	2.31	0.49
1:A:393:ILE:O	1:A:416:PHE:HD1	1.95	0.49
1:A:498:ASP:CB	1:A:538:ALA:HB2	2.42	0.49
1:A:238:LYS:HE3	1:A:315:HIS:CE1	2.48	0.49
1:A:271:TYR:CE1	1:A:314:VAL:CG2	2.95	0.49
1:A:328:GLU:OE2	1:A:342:TYR:OH	2.24	0.49
1:A:136:ASN:H	1:A:138:GLU:HG3	1.77	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:52:PRO:CD	1:A:53:GLU:N	2.74	0.49
1:B:339:TYR:O	1:B:351:THR:HA	2.12	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:B:12:LEU:CD1	1:B:127:TYR:CZ	2.96	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:B:178:ILE:HD11	1:B:201:LYS:HG2	1.95	0.49
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: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:A:1:PRO:O	1:A:2:ILE:CG1	2.61	0.49
1:B:266:TRP:CH2	1:B:427:TYR:OH	2.63	0.49
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.12	0.49
1:A:249:LYS:CB	1:A:249:LYS:NZ	2.75	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:27:THR:HG22	1:A:30:LYS:H	1.78	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:308:GLU:HA	1:A:311:LYS:HD2	1.95	0.48
1:B:360:ALA:HB2	1:B:366:LYS:NZ	2.28	0.48
1:A:246:LEU:HD21	1:A:310:LEU:HD13	1.95	0.48
1:A:194:GLU:C	1:A:196:GLY:H	2.17	0.48
1:A:358:ARG:HA	1:A:358:ARG:NE	2.28	0.48
1:A:79:GLU:CG	1:A:83:ARG:HH11	2.26	0.48
1:B:44:GLU:HB2	1:B:46:LYS:HG3	1.95	0.48
1:A:486:LEU:HD13	1:A:524:GLN:CB	2.43	0.48
1:A:529:GLU:HG3	1:A:529:GLU:O	2.12	0.48
1:B:41:MET:HE2	1:B:47:ILE:HG23	1.95	0.48
1:B:22:LYS:HD3	3:B:2007:HOH:O	2.14	0.48
1:B:242:GLN:O	1:B:242:GLN:OE1	2.31	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:402:TRP:O	1:B:406:TRP:HB2	2.14	0.48
1:B:103:LYS:HG2	1:B:190:GLY:CA	2.43	0.48
1:A:52:PRO:HD2	1:A:53:GLU:H	1.79	0.48
1:A:175:ASN:HD21	1:A:201:LYS:HE3	1.79	0.48
1:A:168:LEU:HD11	1:A:187:LEU:HD21	1.95	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:97:PRO:HG2	1:A:232:TYR:CD2	2.49	0.48
1:A:195:ILE:HB	1:A:199:ARG:HD3	1.95	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:B:118:VAL:HG12	1:B:149:LEU:CG	2.38	0.48
1:A:402:TRP:CD1	1:A:403:THR:N	2.82	0.48
1:A:194:GLU:C	1:A:196:GLY:N	2.67	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:B:209:LEU:HD22	1:B:214:LEU:CD1	2.32	0.47
3:A:2140:HOH:O	1:B:422:LEU:HB2	2.14	0.47
1:B:361:HIS:HB2	3:B:2076:HOH:O	2.14	0.47
1:A:14:PRO:C	1:A:16:MET:H	2.17	0.47
1:A:479:LEU:HB2	1:A:517:LEU:HD13	1.95	0.47
1:A:490:GLY:O	1:A:492:GLU:N	2.47	0.47
1:A:228:LEU:CD1	1:A:242:GLN:NE2	2.75	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:448:ARG:HG2	1:A:448:ARG:H	1.55	0.47
1:A:183:TYR:O	1:A:186:ASP:HB2	2.14	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:23:GLN:HE22	1:A:60:VAL:N	2.10	0.47
1:A:209:LEU:O	1:A:212:TRP:N	2.46	0.47
1:A:4:PRO:HG2	1:A:212:TRP:CE3	2.50	0.47
1:A:339:TYR:OH	1:A:378:GLU:OE1	2.30	0.47
1:A:79:GLU:O	1:A:82:LYS:N	2.47	0.47
1:A:276:VAL:HG13	1:A:276:VAL:O	2.14	0.47
1:B:30:LYS:O	1:B:34:LEU:HG	2.14	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:77:PHE:CD1	1:A:80:LEU:HD23	2.49	0.47
1:B:120:LEU:O	1:B:125:ARG:NH2	2.36	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:195:ILE:HB	1:A:199:ARG:CD	2.45	0.47
1:A:365:VAL:HG11	1:A:401:TRP:CE3	2.50	0.47
1:B:84:THR:HG21	1:B:153:TRP:CE2	2.48	0.47
1:B:363:ASN:CB	1:B:366:LYS:HB2	2.44	0.47
1:A:460:ASN:CB	1:B:286:THR:O	2.63	0.47
1:B:278:GLN:HG3	1:B:299:ALA:N	2.30	0.47
1:A:88:TRP:O	1:A:90:VAL:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:H	1:A:176:PRO:CD	2.28	0.47
1:B:360:ALA:HB1	3:B:2078:HOH:O	2.14	0.47
1:A:350:LYS:CG	1:A:351:THR:N	2.78	0.47
1:A:89:GLU:OE1	1:A:89:GLU:O	2.33	0.47
1:B:148:VAL:O	1:B:149:LEU:C	2.54	0.46
1:A:461:ARG:CG	1:A:461:ARG:NH1	2.72	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:26:LEU:HD12	1:A:133:PRO:HD2	1.96	0.46
1:B:391:LEU:HD12	1:B:414:TRP:HB2	1.97	0.46
1:A:100:LEU:HD21	2:A:1546:I15:N1	2.30	0.46
1:A:459:THR:HG23	1:A:463:ARG:HB2	1.98	0.46
1:B:50:ILE:HD12	1:B:54:ASN:ND2	2.30	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:B:266:TRP:HZ3	1:B:427:TYR:CZ	2.34	0.46
1:A:93:GLY:C	1:B:137:ASN:ND2	2.68	0.46
1:A:277:ARG:HH11	1:A:277:ARG:HG2	1.80	0.46
1:B:266:TRP:CD2	1:B:426:TRP:CD1	3.04	0.46
1:B:356:ARG:HD2	1:B:358:ARG:HA	1.98	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:A:536:VAL:HG11	1:A:542:ILE:HG21	1.97	0.46
1:A:317:VAL:HG13	1:A:318:TYR:N	2.30	0.46
1:A:167:ILE:CD1	1:A:214:LEU:HD12	2.45	0.46
1:A:486:LEU:HA	1:A:486:LEU:HD23	1.62	0.46
1:A:406:TRP:CZ3	1:B:418:ASN:HA	2.45	0.46
1:B:183:TYR:CE2	1:B:184:MET:CE	2.99	0.46
1:A:249:LYS:HG2	1:A:251:SER:O	2.16	0.46
1:A:27:THR:HG22	1:A:30:LYS:HG2	1.97	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: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:23:GLN:HG2	1:A:57:ASN:HD21	1.81	0.45
1:B:247:PRO:C	1:B:307:ARG:HH12	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:GLN:HB2	1:B:429:LEU:HD11	1.98	0.45
1:A:337:TRP:NE1	1:A:367:GLN:NE2	2.58	0.45
1:A:434:ILE:HG21	1:A:492:GLU:HB3	1.97	0.45
1:A:180:ILE:HG22	1:A:187:LEU:CD1	2.46	0.45
1:A:411:ILE:CG2	1:A:414:TRP:CD1	2.98	0.45
1:A:270:ILE:HG23	1:A:271:TYR:CD2	2.51	0.45
1:B:195:ILE:O	1:B:199:ARG:HG2	2.16	0.45
1:B:26:LEU:HA	1:B:26:LEU:HD23	1.49	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:479:LEU:CD1	1:A:501:TYR:HE2	2.29	0.45
1:A:440:PHE:CD1	1:A:493:VAL:CG2	2.99	0.45
1:B:47:ILE:HB	1:B:145:GLN:O	2.17	0.45
1:A:277:ARG:NH1	1:A:277:ARG:HG2	2.31	0.45
1:A:447:ASN:O	1:A:451:LYS:N	2.46	0.45
1:A:379:SER:HA	1:A:383:TRP:CE3	2.52	0.45
1:A:135:ILE:HB	1:A:138:GLU:OE2	2.15	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:288:ALA:HB3	1:A:291:GLU:OE1	2.17	0.45
1:B:245:VAL:CG2	1:B:429:LEU:CD2	2.94	0.45
1:A:357:MET:C	1:A:359:GLY:N	2.68	0.45
1:B:266:TRP:HZ3	1:B:427:TYR:HH	1.55	0.45
1:B:312:GLU:HA	1:B:313:PRO:HD2	1.11	0.45
1:A:264:LEU:HA	1:A:264:LEU:HD23	1.84	0.45
1:A:38:CYS:HB3	1:A:144:TYR:CZ	2.52	0.45
1:A:71:TRP:H	1:A:71:TRP:HD1	1.64	0.45
1:A:244:ILE:HG12	3:A:2083:HOH:O	2.16	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: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:226:PRO:HA	1:A:234:LEU:O	2.17	0.45
1:A:52:PRO:CD	1:A:53:GLU:HG2	2.28	0.45
1:A:529:GLU:O	1:A:530:LYS:HG2	2.16	0.45
1:A:167:ILE:HD13	1:A:214:LEU:HD12	1.98	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:B:92:LEU:N	1:B:92:LEU:CD2	2.79	0.44
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.76	0.44
1:A:406:TRP:CZ3	1:A:407:GLN:NE2	2.86	0.44
1:B:249:LYS:O	1:B:250:ASP:HB2	2.16	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:441:TYR:CG	1:A:544:GLY:HA3	2.52	0.44
1:A:401:TRP:CD1	1:A:425:LEU:HD11	2.53	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:B:298:GLU:HG3	1:B:298:GLU:H	1.48	0.44
1:A:513:SER:CB	1:A:518:VAL:CG1	2.96	0.44
1:B:20:LYS:CE	1:B:55:PRO:HB2	2.45	0.44
1:A:364:ASP:HB2	1:A:423:VAL:HG13	1.99	0.44
1:B:58:THR:CG2	1:B:75:VAL:CG1	2.96	0.44
1:B:261:VAL:HA	1:B:276:VAL:HG21	1.98	0.44
1:A:391:LEU:HA	1:A:392:PRO:HD3	1.78	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: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:64:LYS:HA	1:A:71:TRP:HB3	2.00	0.44
1:A:54:ASN:HA	1:A:55:PRO:HD2	1.68	0.44
1:A:416:PHE:CE1	1:A:422:LEU:HD13	2.52	0.44
1:A:10:VAL:HG11	1:A:153:TRP:HH2	1.83	0.44
1:B:36:GLU:O	1:B:38:CYS:N	2.50	0.44
1:A:136:ASN:HB2	1:A:138:GLU:CG	2.47	0.44
1:B:5:ILE:HD13	1:B:5:ILE:HA	1.69	0.44
1:A:30:LYS:HG2	1:A:30:LYS:H	1.50	0.44
1:B:246:LEU:HB3	1:B:260:LEU:CD1	2.48	0.44
1:A:180:ILE:HG22	1:A:187:LEU:HD11	1.99	0.44
1:A:153:TRP:CD1	1:A:154:LYS:N	2.86	0.44
1:A:79:GLU:O	1:A:81:ASN:N	2.51	0.44
1:A:237:ASP:HB2	3:A:2033:HOH:O	2.18	0.44
1:A:445:ALA:O	1:A:453:GLY:HA3	2.17	0.44
1:A:102:LYS:HB3	1:A:318:TYR:HB2	2.00	0.43
1:B:78:ARG:O	1:B:82:LYS:HG3	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:A:131:THR:OG1	1:A:143:ARG:HG2	2.18	0.43
1:A:27:THR:HB	1:A:30:LYS:CG	2.48	0.43
1:B:246:LEU:HD12	1:B:307:ARG:CG	2.48	0.43
1:A:171:PHE:O	1:A:175:ASN:HB2	2.17	0.43
1:B:341:ILE:HG21	1:B:383:TRP:CZ3	2.52	0.43
1:A:398:TRP:CZ2	1:A:411:ILE:HG13	2.52	0.43
1:B:94:ILE:CD1	1:B:94:ILE:N	2.73	0.43
1:A:441:TYR:HB3	1:A:544:GLY:HA3	2.00	0.43
1:A:136:ASN:HB2	3:A:2048:HOH:O	2.18	0.43
1:B:393:ILE:HG12	1:B:394:GLN:H	1.83	0.43
1:B:214:LEU:N	1:B:214:LEU:CD2	2.79	0.43
1:A:334:GLN:HB2	3:A:2107:HOH:O	2.18	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:A:328:GLU:O	1:A:339:TYR:HA	2.18	0.43
1:A:379:SER:HB3	1:A:383:TRP:CE3	2.53	0.43
1:B:281:LYS:O	1:B:283:LEU:N	2.51	0.43
1:A:357:MET:C	1:A:359:GLY:H	2.21	0.43
1:B:376:THR:HG23	1:B:386:THR:HG22	1.99	0.43
1:B:157:PRO:HG3	1:B:184:MET:O	2.18	0.43
1:A:467:VAL:HG13	1:A:468:THR:N	2.33	0.43
1:A:167:ILE:CD1	1:A:214:LEU:CD1	2.96	0.43
1:B:391:LEU:O	1:B:393:ILE:N	2.52	0.43
1:A:455:ALA:O	1:A:467:VAL:N	2.52	0.43
1:B:243:PRO:C	1:B:245:VAL:N	2.72	0.43
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.33	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:139:THR:HA	1:A:140:PRO:HD3	1.85	0.43
1:B:333:GLY:O	1:B:334:GLN:HB2	2.19	0.43
1:A:356:ARG:HB3	1:A:359:GLY:H	1.82	0.43
1:A:277:ARG:NH2	1:A:334:GLN:CG	2.80	0.43
1:B:367:GLN:HA	1:B:370:GLU:HG3	2.01	0.43
1:A:450:THR:O	1:A:451:LYS:CB	2.67	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:A:448:ARG:NH1	1:A:448:ARG:CG	2.77	0.43
1:A:8:VAL:HA	1:A:9:PRO:HD2	1.46	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:B:175:ASN:N	1:B:175:ASN:OD1	2.51	0.43
1:A:406:TRP:CZ3	1:A:407:GLN:CD	2.93	0.43
1:A:273:GLY:HA3	1:A:309:ILE:HD13	2.00	0.43
1:B:274:ILE:CG2	1:B:275:LYS:N	2.82	0.43
1:B:132:ILE:O	1:B:133:PRO:O	2.36	0.43
1:A:538:ALA:O	1:A:539:HIS:HB2	2.19	0.42
1:A:102:LYS:HE2	1:A:320:ASP:CB	2.30	0.42
1:A:406:TRP:CZ3	1:B:419:THR:N	2.87	0.42
1:A:195:ILE:CB	1:A:199:ARG:CD	2.97	0.42
1:A:433:PRO:CG	1:B:255:ASN:HD22	2.31	0.42
1:A:376:THR:HG23	1:A:386:THR:CG2	2.49	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:A:183:TYR:CE1	1:A:230:MET:SD	3.12	0.42
1:B:51:GLY:HA3	1:B:53:GLU:OE1	2.19	0.42
1:B:244:ILE:O	1:B:245:VAL:HG22	2.18	0.42
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.78	0.42
1:A:206:ARG:HH11	1:A:206:ARG:HG2	1.83	0.42
1:B:350:LYS:HB2	1:B:383:TRP:HH2	1.83	0.42
1:A:136:ASN:C	1:A:138:GLU:N	2.72	0.42
1:B:243:PRO:HB2	1:B:245:VAL:HG13	2.01	0.42
1:A:356:ARG:HB3	1:A:359:GLY:N	2.34	0.42
1:A:255:ASN:O	1:A:258:GLN:HB2	2.19	0.42
1:B:175:ASN:ND2	1:B:201:LYS:CE	2.75	0.42
1:A:246:LEU:HD21	1:A:310:LEU:CD1	2.50	0.42
1:A:328:GLU:OE2	1:A:342:TYR:CE2	2.72	0.42
1:B:421:PRO:CD	1:B:422:LEU:H	2.31	0.42
1:A:263:LYS:HA	1:A:263:LYS:HD3	1.87	0.42
1:A:3:SER:OG	1:A:5:ILE:HB	2.19	0.42
1:A:424:LYS:HE2	1:A:426:TRP:CE2	2.50	0.42
1:A:153:TRP:CG	1:A:154:LYS:N	2.87	0.42
1:B:58:THR:HG21	1:B:75:VAL:HG12	2.00	0.42
1:A:467:VAL:CG1	1:A:468:THR:N	2.82	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:3:SER:HA	1:A:4:PRO:HD2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HG	1:A:302:GLU:OE2	2.20	0.42
1:A:441:TYR:CB	1:A:544:GLY:HA3	2.49	0.42
1:B:50:ILE:HD11	1:B:129:ALA:HB1	2.02	0.42
1:A:379:SER:OG	1:A:387:PRO:HD3	2.19	0.42
1:A:357:MET:HG2	1:A:357:MET:O	2.20	0.42
1:A:3:SER:HA	1:A:213:GLY:HA3	2.01	0.42
1:B:172:ARG:NH1	1:B:172:ARG:HG3	2.35	0.42
1:A:68:SER:C	1:A:70:LYS:H	2.23	0.42
1:A:356:ARG:NH1	1:A:512:GLN:NE2	2.66	0.42
1:A:2:ILE:O	1:A:3:SER:C	2.57	0.42
1:A:277:ARG:CZ	1:A:334:GLN:CG	2.97	0.42
1:A:334:GLN:O	1:A:336:GLN:HG3	2.20	0.42
1:B:271:TYR:HA	1:B:272:PRO:HD2	1.91	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:A:268:SER:O	1:A:351:THR:HG22	2.18	0.42
1:B:111:VAL:HG11	1:B:187:LEU:HG	2.02	0.42
1:B:369:THR:HG22	1:B:398:TRP:CZ3	2.54	0.41
1:B:266:TRP:HH2	1:B:427:TYR:HH	1.61	0.41
1:A:253:THR:OG1	1:A:256:ASP:OD1	2.38	0.41
1:B:425:LEU:HD23	1:B:425:LEU:HA	1.34	0.41
1:B:287:LYS:HD3	1:B:293:ILE:HD11	2.02	0.41
1:A:249:LYS:NZ	1:A:249:LYS:HB2	2.18	0.41
1:B:382:ILE:HG22	1:B:382:ILE:O	2.18	0.41
1:A:501:TYR:O	1:A:505:ILE:HG13	2.20	0.41
1:A:202:ILE:HD12	1:A:202:ILE:HA	1.81	0.41
1:B:419:THR:HA	1:B:420:PRO:HD2	1.94	0.41
1:A:452:LEU:HD23	3:A:2126:HOH:O	2.20	0.41
1:A:271:TYR:HB3	1:A:274:ILE:CD1	2.50	0.41
1:A:256:ASP:HA	1:A:259:LYS:HG3	2.01	0.41
1:A:130:PHE:N	1:A:130:PHE:CD2	2.88	0.41
1:B:205:LEU:HD12	1:B:205:LEU:O	2.19	0.41
1:B:331:LYS:CE	1:B:364:ASP:OD2	2.63	0.41
1:B:34:LEU:HA	1:B:34:LEU:HD23	1.84	0.41
1:B:297:GLU:HA	1:B:300:GLU:HG3	2.01	0.41
1:B:242:GLN:O	1:B:242:GLN:CG	2.68	0.41
1:B:50:ILE:HD12	1:B:54:ASN:CB	2.51	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:266:TRP:CH2	1:B:427:TYR:CZ	3.07	0.41
1:A:195:ILE:CG2	1:A:199:ARG:CD	2.98	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:21:VAL:HG21	1:B:79:GLU:CG	2.50	0.41
1:B:180:ILE:HD13	1:B:189:VAL:HG22	2.02	0.41
1:B:270:ILE:HD13	1:B:270:ILE:HG21	1.85	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:A:257:ILE:CG2	1:A:283:LEU:CD1	2.97	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:B:328:GLU:HG2	1:B:390:LYS:HD2	2.03	0.41
1:B:132:ILE:HA	1:B:133:PRO:HD2	1.65	0.41
1:A:136:ASN:HB2	1:A:138:GLU:HG3	2.02	0.41
1:A:37:ILE:CG2	1:A:41:MET:HE1	2.50	0.41
1:A:542:ILE:HB	1:A:545:ASN:HB3	2.02	0.41
1:A:443:ASP:O	1:A:481:ALA:HB2	2.20	0.41
1:B:363:ASN:HB3	1:B:366:LYS:CB	2.50	0.41
1:B:359:GLY:C	1:B:361:HIS:H	2.24	0.41
1:A:491:LEU:HD13	3:A:2149:HOH:O	2.21	0.41
1:A:284:ARG:O	1:A:285:GLY:O	2.38	0.41
1:B:287:LYS:CD	1:B:293:ILE:HD11	2.51	0.41
1:A:540:LYS:CB	1:A:542:ILE:HD12	2.35	0.41
1:B:264:LEU:CD2	1:B:306:ASN:ND2	2.83	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:440:PHE:HD1	1:A:493:VAL:HG23	1.86	0.41
1:B:160:PHE:CD2	1:B:164:MET:HE2	2.56	0.41
1:B:119:PRO:HA	1:B:148:VAL:HA	2.02	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:450:THR:HB	1:A:452:LEU:CD1	2.51	0.41
1:A:268:SER:O	1:A:351:THR:CG2	2.69	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:A:183:TYR:HE1	1:A:230:MET:SD	2.44	0.41
1:A:37:ILE:CG2	1:A:41:MET:CE	2.99	0.41
1:B:81:ASN:HD22	1:B:154:LYS:HD2	1.82	0.41
1:B:88:TRP:CZ3	1:B:89:GLU:HB2	2.56	0.41
1:B:403:THR:C	1:B:405:TYR:N	2.74	0.41
1:B:100:LEU:HD22	1:B:181:TYR:HB3	2.03	0.41
1:B:103:LYS:CD	1:B:190:GLY:HA3	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:THR:HG22	1:A:409:THR:O	2.21	0.40
1:A:340:GLN:HE21	1:A:340:GLN:HB3	1.57	0.40
1:B:51:GLY:C	1:B:53:GLU:N	2.74	0.40
1:A:493:VAL:HG22	1:A:494:ASN:N	2.36	0.40
1:A:216:THR:CG2	1:A:217:PRO:CD	2.99	0.40
1:A:405:TYR:O	1:B:331:LYS:HD3	2.20	0.40
1:B:356:ARG:HD2	1:B:358:ARG:CA	2.52	0.40
1:A:79:GLU:HG3	1:A:83:ARG:HH11	1.85	0.40
1:A:354:TYR:OH	1:A:370:GLU:OE1	2.37	0.40
1:B:153:TRP:CZ2	1:B:155:GLY:HA3	2.56	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: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:136:ASN:H	1:A:138:GLU:CG	2.34	0.40
1:A:34:LEU:HD22	1:A:73:LYS:HG3	2.04	0.40
1:B:171:PHE:HB2	1:B:208:HIS:CD2	2.57	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:5:ILE:HG22	1:B:5:ILE:O	2.22	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:339:TYR:CD1	1:B:375:ILE:HG12	2.56	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:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.56	0.40
1:A:181:TYR:HB2	1:A:188:TYR:HB2	2.04	0.40
1:A:139:THR:CB	1:A:140:PRO:CD	2.96	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	2.42	7 (33%)	27,34,34	1.98	9 (33%)

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	-7.50	1.45	1.50
2	A	1546	I15	C8-C3	-2.75	1.36	1.41
2	A	1546	I15	C13-C15	-2.67	1.34	1.39
2	A	1546	I15	C4-N9	2.50	1.37	1.33
2	A	1546	I15	C12-C6	3.01	1.44	1.38
2	A	1546	I15	C8-C12	3.33	1.43	1.36
2	A	1546	I15	F1-C6	3.43	1.43	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1546	I15	C12-C6-C2	-3.13	115.23	122.38
2	A	1546	I15	C16-C14-C11	-3.12	115.21	119.47
2	A	1546	I15	C13-C15-C18	-2.07	116.90	119.51
2	A	1546	I15	C11-O5-C2	2.32	122.50	118.47
2	A	1546	I15	C17-C15-C18	2.36	122.50	119.51
2	A	1546	I15	C17-C16-C14	2.44	124.24	119.72
2	A	1546	I15	F1-C6-C12	2.55	124.26	118.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1546	I15	C10-C4-N9	3.10	126.67	119.73
2	A	1546	I15	C8-C3-N7	5.00	138.65	130.22

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, 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	545/566 (96%)	0.42	42 (7%)	16 11	34, 59, 86, 107	0
1	B	416/566 (73%)	0.60	50 (12%)	6 3	36, 58, 95, 119	0
All	All	961/1132 (84%)	0.50	92 (9%)	10 6	34, 59, 90, 119	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	357	MET	9.1
1	B	284	ARG	5.6
1	A	285	GLY	4.8
1	A	291	GLU	4.7
1	A	290	THR	4.6
1	B	4	PRO	4.6
1	A	359	GLY	4.4
1	B	15	GLY	4.4
1	B	14	PRO	4.3
1	B	361	HIS	4.1
1	A	65	LYS	4.1
1	B	251	SER	4.1
1	B	296	THR	4.0
1	A	54	ASN	3.9
1	A	66	LYS	3.9
1	B	39	THR	3.8
1	A	67	ASP	3.7
1	B	3	SER	3.7
1	B	362	THR	3.7
1	B	217	PRO	3.6
1	A	453	GLY	3.5
1	B	70	LYS	3.5
1	B	69	THR	3.4
1	B	232	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	278	GLN	3.4
1	B	16	MET	3.3
1	B	7	THR	3.3
1	A	68	SER	3.3
1	B	13	LYS	3.3
1	A	64	LYS	3.3
1	A	278	GLN	3.2
1	B	40	GLU	3.2
1	B	5	ILE	3.2
1	A	282	LEU	3.2
1	A	292	VAL	3.2
1	B	359	GLY	3.1
1	B	230	MET	3.1
1	A	221	HIS	3.1
1	B	184	MET	3.1
1	A	104	LYS	3.0
1	A	402	TRP	3.0
1	B	356	ARG	2.9
1	B	301	LEU	2.9
1	A	539	HIS	2.9
1	B	43	LYS	2.9
1	B	360	ALA	2.8
1	A	69	THR	2.8
1	A	289	LEU	2.8
1	B	335	GLY	2.7
1	B	6	GLU	2.7
1	B	355	ALA	2.7
1	B	298	GLU	2.7
1	A	541	GLY	2.7
1	B	88	TRP	2.6
1	A	472	THR	2.6
1	B	336	GLN	2.6
1	B	231	GLY	2.6
1	B	186	ASP	2.6
1	A	473	THR	2.5
1	A	70	LYS	2.5
1	A	530	LYS	2.5
1	A	242	GLN	2.4
1	A	545	ASN	2.4
1	A	357	MET	2.4
1	B	297	GLU	2.4
1	A	200	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	24	TRP	2.4
1	A	520	GLN	2.3
1	B	173	LYS	2.3
1	A	358	ARG	2.3
1	A	52	PRO	2.3
1	A	544	GLY	2.3
1	B	358	ARG	2.3
1	B	67	ASP	2.2
1	B	123	ASP	2.2
1	B	152	GLY	2.3
1	A	123	ASP	2.2
1	B	65	LYS	2.2
1	B	295	LEU	2.2
1	B	183	TYR	2.2
1	A	63	ILE	2.2
1	A	506	ILE	2.2
1	A	396	GLU	2.1
1	B	248	GLU	2.1
1	B	410	TRP	2.1
1	B	92	LEU	2.1
1	A	315	HIS	2.0
1	A	434	ILE	2.0
1	B	299	ALA	2.0
1	B	237	ASP	2.0
1	A	301	LEU	2.0
1	A	445	ALA	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, 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	LLDF	B-factors(\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.