



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 09:28 PM 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 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/ValidationPDFNotes.html>

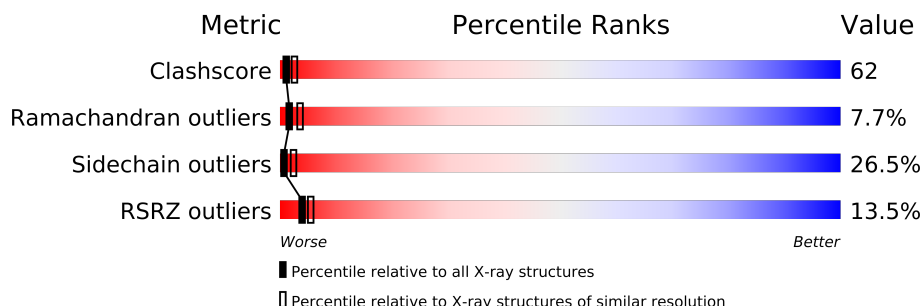
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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.

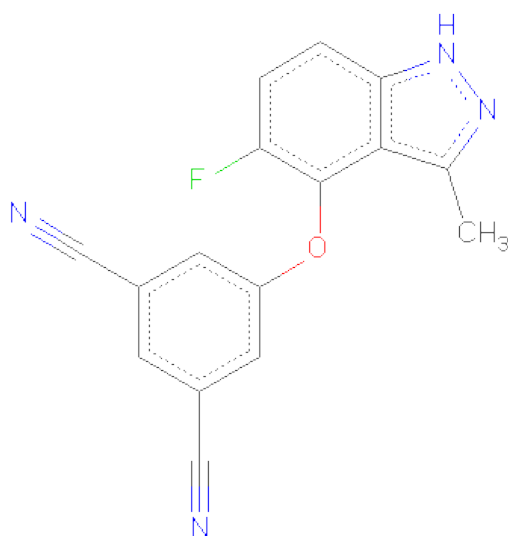
- Molecule 1 is a protein called REVERSE TRANSCRIPTASE/RNASEH.

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
A	350	LYS	ARG	CONFLICT	UNP Q72547
B	103	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.

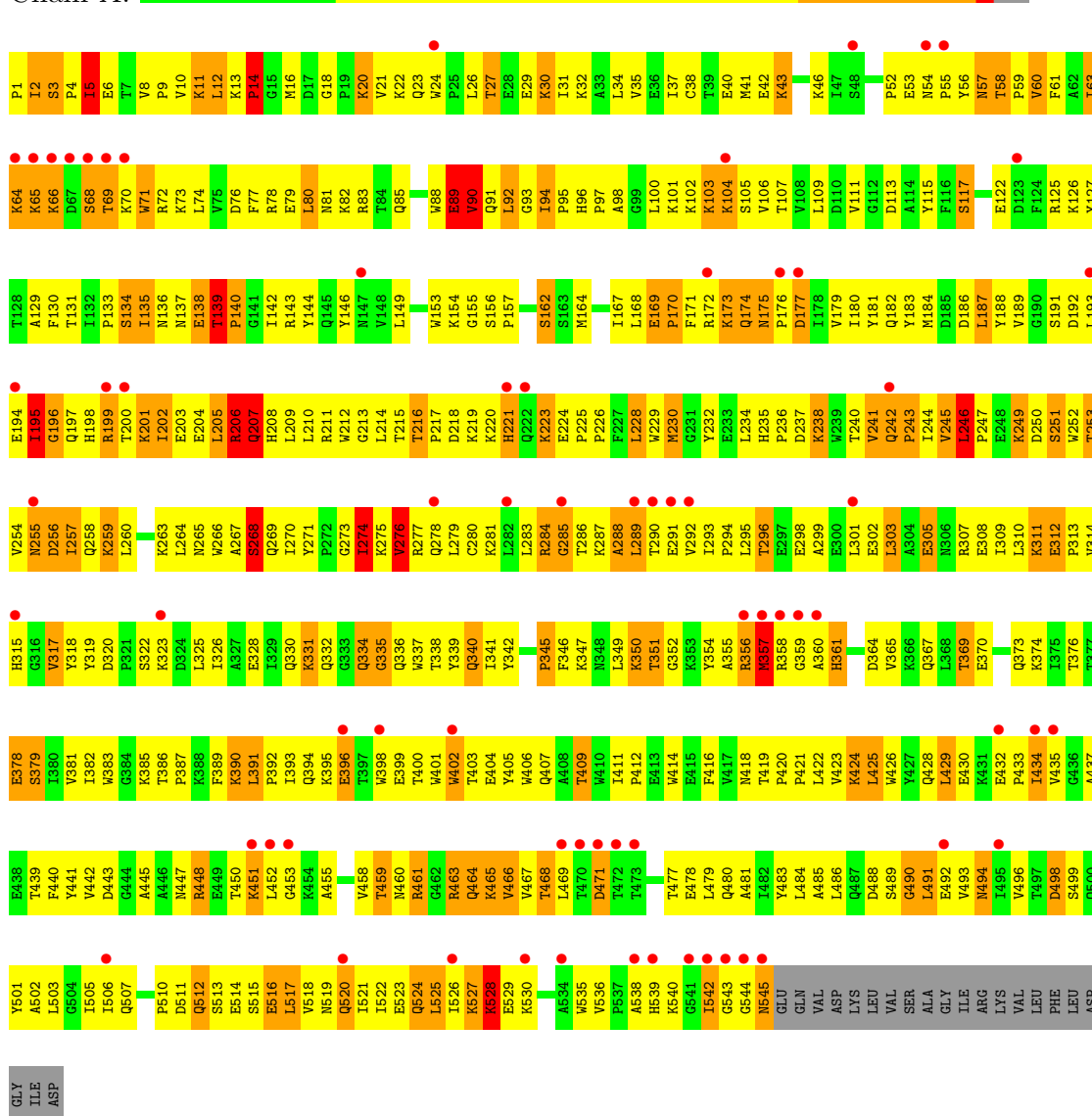
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	0
			152	152		
3	B	87	Total	O	0	0
			87	87		

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.

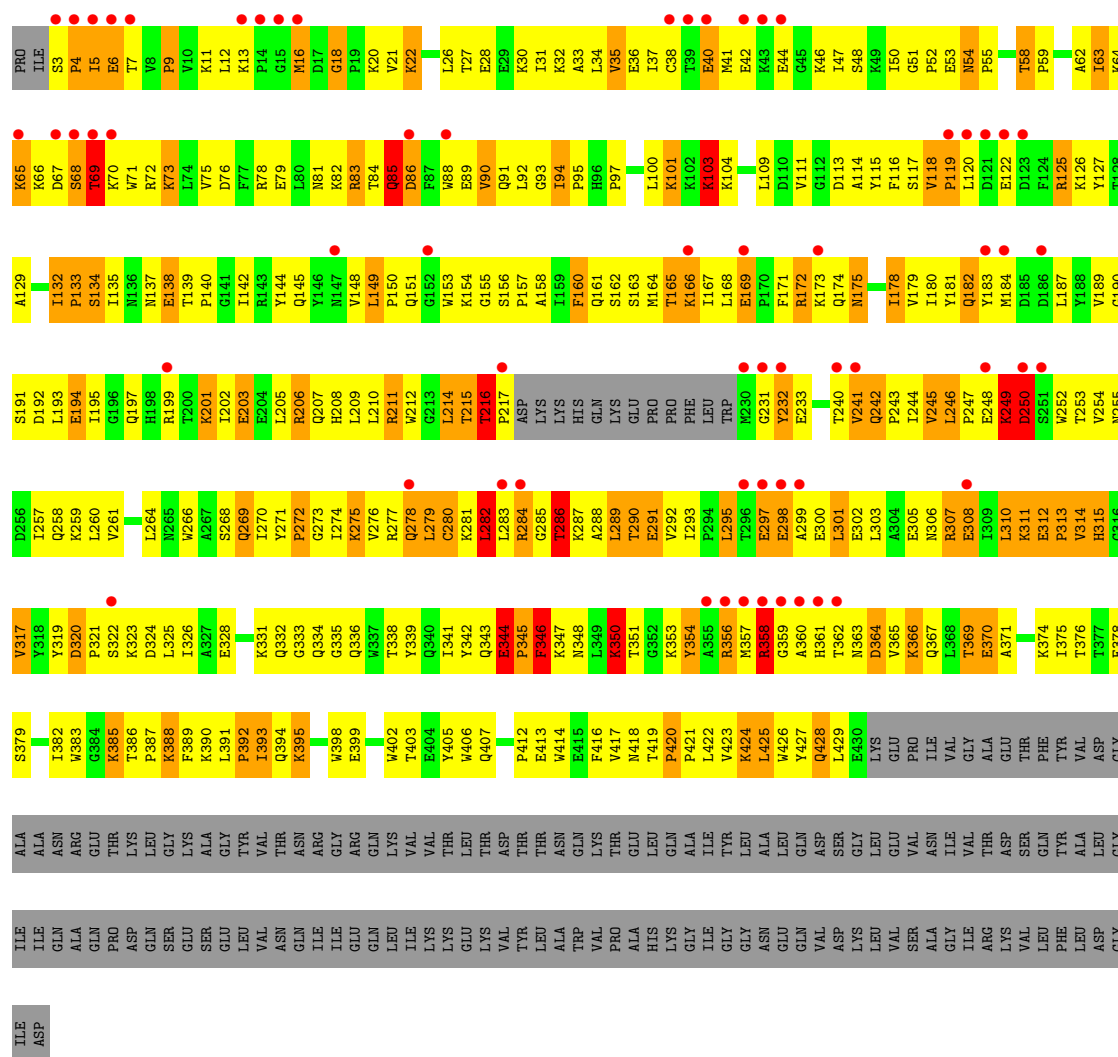
• Molecule 1: REVERSE TRANSCRIPTASE/RNASEH

Chain A:



• Molecule 1: REVERSE TRANSCRIPTASE/RNASEH

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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) 90.5 (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 2.90Å)	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 ²)	66.3	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 79.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.44$	Xtriage
Outliers	3 of 30525 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.90	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 62.

All (989) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:A:104:LYS:CB	1:A:192:ASP:HA	2.04	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	1	2
1	B	375/505 (74%)	278 (74%)	97 (26%)	1	2
All	All	862/1010 (85%)	634 (74%)	228 (26%)	1	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	B	208	HIS
1	B	255	ASN
1	B	278	GLN
1	B	315	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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	-	24,24,24	2.34	6 (25%)	33,34,34	1.68	9 (27%)

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	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1546	I15	C10-C4	-7.24	1.45	1.50
2	A	1546	I15	C4-C1	4.15	1.47	1.39
2	A	1546	I15	C8-C12	3.33	1.43	1.36
2	A	1546	I15	F1-C6	3.29	1.43	1.35
2	A	1546	I15	C12-C6	2.78	1.44	1.38
2	A	1546	I15	C13-C15	-2.59	1.34	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1546	I15	C10-C4-N9	3.22	126.67	119.77
2	A	1546	I15	C12-C6-C2	-3.19	115.23	122.52
2	A	1546	I15	C16-C14-C11	-2.99	115.21	119.24
2	A	1546	I15	C12-C8-C3	2.57	122.79	119.38
2	A	1546	I15	C17-C16-C14	2.40	124.24	119.73
2	A	1546	I15	F1-C6-C12	2.39	124.26	118.47
2	A	1546	I15	C11-O5-C2	2.35	122.50	118.46
2	A	1546	I15	C17-C15-C18	2.27	122.50	119.50
2	A	1546	I15	C15-C13-C11	2.08	122.06	119.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.61	68 (12%) ⓘ ⓘ	34, 59, 86, 107	0
1	B	416/566 (73%)	0.80	62 (14%) ⓘ ⓘ	36, 58, 95, 119	0
All	All	961/1132 (84%)	0.69	130 (13%) ⓘ ⓘ	34, 59, 90, 119	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	357	MET	12.0
1	B	284	ARG	8.3
1	A	359	GLY	6.2
1	A	453	GLY	6.1
1	B	278	GLN	5.6
1	B	4	PRO	5.4
1	A	291	GLU	5.3
1	B	296	THR	5.1
1	A	285	GLY	5.0
1	A	290	THR	4.9
1	B	231	GLY	4.9
1	A	541	GLY	4.8
1	B	7	THR	4.8
1	B	232	TYR	4.7
1	A	545	ASN	4.7
1	A	289	LEU	4.7
1	B	39	THR	4.7
1	B	361	HIS	4.6
1	B	230	MET	4.6
1	B	3	SER	4.6
1	B	251	SER	4.5
1	B	40	GLU	4.5
1	A	68	SER	4.4
1	B	362	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	472	THR	4.3
1	A	67	ASP	4.3
1	B	360	ALA	4.1
1	B	359	GLY	4.0
1	B	358	ARG	4.0
1	B	122	GLU	4.0
1	A	54	ASN	3.9
1	B	298	GLU	3.9
1	A	539	HIS	3.8
1	A	66	LYS	3.7
1	A	278	GLN	3.7
1	A	65	LYS	3.7
1	B	356	ARG	3.7
1	A	471	ASP	3.6
1	B	43	LYS	3.6
1	B	70	LYS	3.6
1	B	248	GLU	3.6
1	B	15	GLY	3.5
1	A	282	LEU	3.5
1	A	358	ARG	3.5
1	A	402	TRP	3.4
1	A	292	VAL	3.4
1	A	452	LEU	3.4
1	A	104	LYS	3.4
1	A	544	GLY	3.4
1	A	470	THR	3.4
1	A	69	THR	3.3
1	B	297	GLU	3.3
1	B	5	ILE	3.3
1	A	357	MET	3.2
1	A	530	LYS	3.2
1	A	70	LYS	3.2
1	A	200	THR	3.2
1	B	69	THR	3.2
1	A	176	PRO	3.1
1	A	473	THR	3.1
1	B	65	LYS	3.0
1	A	323	LYS	3.0
1	A	451	LYS	3.0
1	B	283	LEU	2.9
1	B	217	PRO	2.9
1	A	221	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	16	MET	2.9
1	B	14	PRO	2.9
1	A	506	ILE	2.8
1	B	120	LEU	2.8
1	A	396	GLU	2.8
1	B	13	LYS	2.8
1	A	199	ARG	2.8
1	A	242	GLN	2.8
1	B	184	MET	2.8
1	B	88	TRP	2.8
1	A	434	ILE	2.8
1	A	64	LYS	2.7
1	A	543	GLY	2.7
1	A	526	ILE	2.7
1	A	172	ARG	2.7
1	B	250	ASP	2.7
1	A	469	LEU	2.6
1	B	123	ASP	2.6
1	A	520	GLN	2.6
1	B	38	CYS	2.6
1	A	123	ASP	2.6
1	A	147	ASN	2.6
1	A	194	GLU	2.6
1	A	492	GLU	2.6
1	A	432	GLU	2.5
1	B	308	GLU	2.5
1	B	299	ALA	2.5
1	B	173	LYS	2.5
1	A	24	TRP	2.5
1	B	121	ASP	2.5
1	A	177	ASP	2.4
1	A	255	ASN	2.4
1	A	356	ARG	2.4
1	A	360	ALA	2.4
1	B	241	VAL	2.3
1	A	55	PRO	2.3
1	A	435	VAL	2.3
1	A	193	LEU	2.3
1	A	48	SER	2.3
1	B	186	ASP	2.2
1	B	42	GLU	2.2
1	B	322	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	166	LYS	2.2
1	B	44	GLU	2.2
1	B	183	TYR	2.2
1	B	199	ARG	2.2
1	A	542	ILE	2.2
1	A	301	LEU	2.2
1	B	6	GLU	2.2
1	A	495	ILE	2.1
1	B	240	THR	2.1
1	A	538	ALA	2.1
1	B	152	GLY	2.1
1	A	398	TRP	2.1
1	B	86	ASP	2.1
1	B	119	PRO	2.1
1	B	355	ALA	2.1
1	A	222	GLN	2.1
1	B	147	ASN	2.1
1	A	534	ALA	2.1
1	B	67	ASP	2.0
1	A	315	HIS	2.0
1	B	169	GLU	2.0
1	B	68	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	I15	A	1546	22/22	0.20	-0.62	42,51,55,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.