



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 07:00 AM UTC

PDB ID : 2L5H / pdb_00002l5h
Title : Solution Structure of the H189Q mutant of the Enzyme I dimer Using Residual Dipolar Couplings and Small Angle X-Ray Scattering
Authors : Takayama, Y.D.; Schwieters, C.D.; Grishaev, A.; Guirlando, R.; Clore, G.
Deposited on : 2010-11-01

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

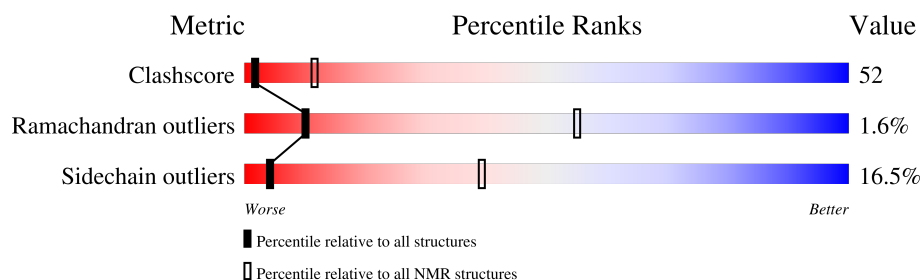
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR, SOLUTION SCATTERING

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	573	51% 35% 14%
1	B	573	52% 33% 14%

2 Ensemble composition and analysis ⓘ

This entry contains 2 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17910 atoms, of which 9028 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Phosphoenolpyruvate-protein phosphotransferase.

Mol	Chain	Residues	Atoms						Trace
1	A	573	Total	C	H	N	O	S	0
			8955	2789	4514	756	875	21	
1	B	573	Total	C	H	N	O	S	0
			8955	2789	4514	756	875	21	

There are 2 discrepancies between the modelled and reference sequences:

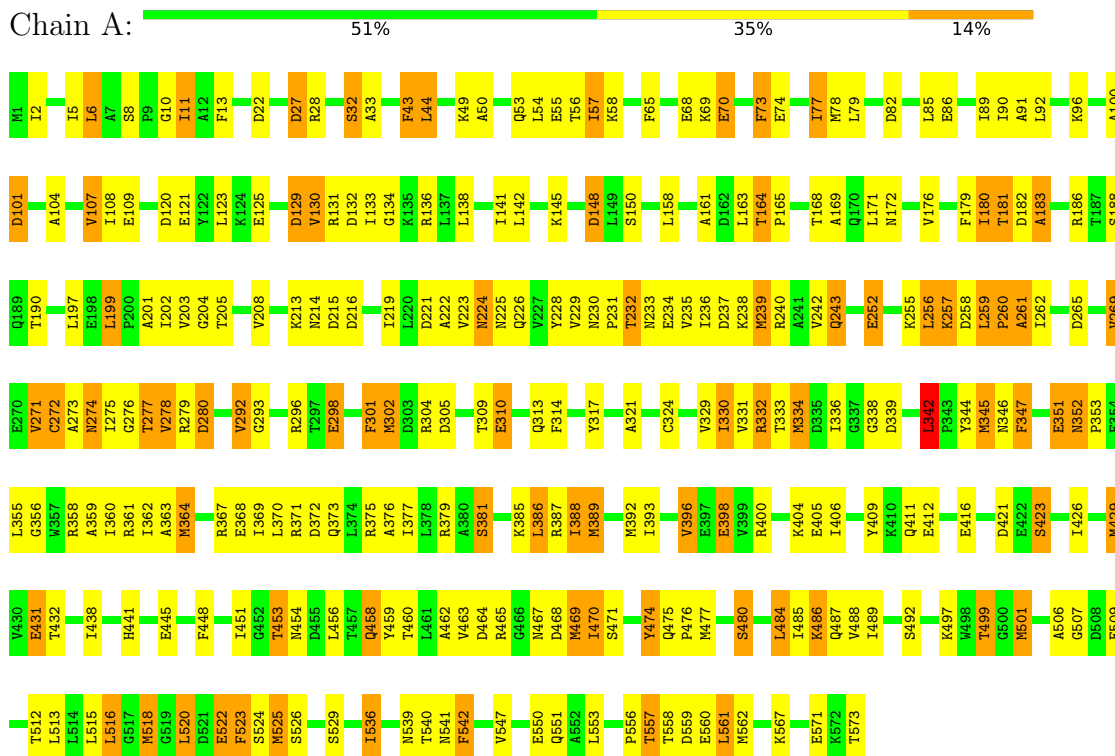
Chain	Residue	Modelled	Actual	Comment	Reference
A	189	GLN	HIS	engineered mutation	UNP P08839
B	189	GLN	HIS	engineered mutation	UNP P08839

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

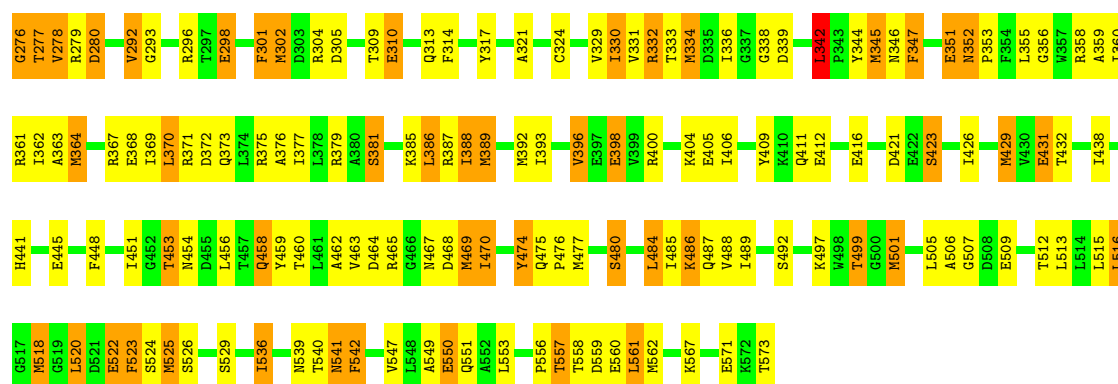
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase



- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase



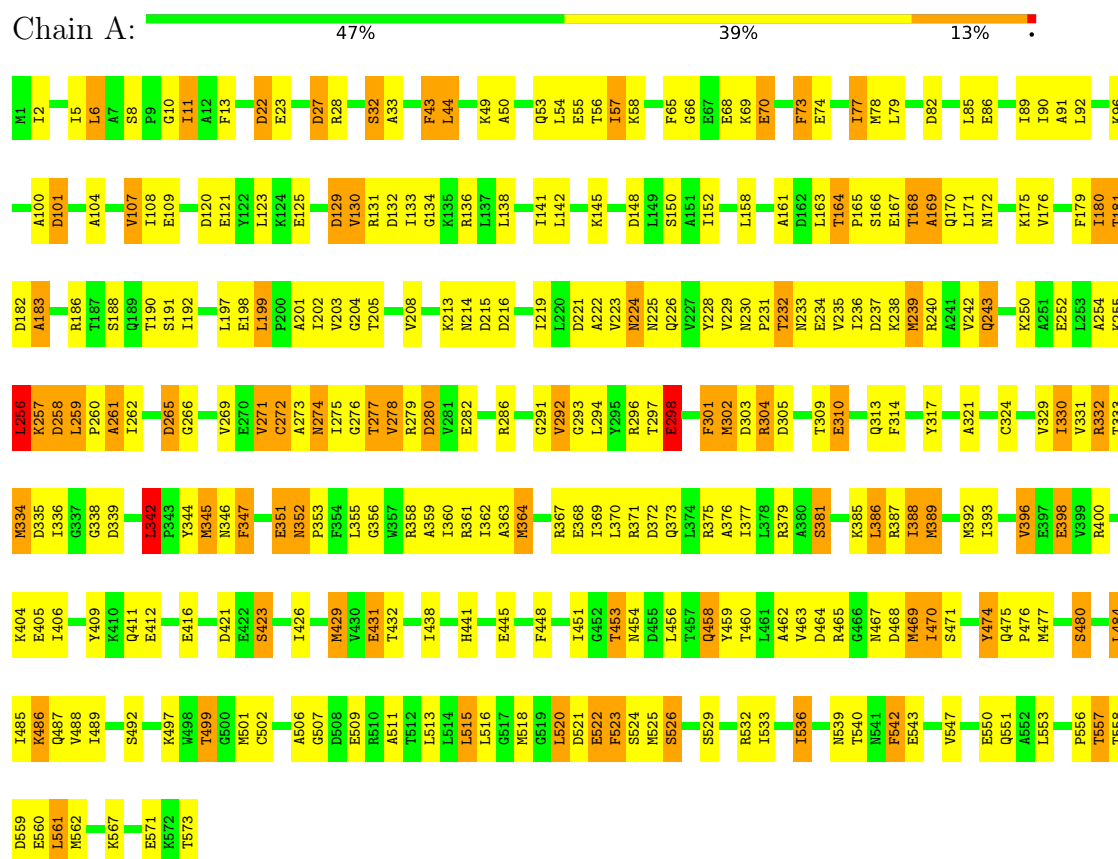


4.2 Scores per residue for each member of the ensemble

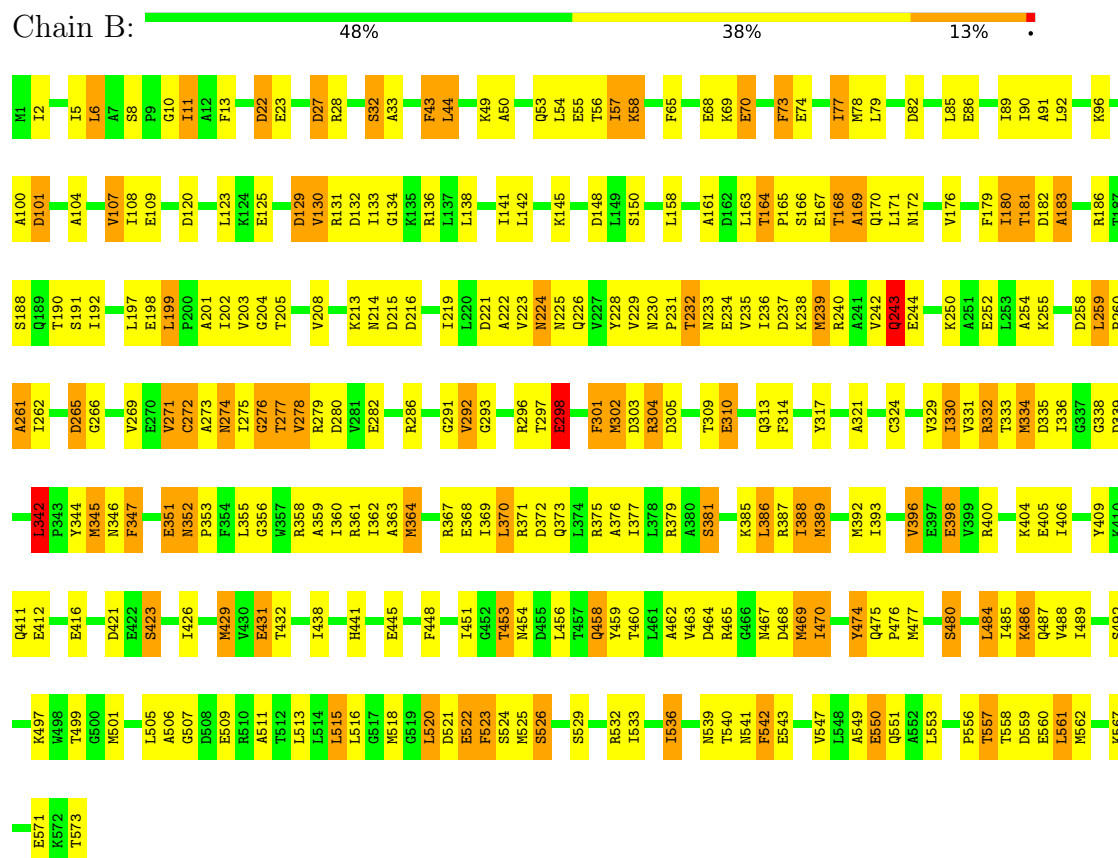
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase

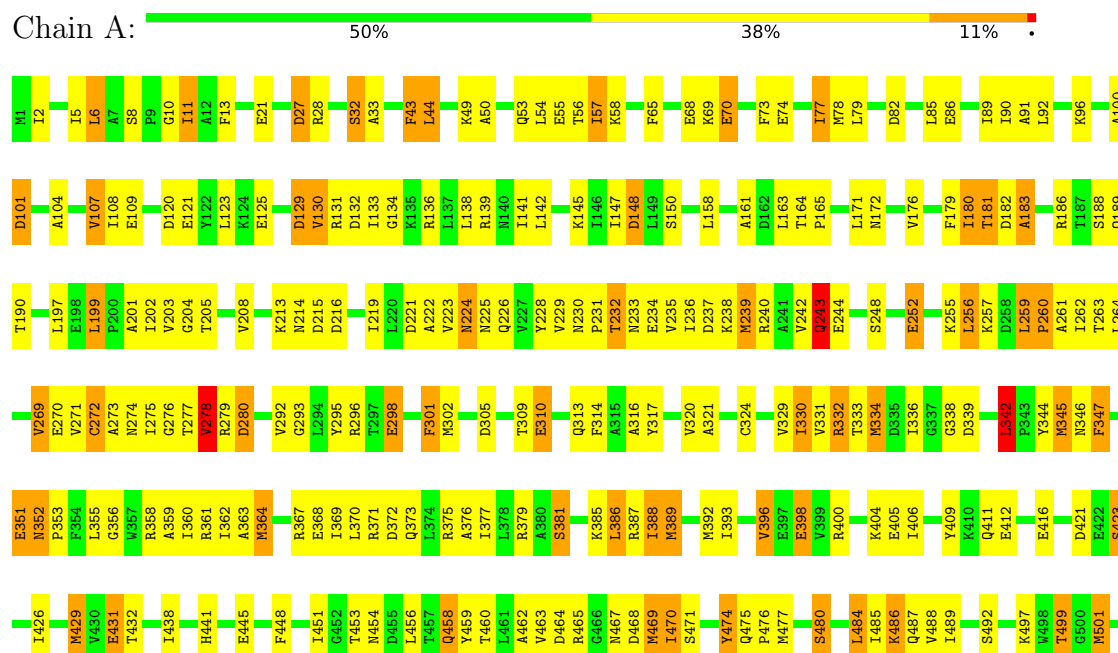


- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase



4.2.2 Score per residue for model 2

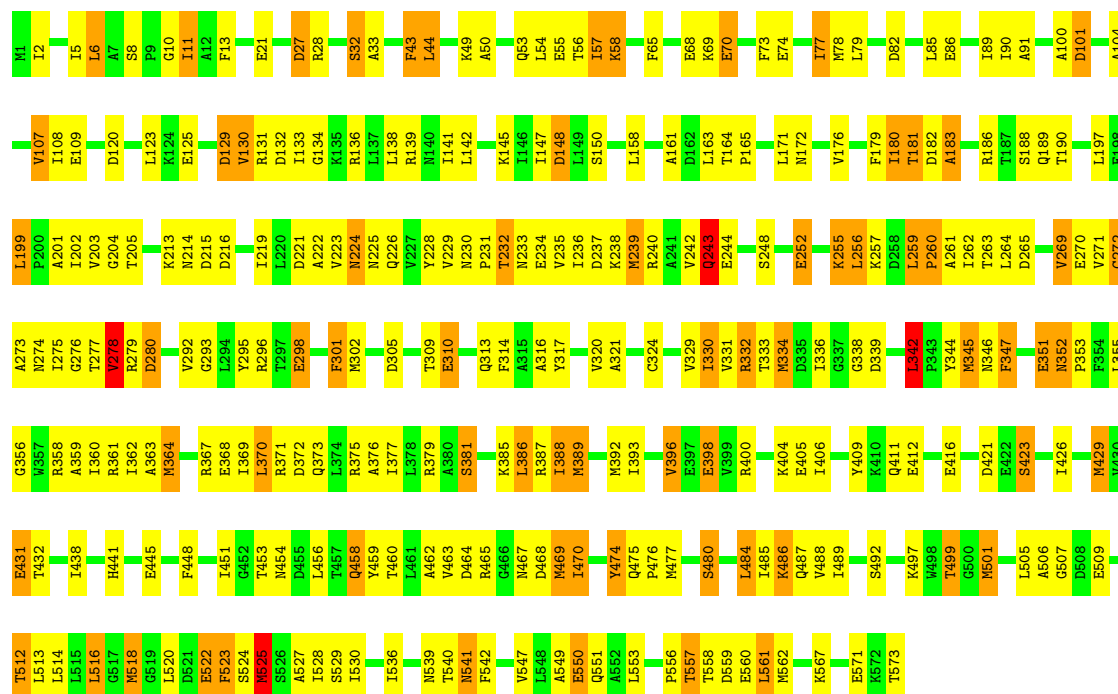
- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase





● Molecule 1: Phosphoenolpyruvate-protein phosphotransferase

Chain B: 50% 37% 12% .



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 120 calculated structures, 2 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Xplor-NIH	structure solution	2.25
Xplor-NIH	refinement	2.25

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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 (average) 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	1.36±0.01	20±0/4493 (0.4± 0.0%)	1.20±0.03	12±2/6058 (0.2± 0.0%)
1	B	1.37±0.01	22±0/4493 (0.5± 0.0%)	1.20±0.03	12±2/6058 (0.2± 0.0%)
All	All	1.37	84/17972 (0.5%)	1.20	47/24232 (0.2%)

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

Mol	Chain	Chirality	Planarity
1	B	0.0±0.0	0.5±0.5
All	All	0	1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	345	MET	SD-CE	13.99	2.14	1.79	1	2
1	A	345	MET	SD-CE	13.96	2.14	1.79	1	2
1	A	469	MET	SD-CE	13.77	2.13	1.79	1	2
1	B	469	MET	SD-CE	13.77	2.13	1.79	1	2
1	A	364	MET	SD-CE	10.62	2.06	1.79	1	2
1	B	364	MET	SD-CE	10.59	2.06	1.79	1	2
1	B	169	ALA	CA-CB	-9.62	1.38	1.53	1	1
1	A	298	GLU	C-O	-9.57	1.12	1.24	1	1
1	B	298	GLU	C-O	-9.27	1.13	1.24	1	1
1	A	169	ALA	CA-CB	-9.04	1.39	1.53	1	1
1	B	562	MET	SD-CE	8.75	2.01	1.79	1	2
1	A	562	MET	SD-CE	8.70	2.01	1.79	1	2
1	A	562	MET	CG-SD	7.56	1.99	1.80	1	2
1	B	562	MET	CG-SD	7.53	1.99	1.80	1	2
1	A	239	MET	SD-CE	7.24	1.97	1.79	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	239	MET	SD-CE	7.18	1.97	1.79	2	2
1	A	364	MET	CG-SD	6.79	1.97	1.80	1	2
1	B	364	MET	CG-SD	6.72	1.97	1.80	1	2
1	A	475	GLN	CA-C	-6.60	1.45	1.52	1	2
1	B	475	GLN	CA-C	-6.57	1.45	1.52	1	2
1	A	525	MET	SD-CE	6.49	1.95	1.79	2	1
1	B	345	MET	CG-SD	6.45	1.96	1.80	1	2
1	B	525	MET	SD-CE	6.42	1.95	1.79	2	1
1	A	345	MET	CG-SD	6.42	1.96	1.80	1	2
1	A	334	MET	CG-SD	6.20	1.96	1.80	1	2
1	A	501	MET	CG-SD	6.16	1.96	1.80	2	1
1	B	334	MET	CG-SD	6.14	1.96	1.80	1	2
1	B	501	MET	CG-SD	6.09	1.96	1.80	2	1
1	A	389	MET	SD-CE	5.97	1.94	1.79	1	2
1	B	243	GLN	CA-CB	5.95	1.62	1.53	1	1
1	B	389	MET	SD-CE	5.92	1.94	1.79	1	2
1	A	239	MET	CG-SD	5.83	1.95	1.80	1	2
1	B	239	MET	CG-SD	5.79	1.95	1.80	1	2
1	A	475	GLN	C-O	-5.75	1.19	1.24	1	2
1	B	475	GLN	C-O	-5.71	1.19	1.24	1	2
1	B	477	MET	SD-CE	5.49	1.93	1.79	1	2
1	A	477	MET	SD-CE	5.49	1.93	1.79	1	2
1	B	120	ASP	N-CA	5.43	1.52	1.46	2	2
1	A	429	MET	SD-CE	5.30	1.92	1.79	1	2
1	B	429	MET	SD-CE	5.23	1.92	1.79	1	2
1	B	334	MET	SD-CE	5.20	1.92	1.79	1	2
1	A	334	MET	SD-CE	5.13	1.92	1.79	1	2
1	B	525	MET	CG-SD	5.07	1.93	1.80	2	1
1	A	525	MET	CG-SD	5.07	1.93	1.80	2	1
1	B	469	MET	CG-SD	5.06	1.93	1.80	1	2
1	A	469	MET	CG-SD	5.04	1.93	1.80	1	2
1	B	550	GLU	N-CA	-5.01	1.40	1.46	1	2
1	A	66	GLY	N-CA	5.00	1.50	1.44	1	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	164	THR	CB-CA-C	19.79	137.36	108.86	1	1
1	B	164	THR	CB-CA-C	19.72	137.26	108.86	1	1
1	B	164	THR	N-CA-CB	-15.93	90.75	110.03	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	164	THR	N-CA-CB	-15.66	91.08	110.03	1	1
1	B	298	GLU	CA-C-O	8.62	129.94	120.63	1	1
1	A	298	GLU	CA-C-O	8.26	129.55	120.63	1	1
1	A	243	GLN	CB-CA-C	-8.01	97.50	110.79	1	2
1	B	243	GLN	CB-CA-C	-7.32	98.64	110.79	1	2
1	A	561	LEU	CA-CB-CG	6.63	139.50	116.30	1	2
1	B	561	LEU	CA-CB-CG	6.63	139.49	116.30	1	2
1	A	169	ALA	N-CA-CB	6.56	119.58	110.07	1	1
1	B	298	GLU	O-C-N	-6.34	115.40	122.12	1	1
1	A	278	VAL	CB-CA-C	-6.25	101.05	111.29	2	1
1	B	278	VAL	CB-CA-C	-6.24	101.06	111.29	2	1
1	A	298	GLU	O-C-N	-5.91	115.86	122.12	1	1
1	B	487	GLN	N-CA-C	-5.76	105.14	111.82	1	2
1	A	487	GLN	N-CA-C	-5.75	105.15	111.82	1	2
1	A	224	ASN	N-CA-C	-5.38	106.39	113.17	1	2
1	B	338	GLY	N-CA-C	-5.34	100.52	113.18	1	2
1	A	338	GLY	N-CA-C	-5.34	100.52	113.18	1	2
1	B	224	ASN	N-CA-C	-5.31	106.48	113.17	2	2
1	A	342	LEU	CA-C-N	5.23	126.38	119.84	1	2
1	A	342	LEU	C-N-CA	5.23	126.38	119.84	1	2
1	B	342	LEU	CA-C-N	5.23	126.38	119.84	1	2
1	B	342	LEU	C-N-CA	5.23	126.38	119.84	1	2
1	A	73	PHE	CA-CB-CG	-5.09	108.70	113.80	1	2
1	B	73	PHE	CA-CB-CG	-5.06	108.74	113.80	2	2
1	B	476	PRO	N-CA-C	-5.02	107.86	114.03	1	2
1	A	476	PRO	N-CA-C	-5.01	107.86	114.03	1	2

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	276	GLY	Mainchain	1

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	4441	4514	4507	485±19
1	B	4441	4514	4507	478±18
All	All	17764	18056	18028	1876

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 52.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:314:PHE:CE1	1:B:376:ALA:HA	1.56	1.35	1	2
1:A:314:PHE:CE1	1:A:376:ALA:HA	1.55	1.35	1	2
1:B:364:MET:SD	1:B:364:MET:CE	1.42	2.06	1	2
1:A:364:MET:SD	1:A:364:MET:CE	1.42	2.06	1	2
1:B:469:MET:CE	1:B:469:MET:SD	1.36	2.14	1	2
1:A:469:MET:SD	1:A:469:MET:CE	1.36	2.14	1	2
1:A:345:MET:SD	1:A:345:MET:CE	1.36	2.14	1	2
1:B:345:MET:SD	1:B:345:MET:CE	1.35	2.14	1	2
1:A:314:PHE:CE1	1:A:376:ALA:CA	1.26	2.19	1	2
1:B:314:PHE:CE1	1:B:376:ALA:CA	1.24	2.19	1	2
1:A:317:TYR:OH	1:A:373:GLN:NE2	1.23	1.72	2	2
1:B:317:TYR:OH	1:B:373:GLN:NE2	1.22	1.73	2	2
1:A:73:PHE:CZ	1:A:169:ALA:HB3	1.21	1.67	1	1
1:B:301:PHE:CE1	1:B:342:LEU:CD2	1.21	2.22	1	2
1:B:272:CYS:SG	1:B:293:GLY:N	1.21	2.13	2	2
1:A:301:PHE:CE1	1:A:342:LEU:CD2	1.21	2.22	1	2
1:A:272:CYS:SG	1:A:293:GLY:N	1.20	2.13	2	2
1:B:301:PHE:HD1	1:B:302:MET:N	1.20	1.34	2	2
1:B:301:PHE:CE2	1:B:342:LEU:HD21	1.19	1.72	2	2
1:B:73:PHE:CZ	1:B:169:ALA:HB3	1.19	1.72	1	1
1:A:301:PHE:CE2	1:A:342:LEU:HD21	1.18	1.71	2	2
1:A:301:PHE:HD1	1:A:302:MET:N	1.18	1.34	2	2
1:A:389:MET:SD	1:A:448:PHE:HZ	1.16	1.63	1	2
1:B:389:MET:SD	1:B:448:PHE:HZ	1.15	1.64	1	2
1:A:301:PHE:CD1	1:A:342:LEU:HD22	1.14	1.77	1	2
1:A:301:PHE:CZ	1:A:342:LEU:HD21	1.14	1.77	2	2
1:A:314:PHE:CZ	1:A:376:ALA:HA	1.13	1.78	1	2
1:B:523:PHE:CD1	1:B:523:PHE:C	1.13	2.24	2	2
1:B:301:PHE:CZ	1:B:342:LEU:HD21	1.13	1.78	2	2
1:A:314:PHE:CD1	1:A:376:ALA:HA	1.12	1.77	1	2
1:B:314:PHE:CD1	1:B:376:ALA:HA	1.12	1.77	1	2
1:B:314:PHE:CZ	1:B:376:ALA:HA	1.12	1.78	1	2
1:B:298:GLU:O	1:B:301:PHE:CD1	1.11	2.03	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:301:PHE:CE1	1:B:342:LEU:HD21	1.10	1.78	1	1
1:B:301:PHE:CD1	1:B:342:LEU:HD22	1.10	1.81	1	2
1:A:298:GLU:O	1:A:301:PHE:CD1	1.10	2.03	1	1
1:A:523:PHE:CD1	1:A:523:PHE:C	1.09	2.23	2	2
1:B:43:PHE:CZ	1:B:104:ALA:HB2	1.09	1.82	1	2
1:B:298:GLU:CB	1:B:301:PHE:CZ	1.09	2.35	1	2
1:A:43:PHE:CZ	1:A:104:ALA:HB2	1.09	1.81	1	2
1:B:298:GLU:HA	1:B:301:PHE:CE2	1.09	1.81	1	2
1:A:298:GLU:HA	1:A:301:PHE:CE2	1.08	1.82	1	2
1:A:301:PHE:CE1	1:A:342:LEU:HD21	1.08	1.80	1	1
1:A:298:GLU:CB	1:A:301:PHE:CZ	1.07	2.37	1	2
1:B:388:ILE:C	1:B:389:MET:SD	1.07	2.38	1	2
1:A:301:PHE:CD1	1:A:342:LEU:CD2	1.06	2.35	1	2
1:A:489:ILE:HA	1:A:499:THR:HG21	1.06	1.26	1	2
1:A:388:ILE:C	1:A:389:MET:SD	1.05	2.38	1	2
1:B:301:PHE:CD1	1:B:342:LEU:CD2	1.04	2.37	1	2
1:A:301:PHE:CD1	1:A:302:MET:N	1.03	2.26	2	2
1:B:73:PHE:CZ	1:B:169:ALA:CB	1.03	2.41	1	1
1:B:301:PHE:CD1	1:B:302:MET:N	1.02	2.26	2	2
1:B:298:GLU:HB2	1:B:301:PHE:CZ	1.02	1.90	2	2
1:B:301:PHE:CZ	1:B:342:LEU:CD2	1.02	2.41	2	2
1:A:73:PHE:CZ	1:A:169:ALA:CB	1.02	2.41	1	1
1:A:301:PHE:CZ	1:A:342:LEU:CD2	1.02	2.41	2	2
1:A:223:VAL:HG21	1:A:242:VAL:HG11	1.02	1.32	2	2
1:B:501:MET:SD	1:B:515:LEU:HD21	1.01	1.95	1	1
1:B:301:PHE:CE2	1:B:336:ILE:CG2	1.01	2.43	1	2
1:A:298:GLU:HB2	1:A:301:PHE:CZ	1.01	1.90	2	2
1:B:223:VAL:HG21	1:B:242:VAL:HG11	1.01	1.32	2	2
1:A:221:ASP:HA	1:A:239:MET:CE	1.00	1.87	1	2
1:A:232:THR:CG2	1:A:233:ASN:H	1.00	1.69	2	2
1:B:232:THR:CG2	1:B:233:ASN:H	0.99	1.69	2	2
1:A:301:PHE:CE2	1:A:336:ILE:CG2	0.99	2.45	1	2
1:B:389:MET:SD	1:B:448:PHE:CZ	0.99	2.56	1	2
1:B:298:GLU:HA	1:B:301:PHE:CD2	0.99	1.93	1	2
1:A:389:MET:SD	1:A:448:PHE:CZ	0.99	2.55	1	2
1:B:221:ASP:HA	1:B:239:MET:CE	0.99	1.87	1	2
1:B:232:THR:CG2	1:B:233:ASN:N	0.98	2.26	1	2
1:A:298:GLU:HA	1:A:301:PHE:CD2	0.98	1.92	1	2
1:A:232:THR:CG2	1:A:233:ASN:N	0.98	2.27	2	2
1:A:221:ASP:OD2	1:A:225:ASN:N	0.98	1.96	2	2
1:A:232:THR:HG22	1:A:233:ASN:N	0.98	1.71	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:232:THR:HG22	1:B:233:ASN:N	0.97	1.71	1	2
1:A:11:ILE:HG13	1:A:243:GLN:CB	0.97	1.89	2	2
1:B:221:ASP:OD2	1:B:225:ASN:N	0.97	1.96	1	2
1:A:301:PHE:CE2	1:A:336:ILE:HG22	0.96	1.95	2	2
1:B:301:PHE:CE2	1:B:336:ILE:HG22	0.96	1.95	2	2
1:B:43:PHE:CZ	1:B:100:ALA:O	0.96	2.19	2	2
1:A:43:PHE:CZ	1:A:100:ALA:O	0.96	2.19	2	2
1:A:492:SER:OG	1:A:499:THR:HG22	0.95	1.59	1	1
1:B:298:GLU:CB	1:B:301:PHE:CE2	0.95	2.49	2	2
1:B:11:ILE:HG13	1:B:243:GLN:CB	0.95	1.91	2	2
1:A:298:GLU:CB	1:A:301:PHE:CE2	0.94	2.49	2	2
1:A:298:GLU:CA	1:A:301:PHE:CE2	0.94	2.50	1	2
1:B:298:GLU:CA	1:B:301:PHE:CE2	0.94	2.50	1	2
1:B:221:ASP:HA	1:B:239:MET:HE2	0.93	1.41	1	2
1:A:314:PHE:CE1	1:A:379:ARG:CB	0.93	2.52	1	2
1:B:11:ILE:HG13	1:B:243:GLN:HB2	0.92	1.40	1	2
1:A:73:PHE:HZ	1:A:169:ALA:HB3	0.92	1.02	1	1
1:A:73:PHE:CE2	1:A:169:ALA:CB	0.92	2.52	1	1
1:B:132:ASP:OD1	1:B:164:THR:CB	0.92	2.18	1	1
1:B:314:PHE:CE1	1:B:379:ARG:CB	0.92	2.52	1	2
1:B:136:ARG:NH2	1:B:167:GLU:HG3	0.92	1.80	1	1
1:A:132:ASP:OD1	1:A:164:THR:HB	0.91	1.65	1	1
1:B:387:ARG:O	1:B:389:MET:HE1	0.91	1.64	1	2
1:B:330:ILE:HG23	1:B:389:MET:HE3	0.91	1.43	1	2
1:A:387:ARG:O	1:A:389:MET:HE1	0.91	1.65	1	2
1:A:132:ASP:OD1	1:A:164:THR:CB	0.91	2.18	1	1
1:A:221:ASP:HA	1:A:239:MET:HE2	0.91	1.41	2	2
1:B:132:ASP:OD1	1:B:164:THR:HB	0.91	1.65	1	1
1:A:456:LEU:HD13	1:A:484:LEU:HD21	0.90	1.43	1	2
1:B:43:PHE:CZ	1:B:104:ALA:CB	0.90	2.54	2	2
1:A:43:PHE:CZ	1:A:104:ALA:CB	0.90	2.54	2	2
1:B:73:PHE:HZ	1:B:169:ALA:HB3	0.90	1.03	1	1
1:B:523:PHE:C	1:B:523:PHE:HD1	0.90	1.73	2	2
1:B:73:PHE:CE2	1:B:169:ALA:CB	0.90	2.54	1	1
1:A:330:ILE:HG23	1:A:389:MET:HE3	0.89	1.41	1	2
1:A:523:PHE:CD1	1:A:525:MET:SD	0.89	2.66	1	2
1:A:272:CYS:SG	1:A:292:VAL:CA	0.89	2.61	1	1
1:B:456:LEU:HD13	1:B:484:LEU:HD21	0.88	1.43	1	2
1:A:221:ASP:CG	1:A:226:GLN:H	0.88	1.77	1	2
1:B:272:CYS:SG	1:B:292:VAL:HA	0.88	2.08	1	1
1:B:523:PHE:CD1	1:B:525:MET:SD	0.88	2.66	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:386:LEU:HD12	1:A:387:ARG:N	0.88	1.84	1	2
1:B:272:CYS:SG	1:B:292:VAL:CA	0.88	2.61	1	1
1:A:272:CYS:SG	1:A:292:VAL:HA	0.88	2.08	1	1
1:B:386:LEU:HD12	1:B:387:ARG:N	0.88	1.82	1	2
1:A:484:LEU:HD23	1:A:485:ILE:N	0.88	1.84	1	2
1:A:228:TYR:HB3	1:A:231:PRO:HG3	0.88	1.45	1	2
1:B:221:ASP:CG	1:B:226:GLN:H	0.88	1.77	2	2
1:B:453:THR:OG1	1:B:501:MET:HE2	0.88	1.69	1	1
1:B:73:PHE:CE2	1:B:169:ALA:HB1	0.87	2.04	1	1
1:A:43:PHE:CD2	1:A:100:ALA:HB1	0.87	2.04	1	2
1:A:11:ILE:HG13	1:A:243:GLN:HB2	0.87	1.45	1	2
1:A:314:PHE:CE1	1:A:379:ARG:HB2	0.87	2.05	1	2
1:B:523:PHE:CE1	1:B:525:MET:SD	0.87	2.67	1	2
1:B:359:ALA:O	1:B:362:ILE:HG22	0.87	1.70	1	2
1:B:484:LEU:HD23	1:B:485:ILE:N	0.87	1.84	1	2
1:B:515:LEU:HD23	1:B:520:LEU:HD13	0.87	1.45	1	1
1:A:523:PHE:C	1:A:523:PHE:HD1	0.86	1.73	2	2
1:B:43:PHE:CD2	1:B:100:ALA:HB1	0.86	2.05	2	2
1:B:228:TYR:HB3	1:B:231:PRO:HG3	0.86	1.45	1	2
1:B:314:PHE:CE1	1:B:379:ARG:HB2	0.86	2.05	1	2
1:A:523:PHE:CE1	1:A:525:MET:SD	0.85	2.68	1	2
1:A:331:VAL:O	1:A:389:MET:HE2	0.85	1.72	1	2
1:B:272:CYS:SG	1:B:273:ALA:N	0.85	2.50	1	2
1:B:331:VAL:O	1:B:389:MET:HE2	0.85	1.72	1	2
1:B:388:ILE:HD12	1:B:389:MET:N	0.85	1.87	1	2
1:A:272:CYS:SG	1:A:273:ALA:N	0.84	2.50	1	2
1:A:388:ILE:HD12	1:A:389:MET:N	0.84	1.88	1	2
1:A:359:ALA:O	1:A:362:ILE:HG22	0.84	1.70	1	2
1:A:259:LEU:HD22	1:A:259:LEU:H	0.84	1.32	1	1
1:A:523:PHE:HD1	1:A:524:SER:N	0.84	1.70	2	1
1:B:43:PHE:HZ	1:B:104:ALA:CB	0.84	1.85	1	2
1:B:136:ARG:NH2	1:B:167:GLU:CG	0.83	2.41	1	1
1:B:176:VAL:HG11	1:B:179:PHE:CE1	0.83	2.08	2	2
1:A:43:PHE:HZ	1:A:104:ALA:CB	0.83	1.85	1	2
1:B:523:PHE:HD1	1:B:524:SER:N	0.83	1.70	2	1
1:B:301:PHE:HD1	1:B:302:MET:H	0.83	1.16	2	1
1:B:271:VAL:HB	1:B:523:PHE:CE2	0.83	2.08	2	2
1:A:176:VAL:HG11	1:A:179:PHE:CE1	0.83	2.09	2	2
1:A:199:LEU:HD23	1:A:199:LEU:O	0.83	1.72	2	2
1:A:298:GLU:HB3	1:A:301:PHE:CE2	0.82	2.07	2	2
1:B:259:LEU:H	1:B:259:LEU:HD22	0.82	1.33	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:271:VAL:HB	1:A:523:PHE:CE2	0.82	2.08	2	2
1:B:272:CYS:SG	1:B:292:VAL:C	0.82	2.62	1	1
1:B:301:PHE:HE2	1:B:336:ILE:HG22	0.82	1.34	2	1
1:B:199:LEU:HD23	1:B:199:LEU:O	0.82	1.73	2	2
1:B:298:GLU:HB3	1:B:301:PHE:CE2	0.82	2.07	2	2
1:B:523:PHE:CD1	1:B:523:PHE:O	0.82	2.33	2	2
1:B:11:ILE:CG1	1:B:243:GLN:HB2	0.82	2.04	1	2
1:A:272:CYS:SG	1:A:292:VAL:C	0.82	2.62	1	1
1:A:301:PHE:HD1	1:A:302:MET:H	0.82	1.17	2	1
1:A:314:PHE:CZ	1:A:376:ALA:CA	0.81	2.54	1	2
1:A:474:TYR:CG	1:A:474:TYR:O	0.81	2.33	1	2
1:B:314:PHE:CZ	1:B:376:ALA:CA	0.81	2.54	1	2
1:A:73:PHE:CE2	1:A:169:ALA:HB1	0.81	2.09	1	1
1:B:298:GLU:O	1:B:301:PHE:CE1	0.81	2.33	1	1
1:A:515:LEU:HD23	1:A:520:LEU:HD13	0.81	1.51	1	1
1:A:556:PRO:HB3	1:B:441:HIS:ND1	0.81	1.89	1	2
1:B:474:TYR:O	1:B:474:TYR:CG	0.80	2.33	1	2
1:B:298:GLU:CA	1:B:301:PHE:CZ	0.80	2.64	1	1
1:A:523:PHE:CD1	1:A:523:PHE:O	0.80	2.32	2	2
1:A:298:GLU:O	1:A:301:PHE:CE1	0.80	2.35	1	1
1:B:181:THR:CG2	1:B:183:ALA:H	0.79	1.91	1	2
1:A:301:PHE:HE2	1:A:336:ILE:HG22	0.79	1.33	2	1
1:A:292:VAL:CG1	1:A:329:VAL:HG12	0.79	2.07	1	1
1:B:259:LEU:N	1:B:259:LEU:HD13	0.79	1.92	1	1
1:B:314:PHE:CD1	1:B:376:ALA:CA	0.79	2.58	1	2
1:A:259:LEU:HD13	1:A:259:LEU:N	0.79	1.91	1	1
1:A:243:GLN:HG3	1:A:244:GLU:N	0.79	1.92	2	1
1:B:389:MET:CG	1:B:448:PHE:CZ	0.79	2.65	1	2
1:A:336:ILE:HD13	1:A:345:MET:HE1	0.78	1.55	1	2
1:A:389:MET:CG	1:A:448:PHE:CZ	0.78	2.66	1	2
1:B:272:CYS:SG	1:B:291:GLY:O	0.78	2.41	1	1
1:B:388:ILE:O	1:B:389:MET:SD	0.78	2.42	1	2
1:B:438:ILE:CG2	1:B:441:HIS:HB2	0.78	2.08	1	2
1:A:272:CYS:SG	1:A:291:GLY:O	0.78	2.41	1	1
1:A:181:THR:CG2	1:A:183:ALA:H	0.77	1.91	2	2
1:A:129:ASP:CG	1:A:165:PRO:HG2	0.77	2.05	2	1
1:B:314:PHE:CE1	1:B:379:ARG:HB3	0.77	2.14	1	2
1:A:438:ILE:CG2	1:A:441:HIS:HB2	0.77	2.08	1	2
1:B:136:ARG:HH22	1:B:167:GLU:HG3	0.77	1.35	1	1
1:B:292:VAL:CG1	1:B:329:VAL:HG12	0.77	2.08	1	1
1:A:13:PHE:CZ	1:A:240:ARG:HD2	0.77	2.15	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:ARG:NH2	1:A:167:GLU:HG3	0.77	1.93	1	1
1:A:298:GLU:CA	1:A:301:PHE:CZ	0.77	2.67	1	2
1:A:388:ILE:O	1:A:389:MET:SD	0.77	2.43	1	2
1:B:336:ILE:HD13	1:B:345:MET:HE1	0.77	1.56	1	2
1:B:129:ASP:CG	1:B:165:PRO:HG2	0.77	2.05	2	1
1:B:13:PHE:CZ	1:B:240:ARG:HD2	0.77	2.15	2	2
1:B:301:PHE:CE1	1:B:342:LEU:HD22	0.77	2.13	2	2
1:A:301:PHE:CE1	1:A:342:LEU:HD22	0.76	2.13	2	2
1:A:314:PHE:CE1	1:A:379:ARG:HB3	0.76	2.14	1	2
1:A:352:ASN:CG	1:B:352:ASN:CG	0.76	2.53	1	2
1:B:295:TYR:CZ	1:B:320:VAL:HG21	0.76	2.16	2	1
1:A:295:TYR:CZ	1:A:320:VAL:HG21	0.76	2.16	2	1
1:A:314:PHE:CE1	1:A:376:ALA:C	0.75	2.64	1	2
1:A:314:PHE:CZ	1:A:375:ARG:C	0.75	2.65	1	2
1:B:314:PHE:CE1	1:B:376:ALA:C	0.75	2.64	1	2
1:A:73:PHE:HE2	1:A:169:ALA:HB1	0.74	1.42	1	1
1:A:275:ILE:HG23	1:A:280:ASP:CB	0.74	2.12	2	2
1:B:314:PHE:CZ	1:B:375:ARG:C	0.74	2.65	1	2
1:B:73:PHE:HE2	1:B:169:ALA:HB1	0.74	1.40	1	1
1:B:275:ILE:HG23	1:B:280:ASP:CB	0.74	2.12	2	2
1:B:275:ILE:HG23	1:B:280:ASP:HB2	0.74	1.57	1	2
1:A:11:ILE:CG1	1:A:243:GLN:HB2	0.74	2.12	2	2
1:A:86:GLU:O	1:A:90:ILE:HG23	0.74	1.83	1	2
1:B:352:ASN:OD1	1:B:355:LEU:HD12	0.74	1.82	1	2
1:B:372:ASP:CG	1:B:373:GLN:N	0.74	2.45	1	2
1:B:386:LEU:HD12	1:B:386:LEU:C	0.74	2.08	1	2
1:B:243:GLN:HG3	1:B:244:GLU:N	0.74	1.96	2	1
1:A:223:VAL:HG21	1:A:242:VAL:CG1	0.73	2.13	1	2
1:B:86:GLU:O	1:B:90:ILE:HG23	0.73	1.83	2	2
1:A:352:ASN:HD22	1:A:352:ASN:C	0.73	1.91	1	2
1:A:352:ASN:OD1	1:A:355:LEU:HD12	0.73	1.82	1	2
1:B:507:GLY:HA2	1:B:525:MET:SD	0.73	2.23	1	2
1:B:228:TYR:CB	1:B:231:PRO:HG3	0.73	2.14	2	2
1:A:228:TYR:CD1	1:A:235:VAL:HG11	0.73	2.19	2	2
1:A:232:THR:O	1:A:236:ILE:HG13	0.73	1.84	2	2
1:A:295:TYR:OH	1:A:320:VAL:HG21	0.73	1.84	2	1
1:A:362:ILE:CG2	1:A:363:ALA:N	0.72	2.52	1	2
1:A:372:ASP:CG	1:A:373:GLN:N	0.72	2.45	1	2
1:B:301:PHE:CD1	1:B:301:PHE:C	0.72	2.65	2	2
1:A:275:ILE:HG23	1:A:280:ASP:HB2	0.72	1.61	2	2
1:A:301:PHE:HE2	1:A:336:ILE:CG2	0.72	1.97	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:228:TYR:CD1	1:B:235:VAL:HG11	0.72	2.19	2	2
1:B:295:TYR:OH	1:B:320:VAL:HG21	0.72	1.84	2	1
1:A:228:TYR:CB	1:A:231:PRO:HG3	0.72	2.14	2	2
1:B:232:THR:O	1:B:236:ILE:HG13	0.72	1.84	2	2
1:A:302:MET:O	1:A:302:MET:SD	0.72	2.47	1	2
1:B:136:ARG:HH22	1:B:167:GLU:CG	0.72	1.97	1	1
1:B:272:CYS:SG	1:B:293:GLY:CA	0.72	2.77	2	1
1:A:441:HIS:ND1	1:B:556:PRO:HB3	0.72	1.99	1	2
1:A:272:CYS:SG	1:A:293:GLY:CA	0.72	2.78	2	1
1:B:223:VAL:HG21	1:B:242:VAL:CG1	0.72	2.14	2	2
1:B:302:MET:O	1:B:302:MET:SD	0.72	2.47	1	2
1:B:314:PHE:CD1	1:B:376:ALA:O	0.72	2.42	1	2
1:B:362:ILE:CG2	1:B:363:ALA:N	0.72	2.52	1	2
1:A:301:PHE:CD2	1:A:342:LEU:HD21	0.71	2.20	2	1
1:A:274:ASN:HD22	1:A:275:ILE:N	0.71	1.83	1	2
1:B:431:GLU:HA	1:B:456:LEU:HG	0.71	1.62	1	2
1:B:331:VAL:O	1:B:389:MET:CE	0.71	2.39	1	2
1:B:362:ILE:HG23	1:B:363:ALA:N	0.71	2.00	1	2
1:A:57:ILE:CG1	1:A:170:GLN:HB3	0.71	2.15	1	1
1:A:362:ILE:HG23	1:A:363:ALA:N	0.71	2.00	1	2
1:A:507:GLY:HA2	1:A:525:MET:SD	0.71	2.24	1	2
1:A:431:GLU:HA	1:A:456:LEU:HG	0.71	1.62	1	2
1:B:272:CYS:HG	1:B:292:VAL:HA	0.71	1.44	1	1
1:A:219:ILE:HD11	1:A:236:ILE:HG12	0.71	1.62	2	2
1:A:314:PHE:CD1	1:A:376:ALA:O	0.71	2.42	1	2
1:B:108:ILE:HD12	1:B:109:GLU:N	0.71	2.01	2	2
1:A:43:PHE:CE2	1:A:100:ALA:HB1	0.71	2.21	1	2
1:B:219:ILE:HD11	1:B:236:ILE:HG12	0.71	1.62	1	2
1:A:511:ALA:HB1	1:A:515:LEU:CD1	0.70	2.15	1	1
1:B:107:VAL:CG1	1:B:108:ILE:N	0.70	2.54	2	2
1:B:298:GLU:HB3	1:B:301:PHE:CZ	0.70	2.18	1	1
1:A:331:VAL:O	1:A:389:MET:CE	0.70	2.39	1	2
1:A:567:LYS:O	1:A:571:GLU:HG3	0.70	1.87	1	2
1:B:501:MET:SD	1:B:515:LEU:CD2	0.70	2.79	1	1
1:A:301:PHE:CD1	1:A:301:PHE:C	0.70	2.65	2	2
1:A:107:VAL:CG1	1:A:108:ILE:N	0.70	2.54	1	2
1:A:298:GLU:CA	1:A:301:PHE:CD2	0.70	2.75	2	2
1:A:171:LEU:HD21	1:A:179:PHE:CE1	0.70	2.21	1	2
1:A:275:ILE:CG2	1:A:276:GLY:N	0.70	2.53	2	2
1:A:314:PHE:CZ	1:A:376:ALA:N	0.70	2.59	1	2
1:B:171:LEU:HD21	1:B:179:PHE:CE1	0.70	2.21	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:PHE:CE2	1:B:100:ALA:HB1	0.70	2.21	1	2
1:A:6:LEU:C	1:A:6:LEU:HD13	0.70	2.12	1	2
1:A:292:VAL:HG11	1:A:329:VAL:HG12	0.70	1.63	1	1
1:B:314:PHE:CZ	1:B:376:ALA:N	0.70	2.59	1	2
1:B:6:LEU:HD13	1:B:6:LEU:C	0.69	2.12	2	2
1:B:301:PHE:HE2	1:B:336:ILE:CG2	0.69	1.97	2	2
1:B:567:LYS:O	1:B:571:GLU:HG3	0.69	1.87	1	2
1:B:275:ILE:CG2	1:B:276:GLY:N	0.69	2.54	2	2
1:A:255:LYS:O	1:A:257:LYS:N	0.69	2.25	2	1
1:A:228:TYR:CG	1:A:235:VAL:HG11	0.69	2.23	1	2
1:A:271:VAL:HG23	1:A:523:PHE:CZ	0.69	2.22	1	1
1:B:13:PHE:CE2	1:B:240:ARG:HD2	0.69	2.23	2	2
1:B:43:PHE:CG	1:B:100:ALA:HB1	0.69	2.22	2	2
1:B:57:ILE:CG1	1:B:170:GLN:HB3	0.69	2.16	1	1
1:B:232:THR:HG23	1:B:233:ASN:H	0.69	1.48	2	2
1:B:511:ALA:HB1	1:B:515:LEU:CD1	0.69	2.17	1	1
1:A:108:ILE:HD12	1:A:109:GLU:N	0.69	2.03	2	2
1:A:129:ASP:OD1	1:A:129:ASP:N	0.69	2.26	2	2
1:B:228:TYR:CG	1:B:235:VAL:HG11	0.69	2.23	1	2
1:B:298:GLU:CA	1:B:301:PHE:CD2	0.69	2.75	2	1
1:A:386:LEU:HD12	1:A:387:ARG:C	0.69	2.13	1	2
1:A:13:PHE:CE2	1:A:240:ARG:HD2	0.69	2.22	1	2
1:A:43:PHE:CG	1:A:100:ALA:HB1	0.69	2.22	2	2
1:A:314:PHE:CD1	1:A:376:ALA:CA	0.69	2.58	1	2
1:A:556:PRO:HB3	1:B:441:HIS:CG	0.69	2.23	1	2
1:A:130:VAL:O	1:A:133:ILE:HG22	0.68	1.88	2	2
1:B:130:VAL:O	1:B:133:ILE:HG22	0.68	1.88	1	2
1:B:301:PHE:CD2	1:B:342:LEU:HD21	0.68	2.20	2	1
1:B:301:PHE:CD1	1:B:342:LEU:HD21	0.68	2.15	1	1
1:A:163:LEU:HB2	1:A:190:THR:HG21	0.68	1.66	1	1
1:B:129:ASP:OD1	1:B:129:ASP:N	0.68	2.26	1	2
1:B:389:MET:HE2	1:B:389:MET:N	0.68	2.03	1	2
1:B:264:LEU:C	1:B:264:LEU:HD23	0.68	2.13	2	1
1:A:386:LEU:HD12	1:A:386:LEU:C	0.68	2.14	1	2
1:A:298:GLU:HB3	1:A:301:PHE:CZ	0.67	2.21	1	1
1:B:163:LEU:HB2	1:B:190:THR:HG21	0.67	1.64	1	1
1:B:13:PHE:CG	1:B:240:ARG:NH1	0.67	2.63	2	2
1:B:221:ASP:OD2	1:B:224:ASN:C	0.67	2.37	2	2
1:B:271:VAL:HG23	1:B:523:PHE:CZ	0.67	2.24	1	1
1:B:370:LEU:HD13	1:B:370:LEU:O	0.67	1.89	1	2
1:A:264:LEU:HD23	1:A:264:LEU:C	0.67	2.14	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:259:LEU:N	1:B:260:PRO:CD	0.67	2.58	2	1
1:A:272:CYS:HG	1:A:292:VAL:HA	0.67	1.48	1	1
1:A:370:LEU:HD13	1:A:370:LEU:O	0.67	1.90	1	2
1:A:13:PHE:CG	1:A:240:ARG:NH1	0.67	2.63	1	2
1:B:181:THR:HG22	1:B:183:ALA:H	0.67	1.50	2	2
1:B:489:ILE:HA	1:B:499:THR:HG21	0.67	1.64	1	2
1:B:536:ILE:O	1:B:540:THR:HG23	0.67	1.89	1	1
1:A:259:LEU:N	1:A:260:PRO:CD	0.67	2.57	2	1
1:A:232:THR:HG23	1:A:233:ASN:H	0.67	1.48	1	2
1:A:389:MET:HE2	1:A:389:MET:N	0.67	2.05	1	2
1:B:292:VAL:HG11	1:B:329:VAL:HG12	0.67	1.64	1	1
1:A:221:ASP:OD2	1:A:224:ASN:C	0.67	2.38	1	2
1:A:389:MET:HG3	1:A:448:PHE:CE1	0.66	2.25	1	2
1:B:10:GLY:O	1:B:222:ALA:HB3	0.66	1.90	1	2
1:B:221:ASP:HA	1:B:239:MET:HE1	0.66	1.66	1	2
1:A:314:PHE:CE1	1:A:375:ARG:O	0.66	2.48	1	2
1:A:389:MET:HG3	1:A:448:PHE:CZ	0.66	2.25	1	2
1:B:232:THR:HG22	1:B:234:GLU:H	0.66	1.51	1	2
1:A:232:THR:HG22	1:A:234:GLU:H	0.66	1.50	2	2
1:B:221:ASP:O	1:B:223:VAL:HG22	0.66	1.90	1	2
1:B:389:MET:HG3	1:B:448:PHE:CE1	0.66	2.25	1	2
1:A:301:PHE:CD1	1:A:342:LEU:HD21	0.66	2.15	1	1
1:A:10:GLY:O	1:A:222:ALA:HB3	0.66	1.90	1	2
1:A:132:ASP:OD1	1:A:164:THR:OG1	0.66	2.13	1	2
1:A:536:ILE:O	1:A:540:THR:HG23	0.66	1.91	1	1
1:B:230:ASN:N	1:B:231:PRO:CD	0.66	2.59	2	2
1:B:301:PHE:CZ	1:B:336:ILE:HG22	0.66	2.25	1	1
1:B:314:PHE:CE1	1:B:375:ARG:O	0.66	2.49	1	2
1:A:230:ASN:N	1:A:231:PRO:CD	0.66	2.59	2	2
1:B:389:MET:HG3	1:B:448:PHE:CZ	0.66	2.25	1	2
1:B:386:LEU:HD12	1:B:387:ARG:C	0.65	2.15	1	2
1:A:507:GLY:CA	1:A:525:MET:SD	0.65	2.85	1	2
1:B:230:ASN:N	1:B:231:PRO:HD3	0.65	2.06	2	2
1:B:507:GLY:CA	1:B:525:MET:SD	0.65	2.84	1	2
1:A:271:VAL:HG12	1:A:523:PHE:CD2	0.65	2.27	2	1
1:A:221:ASP:O	1:A:223:VAL:HG22	0.65	1.90	1	2
1:A:377:ILE:HG22	1:A:386:LEU:HD21	0.65	1.66	1	2
1:A:406:ILE:HD13	1:A:426:ILE:HD13	0.65	1.68	1	2
1:B:406:ILE:HD13	1:B:426:ILE:HD13	0.65	1.68	1	2
1:B:492:SER:OG	1:B:499:THR:CG2	0.65	2.44	1	1
1:A:352:ASN:C	1:A:352:ASN:ND2	0.65	2.54	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:THR:HG22	1:A:183:ALA:H	0.65	1.50	2	2
1:B:43:PHE:CE2	1:B:104:ALA:HB2	0.65	2.27	1	2
1:B:314:PHE:CD1	1:B:379:ARG:HB3	0.65	2.26	1	2
1:A:230:ASN:N	1:A:231:PRO:HD3	0.64	2.06	2	2
1:A:275:ILE:CG2	1:A:277:THR:H	0.64	2.05	2	2
1:A:377:ILE:HG22	1:A:386:LEU:CD2	0.64	2.22	1	2
1:B:352:ASN:C	1:B:352:ASN:HD22	0.64	1.96	1	2
1:A:221:ASP:HA	1:A:239:MET:HE1	0.64	1.66	2	2
1:B:454:ASN:O	1:B:458:GLN:NE2	0.64	2.31	1	2
1:B:456:LEU:HD22	1:B:484:LEU:HD11	0.64	1.69	1	2
1:B:132:ASP:OD1	1:B:164:THR:OG1	0.64	2.14	1	2
1:B:298:GLU:C	1:B:301:PHE:CE1	0.64	2.76	1	1
1:B:386:LEU:HD12	1:B:387:ARG:CA	0.64	2.22	1	2
1:B:255:LYS:O	1:B:257:LYS:N	0.64	2.30	2	1
1:A:314:PHE:CD1	1:A:379:ARG:HB3	0.64	2.26	1	2
1:B:274:ASN:HD22	1:B:275:ILE:N	0.64	1.89	1	2
1:B:377:ILE:HG22	1:B:386:LEU:CD2	0.64	2.23	1	2
1:A:454:ASN:O	1:A:458:GLN:NE2	0.64	2.31	1	2
1:B:271:VAL:HG12	1:B:523:PHE:CD2	0.64	2.27	2	1
1:A:255:LYS:O	1:A:256:LEU:O	0.64	2.15	1	1
1:A:43:PHE:CD2	1:A:100:ALA:CB	0.64	2.81	2	2
1:B:275:ILE:CG2	1:B:277:THR:H	0.64	2.05	2	2
1:B:377:ILE:HG22	1:B:386:LEU:HD21	0.64	1.69	1	2
1:B:314:PHE:CE1	1:B:376:ALA:O	0.63	2.52	1	2
1:A:171:LEU:HD11	1:A:176:VAL:HG21	0.63	1.70	2	1
1:B:232:THR:HG22	1:B:233:ASN:H	0.63	1.34	2	1
1:A:275:ILE:HG22	1:A:276:GLY:N	0.63	2.08	2	2
1:B:125:GLU:O	1:B:129:ASP:OD1	0.63	2.17	1	2
1:B:506:ALA:C	1:B:525:MET:SD	0.63	2.81	1	2
1:A:456:LEU:HD22	1:A:484:LEU:HD11	0.63	1.69	1	2
1:B:104:ALA:O	1:B:107:VAL:HG12	0.63	1.94	2	2
1:A:314:PHE:CE1	1:A:376:ALA:O	0.63	2.52	1	2
1:B:336:ILE:HD12	1:B:336:ILE:C	0.63	2.19	1	2
1:A:332:ARG:NE	1:A:429:MET:SD	0.63	2.72	1	2
1:A:352:ASN:OD1	1:A:355:LEU:CD1	0.63	2.47	1	2
1:B:43:PHE:CD2	1:B:100:ALA:CB	0.63	2.82	1	2
1:A:104:ALA:O	1:A:107:VAL:HG12	0.63	1.94	2	2
1:A:125:GLU:O	1:A:129:ASP:OD1	0.63	2.17	2	2
1:A:301:PHE:CZ	1:A:336:ILE:HG22	0.63	2.28	1	1
1:A:330:ILE:CG2	1:A:389:MET:HE3	0.63	2.22	1	2
1:A:392:MET:N	1:A:431:GLU:OE2	0.63	2.32	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:275:ILE:HG22	1:B:276:GLY:N	0.63	2.08	2	2
1:B:171:LEU:HD11	1:B:176:VAL:HG21	0.63	1.71	2	1
1:A:240:ARG:O	1:A:243:GLN:HB3	0.62	1.93	1	1
1:B:352:ASN:C	1:B:352:ASN:ND2	0.62	2.56	1	2
1:A:11:ILE:HG13	1:A:243:GLN:CA	0.62	2.24	2	2
1:A:296:ARG:NH2	1:A:335:ASP:HB3	0.62	2.09	1	1
1:A:441:HIS:CG	1:B:556:PRO:HB3	0.62	2.28	1	2
1:B:275:ILE:HG22	1:B:277:THR:H	0.62	1.54	2	1
1:A:330:ILE:HG23	1:A:389:MET:CE	0.62	2.20	1	2
1:A:336:ILE:C	1:A:336:ILE:HD12	0.62	2.19	1	2
1:B:352:ASN:OD1	1:B:355:LEU:CD1	0.62	2.47	1	2
1:A:43:PHE:CE2	1:A:104:ALA:HB2	0.62	2.27	1	2
1:A:389:MET:CG	1:A:448:PHE:CE1	0.62	2.82	1	2
1:B:332:ARG:NE	1:B:429:MET:SD	0.62	2.72	1	2
1:A:298:GLU:C	1:A:301:PHE:CE1	0.62	2.78	1	1
1:B:228:TYR:HB3	1:B:231:PRO:CG	0.62	2.25	2	2
1:B:392:MET:N	1:B:431:GLU:OE2	0.62	2.32	1	2
1:B:513:LEU:HD22	1:B:540:THR:HG21	0.62	1.72	1	1
1:A:506:ALA:C	1:A:525:MET:SD	0.62	2.82	1	2
1:B:11:ILE:HG13	1:B:243:GLN:CA	0.62	2.25	2	2
1:B:336:ILE:HD12	1:B:336:ILE:O	0.62	1.95	1	2
1:B:389:MET:CG	1:B:448:PHE:CE1	0.62	2.82	1	2
1:A:501:MET:SD	1:A:515:LEU:HD21	0.61	2.34	1	1
1:B:389:MET:SD	1:B:389:MET:N	0.61	2.73	1	2
1:A:386:LEU:HD12	1:A:387:ARG:CA	0.61	2.25	1	2
1:A:489:ILE:O	1:A:492:SER:HB2	0.61	1.95	1	2
1:B:296:ARG:NH2	1:B:335:ASP:HB3	0.61	2.09	1	1
1:B:523:PHE:CZ	1:B:525:MET:CE	0.61	2.83	2	1
1:A:336:ILE:HD12	1:A:336:ILE:O	0.61	1.95	1	2
1:B:238:LYS:O	1:B:242:VAL:HG23	0.61	1.96	2	2
1:A:513:LEU:HD22	1:A:540:THR:HG21	0.61	1.70	1	1
1:B:243:GLN:CG	1:B:244:GLU:N	0.61	2.63	2	2
1:A:275:ILE:HG22	1:A:277:THR:H	0.61	1.54	2	1
1:B:22:ASP:OD1	1:B:145:LYS:NZ	0.61	2.34	1	1
1:A:238:LYS:O	1:A:242:VAL:HG23	0.60	1.96	1	2
1:A:389:MET:SD	1:A:389:MET:N	0.60	2.74	1	2
1:B:438:ILE:HG22	1:B:438:ILE:O	0.60	1.95	1	2
1:A:438:ILE:HG22	1:A:438:ILE:O	0.60	1.96	1	2
1:A:22:ASP:OD1	1:A:145:LYS:NZ	0.60	2.34	1	1
1:A:77:ILE:CG2	1:A:78:MET:N	0.60	2.65	1	2
1:A:352:ASN:CG	1:B:352:ASN:ND2	0.60	2.58	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:356:GLY:O	1:A:361:ARG:NH2	0.60	2.34	1	2
1:A:107:VAL:HG13	1:A:108:ILE:N	0.60	2.11	2	2
1:B:489:ILE:O	1:B:492:SER:HB2	0.60	1.95	1	2
1:B:272:CYS:HG	1:B:273:ALA:N	0.60	1.93	2	1
1:A:298:GLU:O	1:A:301:PHE:CG	0.60	2.53	1	1
1:A:492:SER:CB	1:A:499:THR:HG22	0.60	2.27	1	1
1:A:43:PHE:CZ	1:A:100:ALA:C	0.60	2.80	2	2
1:B:77:ILE:CG2	1:B:78:MET:N	0.60	2.65	2	2
1:B:107:VAL:HG13	1:B:108:ILE:N	0.59	2.11	2	2
1:A:228:TYR:HB3	1:A:231:PRO:CG	0.59	2.25	1	2
1:B:221:ASP:OD1	1:B:222:ALA:N	0.59	2.36	1	2
1:A:523:PHE:CZ	1:A:525:MET:CE	0.59	2.85	2	1
1:B:370:LEU:HD13	1:B:370:LEU:C	0.59	2.22	1	2
1:A:272:CYS:HG	1:A:273:ALA:N	0.59	1.94	2	1
1:B:43:PHE:CZ	1:B:100:ALA:C	0.59	2.80	1	2
1:B:296:ARG:HE	1:B:298:GLU:CD	0.59	2.06	1	1
1:A:370:LEU:HD13	1:A:370:LEU:C	0.59	2.23	1	2
1:A:221:ASP:OD1	1:A:222:ALA:N	0.59	2.36	1	2
1:A:43:PHE:CE2	1:A:100:ALA:O	0.59	2.56	2	2
1:A:371:ARG:NH1	1:A:375:ARG:HH11	0.59	1.96	1	2
1:B:259:LEU:HD22	1:B:259:LEU:N	0.59	2.11	1	1
1:B:301:PHE:HE2	1:B:336:ILE:HG23	0.59	1.57	1	1
1:B:356:GLY:O	1:B:361:ARG:NH2	0.59	2.36	1	2
1:B:389:MET:N	1:B:389:MET:CE	0.59	2.66	1	2
1:B:523:PHE:CE1	1:B:525:MET:CE	0.59	2.85	1	1
1:A:523:PHE:CE1	1:A:525:MET:CE	0.59	2.86	1	1
1:B:272:CYS:HG	1:B:291:GLY:C	0.59	2.06	1	1
1:B:387:ARG:C	1:B:389:MET:HE1	0.59	2.23	1	2
1:B:265:ASP:OD1	1:B:265:ASP:N	0.58	2.34	1	1
1:B:484:LEU:HD23	1:B:484:LEU:C	0.58	2.23	1	2
1:B:330:ILE:HG23	1:B:389:MET:CE	0.58	2.22	1	2
1:A:438:ILE:HG22	1:A:441:HIS:HB2	0.58	1.75	1	2
1:B:259:LEU:H	1:B:259:LEU:CD2	0.58	2.10	1	1
1:B:438:ILE:HG23	1:B:441:HIS:HB2	0.58	1.74	1	2
1:B:133:ILE:CG2	1:B:134:GLY:N	0.58	2.67	1	2
1:B:330:ILE:CG2	1:B:389:MET:HE3	0.58	2.24	1	2
1:A:421:ASP:OD1	1:A:423:SER:HB2	0.58	1.99	1	2
1:B:371:ARG:NH1	1:B:375:ARG:HH11	0.58	1.96	1	2
1:A:474:TYR:O	1:A:474:TYR:CD2	0.58	2.57	1	2
1:B:43:PHE:HZ	1:B:100:ALA:O	0.58	1.74	2	2
1:A:389:MET:N	1:A:389:MET:CE	0.58	2.67	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:484:LEU:HD23	1:A:484:LEU:C	0.58	2.23	1	2
1:B:421:ASP:OD1	1:B:423:SER:HB2	0.58	1.99	1	2
1:A:133:ILE:CG2	1:A:134:GLY:N	0.58	2.67	1	2
1:A:269:VAL:HG13	1:A:521:ASP:C	0.58	2.23	1	1
1:B:243:GLN:HG2	1:B:244:GLU:N	0.58	2.14	1	1
1:B:372:ASP:OD1	1:B:373:GLN:N	0.57	2.37	1	2
1:B:316:ALA:O	1:B:320:VAL:HG23	0.57	1.99	2	1
1:B:489:ILE:HG12	1:B:499:THR:HG21	0.57	1.75	2	1
1:B:269:VAL:HG13	1:B:521:ASP:C	0.57	2.23	1	1
1:B:43:PHE:CE2	1:B:100:ALA:O	0.57	2.57	1	2
1:B:474:TYR:O	1:B:474:TYR:CD2	0.57	2.57	1	2
1:A:11:ILE:HD13	1:A:11:ILE:H	0.57	1.60	2	2
1:B:265:ASP:OD1	1:B:541:ASN:HA	0.57	1.98	1	1
1:B:272:CYS:HG	1:B:292:VAL:CA	0.57	2.10	1	1
1:B:298:GLU:O	1:B:301:PHE:CG	0.57	2.57	1	1
1:B:11:ILE:HD13	1:B:11:ILE:N	0.57	2.15	2	2
1:A:489:ILE:HG12	1:A:499:THR:HG21	0.57	1.75	2	1
1:B:11:ILE:HD13	1:B:11:ILE:H	0.57	1.60	1	2
1:A:13:PHE:CD2	1:A:240:ARG:NH1	0.57	2.73	1	2
1:A:352:ASN:OD1	1:B:352:ASN:OD1	0.57	2.21	1	2
1:A:352:ASN:ND2	1:B:352:ASN:CG	0.57	2.62	1	2
1:B:229:VAL:C	1:B:231:PRO:HD3	0.57	2.25	1	2
1:A:260:PRO:O	1:A:262:ILE:N	0.57	2.38	2	1
1:B:260:PRO:O	1:B:262:ILE:N	0.57	2.38	2	1
1:B:13:PHE:CD2	1:B:240:ARG:NH1	0.57	2.73	2	2
1:B:456:LEU:CD2	1:B:484:LEU:HD11	0.57	2.30	1	2
1:A:316:ALA:O	1:A:320:VAL:HG23	0.57	1.99	2	1
1:A:259:LEU:HD23	1:A:262:ILE:HG21	0.57	1.77	1	1
1:A:296:ARG:HE	1:A:298:GLU:CD	0.57	2.07	1	1
1:A:456:LEU:CD2	1:A:484:LEU:HD11	0.57	2.30	1	2
1:B:507:GLY:CA	1:B:525:MET:HG2	0.56	2.30	2	2
1:A:11:ILE:HD13	1:A:11:ILE:N	0.56	2.15	1	2
1:A:136:ARG:NH2	1:A:167:GLU:CG	0.56	2.69	1	1
1:A:486:LYS:HD2	1:A:553:LEU:HD13	0.56	1.76	1	2
1:B:486:LYS:HD2	1:B:553:LEU:HD13	0.56	1.75	1	2
1:A:229:VAL:C	1:A:231:PRO:HD3	0.56	2.25	2	2
1:A:259:LEU:H	1:A:259:LEU:CD2	0.56	2.08	1	1
1:B:412:GLU:O	1:B:416:GLU:HG3	0.56	2.01	1	2
1:A:331:VAL:N	1:A:389:MET:CE	0.55	2.69	1	2
1:A:372:ASP:OD1	1:A:373:GLN:N	0.55	2.38	1	2
1:A:387:ARG:C	1:A:389:MET:HE1	0.55	2.24	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:181:THR:CG2	1:B:182:ASP:N	0.55	2.69	2	2
1:B:240:ARG:O	1:B:243:GLN:HG3	0.55	2.01	2	1
1:A:412:GLU:O	1:A:416:GLU:HG3	0.55	2.01	1	2
1:A:278:VAL:HG13	1:A:279:ARG:N	0.55	2.17	2	1
1:B:295:TYR:CE1	1:B:320:VAL:HG11	0.55	2.36	2	1
1:A:161:ALA:O	1:A:182:ASP:OD1	0.55	2.25	2	2
1:B:301:PHE:CE2	1:B:336:ILE:HG23	0.55	2.29	1	1
1:A:13:PHE:CD1	1:A:13:PHE:N	0.55	2.74	1	2
1:A:507:GLY:CA	1:A:525:MET:HG2	0.55	2.30	2	2
1:B:301:PHE:CE2	1:B:342:LEU:CD2	0.55	2.66	2	1
1:A:136:ARG:HH21	1:A:167:GLU:HG3	0.55	1.57	1	1
1:B:470:ILE:HD12	1:B:470:ILE:H	0.55	1.61	1	2
1:B:243:GLN:C	1:B:243:GLN:CD	0.55	2.75	2	1
1:A:53:GLN:O	1:A:56:THR:OG1	0.55	2.24	1	2
1:A:398:GLU:N	1:A:398:GLU:OE1	0.55	2.40	1	2
1:B:331:VAL:N	1:B:389:MET:CE	0.55	2.69	1	2
1:A:438:ILE:HG23	1:A:441:HIS:HB2	0.55	1.77	1	2
1:B:53:GLN:O	1:B:56:THR:OG1	0.55	2.24	2	2
1:A:181:THR:HG23	1:A:182:ASP:N	0.55	2.17	2	2
1:B:13:PHE:N	1:B:13:PHE:CD1	0.54	2.75	1	2
1:B:43:PHE:CE2	1:B:100:ALA:CA	0.54	2.90	1	2
1:B:161:ALA:O	1:B:182:ASP:OD1	0.54	2.25	1	2
1:B:276:GLY:O	1:B:277:THR:HG22	0.54	2.02	1	1
1:A:386:LEU:CD1	1:A:387:ARG:C	0.54	2.80	1	2
1:B:386:LEU:CD1	1:B:387:ARG:C	0.54	2.80	1	2
1:A:295:TYR:CE1	1:A:320:VAL:HG11	0.54	2.37	2	1
1:A:43:PHE:CE2	1:A:100:ALA:CB	0.54	2.90	2	2
1:A:226:GLN:NE2	1:A:228:TYR:OH	0.54	2.40	1	2
1:B:274:ASN:HD22	1:B:274:ASN:C	0.54	2.10	1	1
1:B:398:GLU:OE1	1:B:398:GLU:N	0.54	2.41	1	2
1:A:355:LEU:CD2	1:B:462:ALA:HA	0.54	2.32	1	2
1:B:182:ASP:OD1	1:B:182:ASP:C	0.54	2.50	1	2
1:B:226:GLN:NE2	1:B:228:TYR:OH	0.54	2.40	1	2
1:A:181:THR:CG2	1:A:182:ASP:N	0.54	2.69	2	2
1:B:181:THR:HG23	1:B:182:ASP:N	0.54	2.17	1	2
1:B:259:LEU:HD23	1:B:262:ILE:HG21	0.54	1.79	1	1
1:B:513:LEU:CD2	1:B:540:THR:HG21	0.54	2.33	1	1
1:A:43:PHE:CE2	1:A:100:ALA:CA	0.54	2.90	2	2
1:A:182:ASP:OD1	1:A:182:ASP:C	0.54	2.50	2	2
1:A:405:GLU:HG3	1:A:409:TYR:CE2	0.54	2.38	1	2
1:A:301:PHE:CE2	1:A:336:ILE:HG23	0.54	2.33	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:PHE:CE2	1:B:100:ALA:CB	0.54	2.91	2	2
1:B:509:GLU:OE2	1:B:532:ARG:NH1	0.54	2.38	1	1
1:A:101:ASP:OD1	1:A:101:ASP:N	0.54	2.41	2	2
1:A:221:ASP:OD2	1:A:226:GLN:N	0.54	2.40	1	2
1:A:347:PHE:CD1	1:A:347:PHE:C	0.54	2.85	1	2
1:A:470:ILE:HD12	1:A:470:ILE:H	0.54	1.62	1	2
1:A:43:PHE:HZ	1:A:100:ALA:O	0.54	1.75	2	2
1:B:339:ASP:OD1	1:B:465:ARG:NH2	0.53	2.41	1	2
1:B:470:ILE:HD12	1:B:470:ILE:N	0.53	2.18	1	2
1:A:514:LEU:O	1:A:518:MET:SD	0.53	2.66	2	1
1:B:278:VAL:HG13	1:B:279:ARG:N	0.53	2.17	2	1
1:B:514:LEU:O	1:B:518:MET:SD	0.53	2.67	2	1
1:B:101:ASP:N	1:B:101:ASP:OD1	0.53	2.41	2	2
1:B:492:SER:OG	1:B:499:THR:HG23	0.53	2.02	1	1
1:A:132:ASP:OD2	1:A:166:SER:CB	0.53	2.56	1	1
1:B:405:GLU:HG3	1:B:409:TYR:CE2	0.53	2.38	1	2
1:B:431:GLU:N	1:B:431:GLU:OE1	0.53	2.41	1	2
1:A:276:GLY:O	1:A:277:THR:HG22	0.53	2.02	1	1
1:A:297:THR:OG1	1:A:317:TYR:OH	0.53	2.27	1	1
1:A:470:ILE:HD12	1:A:470:ILE:N	0.53	2.19	1	2
1:A:501:MET:SD	1:A:520:LEU:HD11	0.53	2.43	1	1
1:A:199:LEU:O	1:A:199:LEU:CD2	0.53	2.52	2	1
1:A:301:PHE:CE2	1:A:342:LEU:CD2	0.53	2.66	2	1
1:B:352:ASN:OD1	1:B:355:LEU:CG	0.53	2.57	1	2
1:A:339:ASP:OD1	1:A:465:ARG:NH2	0.53	2.42	1	2
1:B:132:ASP:OD2	1:B:166:SER:CB	0.53	2.57	1	1
1:B:507:GLY:HA2	1:B:525:MET:CE	0.53	2.33	1	1
1:A:123:LEU:CD2	1:A:123:LEU:N	0.53	2.72	2	2
1:A:431:GLU:N	1:A:431:GLU:OE1	0.53	2.42	1	2
1:B:438:ILE:HG22	1:B:441:HIS:HB2	0.53	1.77	1	2
1:A:507:GLY:HA2	1:A:525:MET:CE	0.52	2.34	1	1
1:B:123:LEU:N	1:B:123:LEU:CD2	0.52	2.72	2	2
1:B:221:ASP:OD2	1:B:226:GLN:N	0.52	2.40	2	2
1:B:221:ASP:CA	1:B:239:MET:CE	0.52	2.78	1	2
1:A:352:ASN:OD1	1:B:352:ASN:CG	0.52	2.52	1	2
1:A:386:LEU:CD1	1:A:387:ARG:O	0.52	2.57	1	2
1:B:511:ALA:HB1	1:B:515:LEU:HD12	0.52	1.82	1	1
1:B:347:PHE:CD1	1:B:347:PHE:C	0.52	2.85	1	2
1:B:199:LEU:O	1:B:199:LEU:CD2	0.52	2.53	2	1
1:B:79:LEU:O	1:B:82:ASP:OD1	0.52	2.27	1	2
1:B:507:GLY:N	1:B:525:MET:SD	0.52	2.83	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:339:ASP:CG	1:A:465:ARG:NH2	0.52	2.68	1	2
1:B:296:ARG:NE	1:B:298:GLU:OE2	0.52	2.43	1	1
1:B:269:VAL:CG1	1:B:270:GLU:N	0.52	2.71	2	1
1:A:85:LEU:HD21	1:A:89:ILE:HD12	0.52	1.82	2	2
1:A:259:LEU:N	1:A:259:LEU:CD1	0.52	2.62	1	1
1:A:314:PHE:CZ	1:A:375:ARG:O	0.52	2.62	1	2
1:B:68:GLU:HB2	1:B:286:ARG:NH2	0.52	2.20	1	1
1:A:274:ASN:HD22	1:A:274:ASN:C	0.52	2.12	1	1
1:A:292:VAL:HG13	1:A:329:VAL:HG12	0.52	1.81	1	1
1:A:388:ILE:C	1:A:388:ILE:HD12	0.52	2.30	1	2
1:B:221:ASP:C	1:B:223:VAL:N	0.52	2.66	2	2
1:B:339:ASP:CG	1:B:465:ARG:NH2	0.52	2.68	1	2
1:A:269:VAL:CG1	1:A:270:GLU:N	0.52	2.71	2	1
1:B:6:LEU:C	1:B:6:LEU:CD1	0.52	2.83	2	2
1:B:43:PHE:HZ	1:B:104:ALA:HB3	0.52	1.64	2	2
1:B:314:PHE:CZ	1:B:375:ARG:O	0.52	2.62	1	2
1:B:386:LEU:C	1:B:386:LEU:CD1	0.52	2.78	1	2
1:A:6:LEU:C	1:A:6:LEU:CD1	0.52	2.83	2	2
1:A:79:LEU:O	1:A:82:ASP:OD1	0.52	2.28	2	2
1:A:330:ILE:C	1:A:389:MET:HE3	0.52	2.30	1	2
1:B:129:ASP:CG	1:B:165:PRO:CG	0.52	2.82	2	1
1:A:309:THR:O	1:A:313:GLN:CG	0.51	2.58	1	2
1:B:74:GLU:O	1:B:77:ILE:HG22	0.51	2.05	2	2
1:B:123:LEU:N	1:B:123:LEU:HD22	0.51	2.20	2	2
1:B:370:LEU:C	1:B:370:LEU:CD1	0.51	2.84	1	2
1:A:431:GLU:OE1	1:A:432:THR:N	0.51	2.44	1	2
1:B:158:LEU:HD21	1:B:163:LEU:HD11	0.51	1.83	1	2
1:B:296:ARG:HH21	1:B:335:ASP:HB3	0.51	1.66	1	1
1:B:330:ILE:C	1:B:389:MET:HE3	0.51	2.30	1	2
1:B:388:ILE:C	1:B:388:ILE:HD12	0.51	2.29	1	2
1:A:221:ASP:C	1:A:223:VAL:N	0.51	2.67	2	2
1:B:309:THR:O	1:B:313:GLN:CG	0.51	2.59	1	2
1:B:557:THR:HB	1:B:560:GLU:OE1	0.51	2.05	1	2
1:A:255:LYS:C	1:A:257:LYS:H	0.51	2.13	2	1
1:A:68:GLU:HB2	1:A:286:ARG:NH2	0.51	2.20	1	1
1:A:123:LEU:N	1:A:123:LEU:HD22	0.51	2.21	2	2
1:A:507:GLY:N	1:A:525:MET:SD	0.51	2.84	1	1
1:B:271:VAL:CB	1:B:523:PHE:CE2	0.51	2.90	2	2
1:B:321:ALA:O	1:B:324:CYS:SG	0.51	2.66	2	2
1:B:451:ILE:HG23	1:B:456:LEU:HD12	0.51	1.83	1	2
1:B:489:ILE:HA	1:B:499:THR:CG2	0.51	2.35	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:232:THR:HG22	1:A:233:ASN:H	0.51	1.34	1	2
1:A:302:MET:O	1:A:302:MET:CG	0.51	2.59	2	2
1:A:370:LEU:C	1:A:370:LEU:CD1	0.51	2.84	1	2
1:B:57:ILE:CD1	1:B:170:GLN:HB3	0.51	2.36	1	1
1:B:292:VAL:HG13	1:B:329:VAL:HG12	0.51	1.82	1	1
1:B:271:VAL:HG23	1:B:271:VAL:O	0.51	2.06	2	1
1:A:11:ILE:N	1:A:11:ILE:CD1	0.51	2.74	2	2
1:A:296:ARG:HH21	1:A:335:ASP:HB3	0.51	1.66	1	1
1:B:431:GLU:OE1	1:B:432:THR:N	0.51	2.44	1	2
1:B:507:GLY:HA3	1:B:525:MET:HG2	0.51	1.83	2	2
1:A:265:ASP:OD1	1:A:265:ASP:N	0.51	2.38	1	1
1:A:507:GLY:HA3	1:A:525:MET:HG2	0.51	1.83	2	2
1:B:158:LEU:O	1:B:180:ILE:HG23	0.51	2.06	1	2
1:A:271:VAL:HG23	1:A:271:VAL:O	0.51	2.06	2	1
1:B:11:ILE:N	1:B:11:ILE:CD1	0.50	2.74	1	2
1:A:243:GLN:O	1:A:243:GLN:NE2	0.50	2.44	2	1
1:B:272:CYS:SG	1:B:293:GLY:HA3	0.50	2.46	2	1
1:B:523:PHE:CD1	1:B:524:SER:N	0.50	2.57	2	1
1:A:163:LEU:CB	1:A:190:THR:HG21	0.50	2.36	1	1
1:A:352:ASN:OD1	1:A:355:LEU:CG	0.50	2.59	1	2
1:A:431:GLU:CA	1:A:456:LEU:HG	0.50	2.35	1	2
1:A:43:PHE:HZ	1:A:104:ALA:HB3	0.50	1.63	1	2
1:A:271:VAL:CB	1:A:523:PHE:CE2	0.50	2.90	2	2
1:A:314:PHE:CG	1:A:376:ALA:HA	0.50	2.37	1	2
1:A:400:ARG:NH2	1:A:445:GLU:OE2	0.50	2.45	1	2
1:A:453:THR:OG1	1:A:501:MET:CE	0.50	2.59	1	1
1:A:147:ILE:HG23	1:A:148:ASP:N	0.50	2.21	2	1
1:A:541:ASN:N	1:A:541:ASN:HD22	0.50	2.05	2	1
1:B:219:ILE:CD1	1:B:236:ILE:HG12	0.50	2.36	2	2
1:A:272:CYS:SG	1:A:293:GLY:HA3	0.50	2.47	2	1
1:A:74:GLU:O	1:A:77:ILE:HG22	0.50	2.06	1	2
1:A:259:LEU:HD22	1:A:259:LEU:N	0.50	2.11	1	1
1:A:301:PHE:HE2	1:A:336:ILE:HG23	0.50	1.60	1	1
1:A:334:MET:SD	1:A:369:ILE:CG2	0.50	3.00	1	2
1:B:240:ARG:O	1:B:243:GLN:CG	0.50	2.60	2	1
1:A:57:ILE:CD1	1:A:170:GLN:HB3	0.50	2.36	1	1
1:A:202:ILE:HD12	1:A:205:THR:HG22	0.50	1.83	1	1
1:A:352:ASN:CG	1:B:352:ASN:OD1	0.50	2.54	1	2
1:A:556:PRO:HB3	1:B:441:HIS:CE1	0.50	2.41	1	2
1:B:132:ASP:OD2	1:B:136:ARG:NH1	0.50	2.45	2	2
1:B:277:THR:O	1:B:278:VAL:C	0.50	2.54	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:302:MET:O	1:B:302:MET:CG	0.50	2.59	2	2
1:B:388:ILE:C	1:B:389:MET:CE	0.50	2.84	1	2
1:B:464:ASP:OD2	1:B:467:ASN:N	0.50	2.45	1	2
1:B:492:SER:CB	1:B:499:THR:HG23	0.50	2.36	1	1
1:A:68:GLU:H	1:A:68:GLU:CD	0.50	2.15	2	2
1:A:269:VAL:HG13	1:A:521:ASP:O	0.50	2.07	1	1
1:B:265:ASP:OD2	1:B:542:PHE:N	0.50	2.45	1	1
1:A:272:CYS:SG	1:A:273:ALA:O	0.50	2.69	2	1
1:B:272:CYS:SG	1:B:273:ALA:O	0.50	2.70	2	1
1:A:464:ASP:OD1	1:A:467:ASN:N	0.50	2.44	1	2
1:A:557:THR:HB	1:A:560:GLU:OE1	0.50	2.05	1	2
1:B:202:ILE:HD12	1:B:205:THR:HG22	0.50	1.83	1	1
1:B:330:ILE:HG22	1:B:330:ILE:O	0.50	2.07	1	2
1:B:509:GLU:O	1:B:512:THR:CG2	0.50	2.60	2	1
1:B:541:ASN:N	1:B:541:ASN:HD22	0.50	2.05	2	1
1:A:132:ASP:OD2	1:A:136:ARG:NH1	0.49	2.45	1	2
1:A:132:ASP:OD2	1:A:166:SER:HB2	0.49	2.07	1	1
1:A:181:THR:CG2	1:A:183:ALA:N	0.49	2.72	1	2
1:A:219:ILE:CD1	1:A:236:ILE:HG12	0.49	2.36	1	2
1:A:272:CYS:SG	1:A:291:GLY:C	0.49	2.95	1	1
1:A:462:ALA:HA	1:B:355:LEU:CD2	0.49	2.37	1	2
1:A:525:MET:O	1:A:526:SER:C	0.49	2.55	1	1
1:B:303:ASP:O	1:B:304:ARG:HD3	0.49	2.07	1	1
1:B:333:THR:HG22	1:B:334:MET:N	0.49	2.22	1	2
1:B:334:MET:SD	1:B:369:ILE:CG2	0.49	3.00	1	2
1:A:240:ARG:O	1:A:243:GLN:CG	0.49	2.60	2	1
1:A:274:ASN:ND2	1:A:275:ILE:N	0.49	2.60	2	1
1:A:57:ILE:HD11	1:A:170:GLN:HB3	0.49	1.84	1	1
1:A:511:ALA:CB	1:A:515:LEU:CD1	0.49	2.89	1	1
1:B:57:ILE:HD11	1:B:170:GLN:HB3	0.49	1.83	1	1
1:B:181:THR:CG2	1:B:183:ALA:N	0.49	2.71	1	2
1:B:274:ASN:ND2	1:B:275:ILE:N	0.49	2.60	2	1
1:A:132:ASP:OD1	1:A:136:ARG:NH1	0.49	2.45	2	2
1:A:459:TYR:HB3	1:B:459:TYR:O	0.49	2.07	1	2
1:A:469:MET:SD	1:A:469:MET:N	0.49	2.85	1	2
1:B:85:LEU:HD21	1:B:89:ILE:HD12	0.49	1.83	2	2
1:B:269:VAL:HG13	1:B:521:ASP:O	0.49	2.07	1	1
1:B:400:ARG:NH2	1:B:445:GLU:OE2	0.49	2.45	1	2
1:A:542:PHE:CD1	1:A:543:GLU:N	0.49	2.81	1	1
1:B:336:ILE:CD1	1:B:345:MET:HE1	0.49	2.36	1	2
1:B:431:GLU:CA	1:B:456:LEU:HG	0.49	2.35	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:458:GLN:OE1	1:B:463:VAL:O	0.49	2.31	1	2
1:A:509:GLU:O	1:A:512:THR:CG2	0.49	2.60	2	1
1:A:303:ASP:O	1:A:304:ARG:HD3	0.49	2.08	1	1
1:A:492:SER:CB	1:A:499:THR:CG2	0.49	2.91	1	1
1:B:314:PHE:CD1	1:B:376:ALA:C	0.49	2.88	1	2
1:A:451:ILE:HG23	1:A:456:LEU:HD12	0.49	1.83	1	2
1:B:388:ILE:C	1:B:388:ILE:CD1	0.49	2.85	1	2
1:B:469:MET:SD	1:B:469:MET:N	0.49	2.86	1	2
1:B:542:PHE:CD1	1:B:543:GLU:N	0.49	2.81	1	1
1:B:259:LEU:H	1:B:260:PRO:CD	0.49	2.20	2	1
1:B:275:ILE:CG1	1:B:280:ASP:HB3	0.49	2.37	2	1
1:B:492:SER:OG	1:B:499:THR:HG22	0.49	2.07	1	1
1:A:527:ALA:O	1:A:530:ILE:HG13	0.49	2.08	2	1
1:A:330:ILE:O	1:A:330:ILE:HG22	0.49	2.08	1	2
1:A:511:ALA:HB1	1:A:515:LEU:HD12	0.49	1.83	1	1
1:B:176:VAL:CG1	1:B:179:PHE:CE1	0.49	2.92	2	2
1:B:333:THR:HG22	1:B:334:MET:H	0.49	1.68	1	2
1:B:68:GLU:CD	1:B:68:GLU:H	0.49	2.14	2	1
1:B:275:ILE:CG2	1:B:276:GLY:H	0.49	2.21	2	1
1:A:233:ASN:O	1:A:237:ASP:OD2	0.49	2.31	2	2
1:B:90:ILE:HG13	1:B:91:ALA:N	0.49	2.22	2	2
1:B:233:ASN:O	1:B:237:ASP:OD2	0.49	2.31	1	2
1:B:147:ILE:HG23	1:B:148:ASP:N	0.49	2.22	2	1
1:B:522:GLU:OE1	1:B:522:GLU:C	0.49	2.56	2	1
1:A:356:GLY:O	1:A:361:ARG:CZ	0.49	2.60	1	2
1:A:489:ILE:HA	1:A:499:THR:CG2	0.49	2.18	1	2
1:A:509:GLU:OE2	1:A:532:ARG:NH1	0.49	2.39	1	1
1:B:258:ASP:C	1:B:259:LEU:HD13	0.49	2.33	1	1
1:A:147:ILE:CG2	1:A:148:ASP:N	0.49	2.76	2	1
1:B:147:ILE:CG2	1:B:148:ASP:N	0.49	2.76	2	1
1:A:158:LEU:HD21	1:A:163:LEU:HD11	0.48	1.84	2	2
1:A:168:THR:CG2	1:A:190:THR:HG22	0.48	2.39	1	1
1:A:258:ASP:C	1:A:259:LEU:HD13	0.48	2.33	1	1
1:A:275:ILE:CG2	1:A:280:ASP:HB2	0.48	2.35	1	1
1:A:333:THR:HG22	1:A:334:MET:N	0.48	2.22	1	2
1:A:523:PHE:HD1	1:A:524:SER:CA	0.48	2.21	2	1
1:A:314:PHE:CD1	1:A:376:ALA:C	0.48	2.88	1	2
1:A:388:ILE:C	1:A:389:MET:CE	0.48	2.86	1	2
1:B:467:ASN:CG	1:B:470:ILE:CD1	0.48	2.86	1	2
1:A:336:ILE:CD1	1:A:345:MET:HE1	0.48	2.35	1	2
1:B:305:ASP:O	1:B:344:TYR:CD1	0.48	2.66	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:275:ILE:CG2	1:A:276:GLY:H	0.48	2.20	2	1
1:A:275:ILE:CG1	1:A:280:ASP:HB3	0.48	2.37	2	1
1:A:294:LEU:HB2	1:A:502:CYS:SG	0.48	2.49	1	1
1:A:352:ASN:OD1	1:B:352:ASN:ND2	0.48	2.46	1	2
1:A:467:ASN:CG	1:A:470:ILE:CD1	0.48	2.86	1	2
1:B:132:ASP:OD1	1:B:136:ARG:NH1	0.48	2.46	2	2
1:A:255:LYS:C	1:A:257:LYS:N	0.48	2.71	2	1
1:A:317:TYR:HH	1:A:373:GLN:NE2	0.48	2.00	2	1
1:A:522:GLU:C	1:A:522:GLU:OE1	0.48	2.56	2	1
1:A:277:THR:O	1:A:278:VAL:C	0.48	2.54	1	2
1:A:513:LEU:CD2	1:A:540:THR:HG21	0.48	2.38	1	1
1:A:524:SER:O	1:A:525:MET:HG3	0.48	2.08	1	1
1:A:557:THR:HG22	1:A:560:GLU:H	0.48	1.69	1	2
1:A:264:LEU:C	1:A:264:LEU:CD2	0.48	2.85	2	1
1:B:527:ALA:O	1:B:530:ILE:HG13	0.48	2.08	2	1
1:A:221:ASP:CA	1:A:239:MET:CE	0.48	2.78	2	2
1:A:305:ASP:O	1:A:344:TYR:CD1	0.48	2.66	1	2
1:A:456:LEU:HD13	1:A:484:LEU:CD2	0.48	2.30	1	2
1:B:68:GLU:H	1:B:68:GLU:CD	0.48	2.14	1	1
1:B:68:GLU:OE1	1:B:68:GLU:N	0.48	2.41	1	2
1:A:458:GLN:OE1	1:A:463:VAL:O	0.48	2.31	1	2
1:A:333:THR:HG22	1:A:334:MET:H	0.48	1.68	1	2
1:A:501:MET:SD	1:A:520:LEU:CD1	0.48	3.02	1	1
1:B:132:ASP:OD2	1:B:166:SER:HB2	0.48	2.08	1	1
1:B:272:CYS:SG	1:B:291:GLY:C	0.48	2.95	1	1
1:B:310:GLU:CD	1:B:310:GLU:H	0.48	2.17	1	2
1:A:269:VAL:CG1	1:A:270:GLU:O	0.48	2.62	2	1
1:B:259:LEU:H	1:B:260:PRO:HD3	0.48	1.68	2	1
1:A:339:ASP:OD2	1:A:465:ARG:NH2	0.48	2.46	1	2
1:A:539:ASN:OD1	1:A:539:ASN:C	0.48	2.57	1	1
1:B:70:GLU:O	1:B:70:GLU:OE2	0.48	2.32	1	2
1:B:275:ILE:CG2	1:B:280:ASP:HB2	0.48	2.35	1	1
1:A:129:ASP:HA	1:A:165:PRO:HG2	0.47	1.85	1	1
1:B:10:GLY:O	1:B:221:ASP:O	0.47	2.32	1	2
1:B:163:LEU:CB	1:B:190:THR:HG21	0.47	2.36	1	1
1:B:221:ASP:O	1:B:223:VAL:N	0.47	2.47	1	2
1:B:386:LEU:CD1	1:B:387:ARG:O	0.47	2.62	1	2
1:B:525:MET:O	1:B:526:SER:C	0.47	2.55	1	1
1:B:557:THR:HG22	1:B:560:GLU:H	0.47	1.69	1	2
1:A:129:ASP:CG	1:A:165:PRO:CG	0.47	2.82	2	1
1:A:278:VAL:CG1	1:A:279:ARG:N	0.47	2.77	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:198:GLU:OE2	1:A:250:LYS:NZ	0.47	2.43	1	1
1:B:314:PHE:CE2	1:B:376:ALA:HA	0.47	2.40	1	2
1:B:356:GLY:O	1:B:361:ARG:CZ	0.47	2.62	1	2
1:B:264:LEU:C	1:B:264:LEU:CD2	0.47	2.84	2	1
1:A:321:ALA:O	1:A:324:CYS:SG	0.47	2.67	2	2
1:A:381:SER:CB	1:A:386:LEU:HD23	0.47	2.39	1	2
1:B:269:VAL:CG1	1:B:270:GLU:O	0.47	2.62	2	1
1:A:453:THR:OG1	1:A:501:MET:HE2	0.47	2.09	1	1
1:A:480:SER:OG	1:B:438:ILE:HG12	0.47	2.09	1	2
1:B:539:ASN:OD1	1:B:539:ASN:C	0.47	2.57	1	1
1:A:523:PHE:CD1	1:A:524:SER:CA	0.47	2.97	2	1
1:A:523:PHE:CD1	1:A:524:SER:N	0.47	2.57	2	1
1:A:260:PRO:O	1:A:261:ALA:C	0.47	2.58	1	1
1:A:501:MET:SD	1:A:515:LEU:CD2	0.47	3.02	1	1
1:B:528:ILE:HG22	1:B:528:ILE:O	0.47	2.09	2	1
1:A:70:GLU:OE2	1:A:70:GLU:O	0.47	2.32	2	2
1:A:221:ASP:O	1:A:223:VAL:N	0.47	2.48	1	2
1:A:456:LEU:O	1:A:460:THR:OG1	0.47	2.30	1	2
1:A:295:TYR:OH	1:A:320:VAL:CG2	0.47	2.62	2	1
1:A:10:GLY:O	1:A:221:ASP:O	0.47	2.32	1	2
1:A:310:GLU:CD	1:A:310:GLU:H	0.47	2.17	1	2
1:B:260:PRO:O	1:B:261:ALA:C	0.47	2.58	1	1
1:A:259:LEU:H	1:A:260:PRO:HD3	0.47	1.69	2	1
1:A:528:ILE:HG22	1:A:528:ILE:O	0.47	2.09	2	1
1:B:275:ILE:HG22	1:B:277:THR:N	0.47	2.24	2	1
1:B:523:PHE:CD1	1:B:524:SER:CA	0.47	2.97	2	1
1:B:523:PHE:HD1	1:B:524:SER:CA	0.47	2.21	2	1
1:A:22:ASP:CG	1:A:145:LYS:NZ	0.47	2.73	1	1
1:A:136:ARG:HH22	1:A:167:GLU:CD	0.47	2.18	1	1
1:B:27:ASP:OD1	1:B:27:ASP:N	0.47	2.48	2	2
1:B:314:PHE:CG	1:B:376:ALA:HA	0.47	2.37	1	2
1:B:339:ASP:OD2	1:B:465:ARG:NH2	0.47	2.47	1	2
1:B:501:MET:HE1	1:B:505:LEU:HD23	0.47	1.85	1	1
1:B:278:VAL:CG1	1:B:279:ARG:N	0.47	2.78	2	1
1:A:150:SER:HA	1:A:172:ASN:ND2	0.47	2.25	1	1
1:A:296:ARG:NE	1:A:298:GLU:OE2	0.47	2.45	1	1
1:B:524:SER:O	1:B:525:MET:HG3	0.47	2.09	1	1
1:A:49:LYS:O	1:A:50:ALA:C	0.47	2.57	1	2
1:A:90:ILE:HG13	1:A:91:ALA:N	0.47	2.25	1	2
1:A:388:ILE:C	1:A:388:ILE:CD1	0.47	2.85	1	2
1:B:49:LYS:O	1:B:50:ALA:C	0.46	2.57	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:298:GLU:C	1:B:301:PHE:CD1	0.46	2.86	1	1
1:B:358:ARG:H	1:B:361:ARG:HE	0.46	1.53	1	2
1:A:139:ARG:NH2	1:A:145:LYS:O	0.46	2.48	2	1
1:A:130:VAL:CG1	1:A:131:ARG:N	0.46	2.79	2	2
1:A:132:ASP:OD2	1:A:166:SER:OG	0.46	2.32	1	1
1:A:163:LEU:C	1:A:164:THR:HG23	0.46	2.31	1	1
1:B:5:ILE:O	1:B:6:LEU:O	0.46	2.34	1	2
1:B:57:ILE:CG2	1:B:58:LYS:N	0.46	2.78	2	2
1:B:150:SER:HA	1:B:172:ASN:ND2	0.46	2.26	1	1
1:A:27:ASP:OD1	1:A:27:ASP:N	0.46	2.49	2	1
1:A:27:ASP:N	1:A:27:ASP:OD1	0.46	2.48	1	1
1:A:179:PHE:O	1:A:201:ALA:HB1	0.46	2.11	1	2
1:A:459:TYR:O	1:B:459:TYR:HB3	0.46	2.10	1	2
1:A:301:PHE:CD2	1:A:342:LEU:CD2	0.46	2.96	2	1
1:B:256:LEU:O	1:B:257:LYS:C	0.46	2.59	2	1
1:A:5:ILE:O	1:A:6:LEU:O	0.46	2.34	1	2
1:A:22:ASP:OD2	1:A:145:LYS:NZ	0.46	2.48	1	1
1:A:158:LEU:O	1:A:180:ILE:HG23	0.46	2.10	1	2
1:A:221:ASP:C	1:A:223:VAL:H	0.46	2.19	1	2
1:B:314:PHE:CE1	1:B:375:ARG:C	0.46	2.93	1	2
1:A:57:ILE:CG2	1:A:58:LYS:N	0.46	2.78	1	2
1:B:22:ASP:OD2	1:B:145:LYS:NZ	0.46	2.49	1	1
1:B:511:ALA:CB	1:B:515:LEU:CD1	0.46	2.90	1	1
1:A:68:GLU:OE1	1:A:68:GLU:N	0.46	2.41	1	2
1:A:332:ARG:CG	1:A:332:ARG:HH11	0.46	2.24	1	2
1:B:86:GLU:O	1:B:90:ILE:CG2	0.46	2.61	1	2
1:B:129:ASP:HA	1:B:165:PRO:HG2	0.46	1.86	1	1
1:A:133:ILE:HG23	1:A:134:GLY:N	0.46	2.26	2	2
1:A:262:ILE:HG23	1:A:262:ILE:O	0.46	2.11	2	2
1:B:8:SER:HB3	1:B:199:LEU:O	0.46	2.11	1	1
1:B:133:ILE:HG23	1:B:134:GLY:N	0.46	2.26	2	2
1:A:271:VAL:CG1	1:A:523:PHE:CD2	0.46	2.98	2	1
1:B:189:GLN:CD	1:B:189:GLN:C	0.46	2.84	2	1
1:B:523:PHE:CZ	1:B:525:MET:HE2	0.46	2.46	2	1
1:A:132:ASP:CG	1:A:136:ARG:NH1	0.46	2.74	1	2
1:B:179:PHE:O	1:B:201:ALA:HB1	0.46	2.10	1	2
1:B:186:ARG:C	1:B:188:SER:H	0.46	2.19	2	2
1:B:221:ASP:C	1:B:223:VAL:H	0.46	2.19	1	2
1:A:525:MET:HE3	1:A:529:SER:OG	0.46	2.10	2	1
1:B:248:SER:O	1:B:252:GLU:CD	0.46	2.59	2	1
1:B:269:VAL:HG12	1:B:270:GLU:O	0.46	2.10	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:276:GLY:C	1:A:277:THR:CG2	0.45	2.89	1	1
1:A:314:PHE:CE1	1:A:375:ARG:C	0.45	2.93	1	2
1:A:314:PHE:CE2	1:A:376:ALA:HA	0.45	2.40	1	2
1:A:259:LEU:H	1:A:260:PRO:CD	0.45	2.21	2	1
1:A:292:VAL:HG22	1:A:329:VAL:HA	0.45	1.88	1	1
1:B:276:GLY:C	1:B:277:THR:CG2	0.45	2.90	1	1
1:B:263:THR:CG2	1:B:516:LEU:HD11	0.45	2.41	2	1
1:A:204:GLY:O	1:A:205:THR:C	0.45	2.59	1	2
1:A:148:ASP:OD2	1:A:150:SER:OG	0.45	2.34	2	1
1:B:255:LYS:C	1:B:257:LYS:H	0.45	2.18	2	1
1:A:314:PHE:HE1	1:A:379:ARG:CB	0.45	2.16	1	2
1:A:367:ARG:O	1:A:368:GLU:C	0.45	2.60	1	2
1:B:456:LEU:HD13	1:B:484:LEU:CD2	0.45	2.30	1	2
1:A:86:GLU:O	1:A:90:ILE:CG2	0.45	2.61	1	2
1:A:257:LYS:C	1:A:258:ASP:CG	0.45	2.85	1	1
1:A:438:ILE:CG2	1:A:438:ILE:O	0.45	2.64	1	2
1:A:468:ASP:OD1	1:A:469:MET:SD	0.45	2.74	1	2
1:B:22:ASP:CG	1:B:145:LYS:NZ	0.45	2.74	1	1
1:B:204:GLY:O	1:B:205:THR:C	0.45	2.60	1	2
1:B:468:ASP:OD1	1:B:469:MET:SD	0.45	2.74	1	2
1:A:248:SER:O	1:A:252:GLU:CD	0.45	2.59	2	1
1:A:269:VAL:HG12	1:A:270:GLU:O	0.45	2.11	2	1
1:B:275:ILE:HG23	1:B:280:ASP:HB3	0.45	1.88	2	1
1:A:265:ASP:CG	1:A:542:PHE:H	0.45	2.18	1	1
1:A:333:THR:CG2	1:A:334:MET:H	0.45	2.25	1	2
1:B:132:ASP:CG	1:B:136:ARG:NH1	0.45	2.75	2	2
1:B:168:THR:CG2	1:B:190:THR:HG22	0.45	2.42	1	1
1:B:221:ASP:OD2	1:B:224:ASN:N	0.45	2.50	1	2
1:B:332:ARG:HH11	1:B:332:ARG:CG	0.45	2.24	1	2
1:B:525:MET:HE1	1:B:533:ILE:CG1	0.45	2.42	1	1
1:A:21:GLU:OE1	1:A:21:GLU:O	0.45	2.34	2	1
1:A:189:GLN:C	1:A:189:GLN:CD	0.45	2.84	2	1
1:A:8:SER:HB3	1:A:199:LEU:O	0.45	2.11	1	1
1:B:367:ARG:O	1:B:368:GLU:C	0.45	2.60	1	2
1:B:21:GLU:C	1:B:21:GLU:OE1	0.45	2.60	2	1
1:B:44:LEU:HD13	1:B:44:LEU:O	0.45	2.12	2	2
1:B:54:LEU:O	1:B:57:ILE:HG22	0.45	2.12	1	2
1:B:314:PHE:HE1	1:B:375:ARG:O	0.45	1.94	1	2
1:A:256:LEU:O	1:A:257:LYS:C	0.45	2.58	2	1
1:B:525:MET:HE3	1:B:529:SER:OG	0.45	2.10	2	1
1:A:507:GLY:N	1:A:525:MET:HG2	0.45	2.27	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:262:ILE:O	1:B:262:ILE:HG23	0.45	2.11	2	2
1:B:507:GLY:N	1:B:525:MET:HG2	0.45	2.27	1	1
1:B:21:GLU:OE1	1:B:21:GLU:O	0.45	2.35	2	1
1:A:5:ILE:CG2	1:A:203:VAL:HG12	0.44	2.43	2	2
1:A:180:ILE:HD11	1:A:208:VAL:HG11	0.44	1.89	1	2
1:A:186:ARG:C	1:A:188:SER:H	0.44	2.20	2	2
1:A:369:ILE:O	1:A:372:ASP:OD2	0.44	2.35	1	2
1:A:525:MET:HE1	1:A:533:ILE:CG1	0.44	2.42	1	1
1:A:556:PRO:O	1:B:396:VAL:CG2	0.44	2.65	1	2
1:B:5:ILE:CG2	1:B:203:VAL:HG12	0.44	2.43	1	2
1:B:148:ASP:OD2	1:B:150:SER:OG	0.44	2.35	2	1
1:B:295:TYR:OH	1:B:320:VAL:CG2	0.44	2.62	2	1
1:A:259:LEU:N	1:A:259:LEU:CD2	0.44	2.76	1	1
1:A:358:ARG:H	1:A:361:ARG:HE	0.44	1.54	1	2
1:B:259:LEU:N	1:B:259:LEU:CD1	0.44	2.63	1	1
1:A:263:THR:CG2	1:A:516:LEU:HD11	0.44	2.42	2	1
1:B:139:ARG:NH2	1:B:145:LYS:O	0.44	2.51	2	1
1:B:275:ILE:HG12	1:B:280:ASP:HB3	0.44	1.89	2	1
1:B:301:PHE:CD2	1:B:342:LEU:CD2	0.44	2.96	2	1
1:B:163:LEU:C	1:B:164:THR:HG23	0.44	2.31	1	1
1:B:292:VAL:HG22	1:B:329:VAL:HA	0.44	1.88	1	1
1:B:369:ILE:O	1:B:372:ASP:OD2	0.44	2.35	1	2
1:B:484:LEU:O	1:B:488:VAL:HG23	0.44	2.12	1	2
1:A:172:ASN:O	1:A:176:VAL:HG23	0.44	2.13	2	1
1:A:55:GLU:C	1:A:55:GLU:CD	0.44	2.86	1	2
1:B:345:MET:O	1:B:346:ASN:CG	0.44	2.60	1	2
1:A:21:GLU:OE1	1:A:21:GLU:C	0.44	2.60	2	1
1:B:271:VAL:CG1	1:B:523:PHE:CD2	0.44	2.98	2	1
1:A:221:ASP:CG	1:A:222:ALA:N	0.44	2.75	2	2
1:A:305:ASP:O	1:A:344:TYR:CE1	0.44	2.71	2	2
1:A:484:LEU:O	1:A:488:VAL:HG23	0.44	2.12	1	2
1:B:138:LEU:O	1:B:141:ILE:CG2	0.44	2.66	1	2
1:A:525:MET:CE	1:A:529:SER:OG	0.44	2.66	2	1
1:B:55:GLU:CD	1:B:55:GLU:C	0.44	2.86	2	2
1:B:277:THR:O	1:B:279:ARG:N	0.44	2.50	1	1
1:B:282:GLU:N	1:B:282:GLU:OE1	0.44	2.47	1	1
1:B:305:ASP:O	1:B:344:TYR:CE1	0.44	2.71	2	2
1:B:332:ARG:CG	1:B:332:ARG:NH1	0.44	2.80	1	2
1:B:172:ASN:O	1:B:176:VAL:HG23	0.44	2.13	2	1
1:A:168:THR:HG23	1:A:190:THR:HG22	0.44	1.90	1	1
1:A:345:MET:O	1:A:346:ASN:CG	0.44	2.60	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:467:ASN:C	1:A:467:ASN:HD22	0.44	2.21	1	2
1:B:171:LEU:HD21	1:B:179:PHE:HE1	0.44	1.68	1	1
1:A:44:LEU:HD13	1:A:44:LEU:O	0.44	2.13	2	2
1:A:54:LEU:O	1:A:57:ILE:HG22	0.44	2.12	1	2
1:B:438:ILE:CG2	1:B:438:ILE:O	0.44	2.63	1	2
1:A:107:VAL:CG1	1:A:108:ILE:H	0.44	2.25	2	2
1:A:351:GLU:OE1	1:A:351:GLU:C	0.44	2.61	1	2
1:A:352:ASN:ND2	1:B:352:ASN:OD1	0.44	2.51	1	2
1:B:333:THR:CG2	1:B:334:MET:H	0.44	2.25	1	2
1:A:277:THR:O	1:A:279:ARG:N	0.43	2.51	1	1
1:A:332:ARG:CG	1:A:332:ARG:NH1	0.43	2.81	1	2
1:B:221:ASP:CG	1:B:222:ALA:N	0.43	2.75	1	2
1:A:92:LEU:O	1:A:96:LYS:N	0.43	2.50	1	2
1:A:138:LEU:O	1:A:141:ILE:CG2	0.43	2.66	2	2
1:A:272:CYS:HG	1:A:291:GLY:C	0.43	2.15	1	1
1:A:310:GLU:O	1:A:314:PHE:CD2	0.43	2.71	1	2
1:A:558:THR:O	1:A:559:ASP:C	0.43	2.62	1	2
1:B:22:ASP:O	1:B:23:GLU:C	0.43	2.60	1	1
1:B:259:LEU:O	1:B:260:PRO:O	0.43	2.36	2	1
1:A:182:ASP:O	1:A:183:ALA:O	0.43	2.37	2	2
1:A:431:GLU:OE1	1:A:431:GLU:C	0.43	2.61	1	2
1:A:507:GLY:HA2	1:A:525:MET:HE3	0.43	1.90	1	1
1:B:198:GLU:OE2	1:B:250:LYS:NZ	0.43	2.49	1	1
1:A:523:PHE:CZ	1:A:525:MET:HE2	0.43	2.48	2	1
1:A:351:GLU:OE2	1:B:464:ASP:OD1	0.43	2.36	1	2
1:A:386:LEU:HD12	1:A:387:ARG:O	0.43	2.10	1	2
1:B:381:SER:CB	1:B:386:LEU:HD23	0.43	2.43	1	2
1:B:467:ASN:C	1:B:467:ASN:HD22	0.43	2.21	1	2
1:A:171:LEU:HD21	1:A:179:PHE:HE1	0.43	1.68	1	1
1:B:310:GLU:O	1:B:314:PHE:CD2	0.43	2.72	1	2
1:A:125:GLU:OE1	1:A:192:ILE:CD1	0.43	2.66	1	1
1:A:221:ASP:OD2	1:A:224:ASN:N	0.43	2.51	2	2
1:B:525:MET:CE	1:B:529:SER:OG	0.43	2.67	2	1
1:A:68:GLU:HG2	1:A:69:LYS:N	0.43	2.29	2	2
1:A:396:VAL:CG2	1:B:556:PRO:O	0.43	2.66	1	2
1:B:85:LEU:HD23	1:B:85:LEU:C	0.43	2.39	1	2
1:B:107:VAL:CG1	1:B:108:ILE:H	0.43	2.25	1	2
1:B:351:GLU:C	1:B:351:GLU:OE1	0.43	2.61	1	2
1:B:381:SER:OG	1:B:386:LEU:CD2	0.43	2.67	1	2
1:A:275:ILE:HG22	1:A:277:THR:N	0.43	2.25	2	1
1:B:274:ASN:ND2	1:B:274:ASN:C	0.43	2.75	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:182:ASP:O	1:B:183:ALA:O	0.43	2.37	2	2
1:B:314:PHE:HE1	1:B:379:ARG:CB	0.43	2.16	1	2
1:B:547:VAL:O	1:B:551:GLN:HG3	0.43	2.14	1	2
1:A:262:ILE:O	1:A:262:ILE:CG2	0.43	2.66	2	1
1:A:255:LYS:O	1:A:256:LEU:C	0.43	2.62	1	1
1:A:310:GLU:CD	1:A:310:GLU:N	0.43	2.76	1	2
1:B:138:LEU:O	1:B:141:ILE:HG22	0.43	2.14	1	2
1:A:275:ILE:HG12	1:A:280:ASP:HB3	0.43	1.89	2	1
1:A:8:SER:CB	1:A:199:LEU:O	0.42	2.67	2	2
1:B:68:GLU:HG2	1:B:69:LYS:N	0.42	2.29	2	2
1:B:297:THR:OG1	1:B:317:TYR:OH	0.42	2.27	1	1
1:B:333:THR:CG2	1:B:334:MET:N	0.42	2.82	1	2
1:A:176:VAL:CG1	1:A:179:PHE:CE1	0.42	2.93	2	1
1:B:262:ILE:O	1:B:262:ILE:CG2	0.42	2.66	2	1
1:A:202:ILE:HD12	1:A:205:THR:CG2	0.42	2.44	1	1
1:A:441:HIS:CE1	1:B:556:PRO:HB3	0.42	2.48	1	2
1:B:202:ILE:HD12	1:B:205:THR:CG2	0.42	2.43	1	1
1:B:259:LEU:N	1:B:259:LEU:CD2	0.42	2.78	1	1
1:A:271:VAL:HG12	1:A:523:PHE:HD2	0.42	1.71	2	1
1:A:32:SER:OG	1:A:33:ALA:N	0.42	2.52	2	2
1:A:85:LEU:C	1:A:85:LEU:HD23	0.42	2.39	1	2
1:B:32:SER:OG	1:B:33:ALA:N	0.42	2.52	2	2
1:B:130:VAL:CG1	1:B:131:ARG:N	0.42	2.82	2	2
1:B:507:GLY:CA	1:B:525:MET:CG	0.42	2.97	1	2
1:A:432:THR:C	1:A:456:LEU:HD21	0.42	2.39	1	2
1:B:8:SER:CB	1:B:199:LEU:O	0.42	2.67	2	2
1:B:186:ARG:C	1:B:188:SER:N	0.42	2.76	2	2
1:B:431:GLU:OE1	1:B:431:GLU:C	0.42	2.61	1	2
1:B:456:LEU:O	1:B:460:THR:OG1	0.42	2.31	1	2
1:A:259:LEU:O	1:A:260:PRO:O	0.42	2.37	2	1
1:A:181:THR:O	1:A:203:VAL:C	0.42	2.63	1	2
1:A:333:THR:CG2	1:A:334:MET:N	0.42	2.82	1	2
1:A:381:SER:OG	1:A:386:LEU:CD2	0.42	2.68	1	2
1:A:393:ILE:O	1:A:432:THR:OG1	0.42	2.36	1	2
1:B:181:THR:O	1:B:203:VAL:C	0.42	2.63	1	2
1:A:186:ARG:C	1:A:188:SER:N	0.42	2.76	1	2
1:A:484:LEU:C	1:A:484:LEU:CD2	0.42	2.90	1	2
1:B:90:ILE:CG1	1:B:91:ALA:N	0.42	2.83	2	2
1:B:372:ASP:OD1	1:B:372:ASP:C	0.42	2.63	1	2
1:B:506:ALA:O	1:B:525:MET:SD	0.42	2.78	1	1
1:B:507:GLY:N	1:B:525:MET:CG	0.42	2.82	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:221:ASP:OD1	1:A:226:GLN:N	0.42	2.52	1	2
1:A:297:THR:CG2	1:A:334:MET:HA	0.42	2.45	1	1
1:A:371:ARG:NH1	1:A:375:ARG:NH1	0.42	2.67	1	2
1:A:438:ILE:HG12	1:B:480:SER:OG	0.42	2.14	1	2
1:A:506:ALA:O	1:A:525:MET:SD	0.42	2.78	1	1
1:A:501:MET:SD	1:A:505:LEU:HB3	0.42	2.55	2	1
1:A:547:VAL:O	1:A:551:GLN:HG3	0.42	2.14	1	2
1:B:274:ASN:C	1:B:274:ASN:ND2	0.42	2.78	1	1
1:B:310:GLU:CD	1:B:310:GLU:N	0.42	2.77	1	2
1:B:484:LEU:C	1:B:484:LEU:CD2	0.42	2.90	1	2
1:B:221:ASP:OD1	1:B:226:GLN:N	0.42	2.52	2	1
1:A:22:ASP:O	1:A:23:GLU:C	0.42	2.62	1	1
1:A:464:ASP:OD2	1:B:351:GLU:OE2	0.42	2.38	1	2
1:A:214:ASN:OD1	1:A:214:ASN:O	0.42	2.38	1	2
1:A:550:GLU:O	1:A:551:GLN:C	0.42	2.62	1	2
1:A:240:ARG:O	1:A:243:GLN:HG3	0.42	2.15	2	1
1:A:274:ASN:ND2	1:A:274:ASN:C	0.42	2.75	2	1
1:A:355:LEU:HD22	1:B:462:ALA:HA	0.41	1.91	1	2
1:A:507:GLY:CA	1:A:525:MET:CG	0.41	2.97	1	2
1:B:214:ASN:OD1	1:B:214:ASN:O	0.41	2.38	2	2
1:A:248:SER:O	1:A:252:GLU:OE2	0.41	2.37	2	1
1:B:276:GLY:C	1:B:277:THR:HG23	0.41	2.40	2	1
1:A:152:ILE:O	1:A:175:LYS:NZ	0.41	2.34	1	1
1:A:280:ASP:N	1:A:280:ASP:OD1	0.41	2.50	1	1
1:A:282:GLU:OE1	1:A:282:GLU:N	0.41	2.53	1	1
1:A:301:PHE:CG	1:A:342:LEU:CD2	0.41	2.99	1	2
1:A:525:MET:HE3	1:A:529:SER:HB2	0.41	1.91	1	1
1:B:226:GLN:NE2	1:B:228:TYR:CZ	0.41	2.88	1	2
1:B:507:GLY:HA2	1:B:525:MET:HE3	0.41	1.90	1	1
1:B:301:PHE:CD2	1:B:342:LEU:HD11	0.41	2.50	2	1
1:B:125:GLU:OE1	1:B:192:ILE:CD1	0.41	2.68	1	1
1:B:136:ARG:NH1	1:B:166:SER:HB2	0.41	2.31	1	1
1:B:297:THR:CG2	1:B:334:MET:HA	0.41	2.45	1	1
1:B:558:THR:O	1:B:559:ASP:C	0.41	2.61	1	2
1:B:501:MET:SD	1:B:505:LEU:HB3	0.41	2.55	2	1
1:A:120:ASP:OD1	1:A:121:GLU:N	0.41	2.54	2	2
1:B:352:ASN:O	1:B:353:PRO:C	0.41	2.63	1	2
1:B:392:MET:HE1	1:B:459:TYR:OH	0.41	2.14	1	2
1:B:549:ALA:O	1:B:550:GLU:C	0.41	2.63	1	2
1:B:255:LYS:C	1:B:257:LYS:N	0.41	2.78	2	1
1:A:226:GLN:NE2	1:A:228:TYR:CZ	0.41	2.88	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:271:VAL:HB	1:A:523:PHE:CD2	0.41	2.50	1	1
1:A:309:THR:O	1:A:313:GLN:HG2	0.41	2.16	1	2
1:B:332:ARG:CZ	1:B:429:MET:SD	0.41	3.08	1	2
1:B:432:THR:C	1:B:456:LEU:HD21	0.41	2.40	1	2
1:B:525:MET:HE3	1:B:529:SER:HB2	0.41	1.93	1	1
1:A:276:GLY:C	1:A:277:THR:HG23	0.41	2.41	2	1
1:A:138:LEU:O	1:A:141:ILE:HG22	0.41	2.15	2	2
1:B:262:ILE:HD11	1:B:266:GLY:HA2	0.41	1.91	1	1
1:B:529:SER:O	1:B:533:ILE:HG12	0.41	2.16	1	1
1:B:295:TYR:HB3	1:B:331:VAL:HA	0.41	1.93	2	1
1:A:332:ARG:CZ	1:A:429:MET:SD	0.41	3.08	1	2
1:A:507:GLY:N	1:A:525:MET:CG	0.41	2.83	1	1
1:B:405:GLU:O	1:B:406:ILE:C	0.41	2.62	1	2
1:B:520:LEU:CD2	1:B:522:GLU:O	0.41	2.68	1	1
1:A:295:TYR:HB3	1:A:331:VAL:HA	0.41	1.93	2	1
1:B:536:ILE:O	1:B:539:ASN:OD1	0.41	2.38	2	1
1:A:136:ARG:NH1	1:A:166:SER:HB2	0.41	2.31	1	1
1:A:136:ARG:CZ	1:A:166:SER:HB2	0.41	2.46	1	1
1:A:296:ARG:NH2	1:A:298:GLU:OE2	0.41	2.54	1	1
1:B:388:ILE:O	1:B:388:ILE:HG13	0.41	2.15	1	2
1:A:11:ILE:CG1	1:A:243:GLN:CB	0.41	2.74	2	1
1:A:221:ASP:CA	1:A:239:MET:HE2	0.41	2.30	2	1
1:A:262:ILE:HD11	1:A:266:GLY:HA2	0.41	1.91	1	1
1:A:301:PHE:CD2	1:A:342:LEU:HD11	0.41	2.50	2	2
1:A:392:MET:HE1	1:A:459:TYR:OH	0.41	2.15	1	2
1:A:456:LEU:HD23	1:A:456:LEU:HA	0.41	1.79	1	2
1:A:470:ILE:O	1:A:471:SER:C	0.41	2.64	1	2
1:B:92:LEU:O	1:B:96:LYS:N	0.41	2.50	1	1
1:B:296:ARG:NH2	1:B:298:GLU:OE2	0.41	2.53	1	1
1:B:179:PHE:CD2	1:B:199:LEU:HD11	0.41	2.51	2	1
1:B:189:GLN:C	1:B:189:GLN:NE2	0.41	2.79	2	1
1:B:248:SER:O	1:B:252:GLU:OE2	0.41	2.38	2	1
1:B:43:PHE:CD1	1:B:100:ALA:HB1	0.41	2.51	1	1
1:B:336:ILE:C	1:B:336:ILE:CD1	0.41	2.92	1	2
1:A:536:ILE:O	1:A:539:ASN:OD1	0.41	2.38	2	1
1:B:176:VAL:HG11	1:B:179:PHE:CD1	0.41	2.49	2	1
1:A:352:ASN:O	1:A:353:PRO:C	0.40	2.63	1	2
1:B:136:ARG:CZ	1:B:166:SER:HB2	0.40	2.46	1	1
1:B:168:THR:HG23	1:B:190:THR:HG22	0.40	1.93	1	1
1:A:176:VAL:HG11	1:A:179:PHE:CD1	0.40	2.49	2	1
1:B:265:ASP:OD2	1:B:541:ASN:OD1	0.40	2.39	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:PHE:CZ	1:A:100:ALA:HB1	0.40	2.51	2	1
1:A:129:ASP:OD2	1:A:165:PRO:CB	0.40	2.69	2	1
1:A:43:PHE:CE2	1:A:100:ALA:C	0.40	3.00	1	1
1:A:520:LEU:CD2	1:A:522:GLU:O	0.40	2.69	1	1
1:A:183:ALA:HB3	1:A:203:VAL:CG2	0.40	2.46	2	1
1:B:108:ILE:CD1	1:B:109:GLU:N	0.40	2.78	2	1
1:B:129:ASP:OD2	1:B:165:PRO:CB	0.40	2.70	2	1
1:A:499:THR:O	1:A:499:THR:OG1	0.40	2.40	1	1
1:A:179:PHE:CE2	1:A:199:LEU:CD1	0.40	3.05	2	1
1:A:189:GLN:C	1:A:189:GLN:NE2	0.40	2.80	2	1
1:B:298:GLU:C	1:B:301:PHE:CZ	0.40	2.97	2	1
1:A:331:VAL:N	1:A:389:MET:HE1	0.40	2.31	1	2
1:A:372:ASP:OD1	1:A:372:ASP:C	0.40	2.63	1	2
1:A:405:GLU:O	1:A:406:ILE:C	0.40	2.62	1	2
1:B:180:ILE:HD11	1:B:208:VAL:HG11	0.40	1.93	1	1
1:B:271:VAL:HB	1:B:523:PHE:CD2	0.40	2.50	1	1
1:B:363:ALA:HB1	1:B:370:LEU:HB2	0.40	1.94	1	2
1:B:393:ILE:O	1:B:393:ILE:CG2	0.40	2.68	1	2
1:A:179:PHE:CD2	1:A:199:LEU:HD11	0.40	2.51	2	1
1:B:43:PHE:CZ	1:B:100:ALA:HB1	0.40	2.51	2	1
1:B:541:ASN:N	1:B:541:ASN:ND2	0.40	2.70	2	1

6.3 Torsion angles

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	571/573 (100%)	535±1 (94±0%)	27±1 (5±0%)	9±0 (2±0%)	10	55
1	B	571/573 (100%)	536±0 (94±0%)	26±0 (5±0%)	9±1 (2±0%)	10	55
All	All	2284/2292 (100%)	2141 (94%)	107 (5%)	36 (2%)	10	55

All 22 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	6	LEU	2
1	A	148	ASP	2
1	A	183	ALA	2
1	A	232	THR	2
1	A	256	LEU	2
1	A	261	ALA	2
1	A	278	VAL	2
1	B	6	LEU	2
1	B	148	ASP	2
1	B	183	ALA	2
1	B	232	THR	2
1	B	255	LYS	2
1	B	261	ALA	2
1	B	278	VAL	2
1	A	254	ALA	1
1	A	257	LYS	1
1	B	254	ALA	1
1	A	259	LEU	1
1	A	260	PRO	1
1	B	256	LEU	1
1	B	259	LEU	1
1	B	260	PRO	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. 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	474/474 (100%)	396±2 (84±0%)	78±2 (16±0%)	4	39
1	B	474/474 (100%)	396±0 (83±0%)	78±0 (17±0%)	4	39
All	All	1896/1896 (100%)	1583 (83%)	313 (17%)	4	39

All 182 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	2	ILE	2
1	A	11	ILE	2
1	A	27	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	28	ARG	2
1	A	32	SER	2
1	A	43	PHE	2
1	A	44	LEU	2
1	A	57	ILE	2
1	A	65	PHE	2
1	A	70	GLU	2
1	A	77	ILE	2
1	A	101	ASP	2
1	A	107	VAL	2
1	A	129	ASP	2
1	A	130	VAL	2
1	A	142	LEU	2
1	A	180	ILE	2
1	A	181	THR	2
1	A	197	LEU	2
1	A	199	LEU	2
1	A	213	LYS	2
1	A	215	ASP	2
1	A	216	ASP	2
1	A	252	GLU	2
1	A	272	CYS	2
1	A	280	ASP	2
1	A	292	VAL	2
1	A	298	GLU	2
1	A	301	PHE	2
1	A	310	GLU	2
1	A	330	ILE	2
1	A	332	ARG	2
1	A	342	LEU	2
1	A	347	PHE	2
1	A	351	GLU	2
1	A	352	ASN	2
1	A	360	ILE	2
1	A	381	SER	2
1	A	385	LYS	2
1	A	386	LEU	2
1	A	388	ILE	2
1	A	396	VAL	2
1	A	398	GLU	2
1	A	404	LYS	2
1	A	411	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	423	SER	2
1	A	431	GLU	2
1	A	453	THR	2
1	A	458	GLN	2
1	A	470	ILE	2
1	A	474	TYR	2
1	A	480	SER	2
1	A	484	LEU	2
1	A	486	LYS	2
1	A	497	LYS	2
1	A	499	THR	2
1	A	516	LEU	2
1	A	518	MET	2
1	A	520	LEU	2
1	A	522	GLU	2
1	A	523	PHE	2
1	A	542	PHE	2
1	A	557	THR	2
1	A	561	LEU	2
1	A	573	THR	2
1	B	2	ILE	2
1	B	11	ILE	2
1	B	27	ASP	2
1	B	28	ARG	2
1	B	32	SER	2
1	B	43	PHE	2
1	B	44	LEU	2
1	B	57	ILE	2
1	B	58	LYS	2
1	B	65	PHE	2
1	B	70	GLU	2
1	B	77	ILE	2
1	B	101	ASP	2
1	B	107	VAL	2
1	B	129	ASP	2
1	B	130	VAL	2
1	B	142	LEU	2
1	B	180	ILE	2
1	B	181	THR	2
1	B	197	LEU	2
1	B	199	LEU	2
1	B	213	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	B	215	ASP	2
1	B	216	ASP	2
1	B	243	GLN	2
1	B	252	GLU	2
1	B	272	CYS	2
1	B	292	VAL	2
1	B	298	GLU	2
1	B	301	PHE	2
1	B	310	GLU	2
1	B	330	ILE	2
1	B	332	ARG	2
1	B	342	LEU	2
1	B	347	PHE	2
1	B	351	GLU	2
1	B	352	ASN	2
1	B	360	ILE	2
1	B	370	LEU	2
1	B	381	SER	2
1	B	385	LYS	2
1	B	386	LEU	2
1	B	388	ILE	2
1	B	396	VAL	2
1	B	398	GLU	2
1	B	404	LYS	2
1	B	411	GLN	2
1	B	423	SER	2
1	B	431	GLU	2
1	B	453	THR	2
1	B	458	GLN	2
1	B	470	ILE	2
1	B	474	TYR	2
1	B	480	SER	2
1	B	484	LEU	2
1	B	486	LYS	2
1	B	497	LYS	2
1	B	516	LEU	2
1	B	518	MET	2
1	B	520	LEU	2
1	B	522	GLU	2
1	B	523	PHE	2
1	B	542	PHE	2
1	B	557	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	B	561	LEU	2
1	B	573	THR	2
1	A	22	ASP	1
1	A	168	THR	1
1	A	191	SER	1
1	A	256	LEU	1
1	A	258	ASP	1
1	A	259	LEU	1
1	A	265	ASP	1
1	A	271	VAL	1
1	A	274	ASN	1
1	A	277	THR	1
1	A	302	MET	1
1	A	304	ARG	1
1	A	515	LEU	1
1	A	526	SER	1
1	A	536	ILE	1
1	B	22	ASP	1
1	B	168	THR	1
1	B	191	SER	1
1	B	259	LEU	1
1	B	265	ASP	1
1	B	271	VAL	1
1	B	274	ASN	1
1	B	277	THR	1
1	B	302	MET	1
1	B	304	ARG	1
1	B	515	LEU	1
1	B	526	SER	1
1	B	536	ILE	1
1	A	190	THR	1
1	A	202	ILE	1
1	A	243	GLN	1
1	A	269	VAL	1
1	A	296	ARG	1
1	A	329	VAL	1
1	A	512	THR	1
1	A	513	LEU	1
1	A	525	MET	1
1	A	540	THR	1
1	A	541	ASN	1
1	B	190	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	B	202	ILE	1
1	B	269	VAL	1
1	B	280	ASP	1
1	B	296	ARG	1
1	B	329	VAL	1
1	B	499	THR	1
1	B	512	THR	1
1	B	513	LEU	1
1	B	525	MET	1
1	B	540	THR	1
1	B	541	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided