



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 01:49 AM UTC

PDB ID : 2KX9 / pdb_00002kx9
Title : Solution Structure of the Enzyme I dimer Using Residual Dipolar Couplings and Small Angle X-Ray Scattering
Authors : Schwieters, C.D.; Suh, J.; Grishaev, A.; Takayama, Y.; Guirlando, R.; Clore, G.
Deposited on : 2010-04-29

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

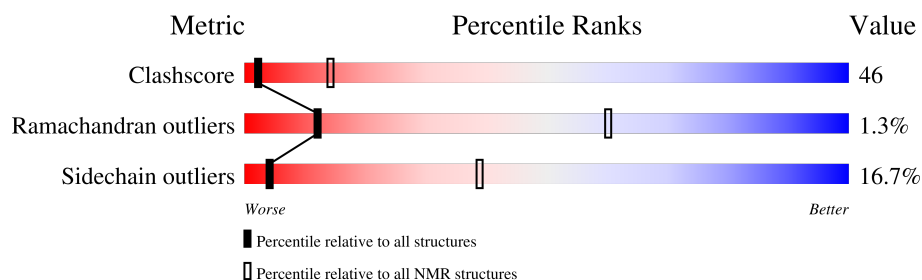
1 Overall quality at a glance

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	
1	B	573	

2 Ensemble composition and analysis ⓘ

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 17912 atoms, of which 9028 are hydrogens and 0 are deuteriums.

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

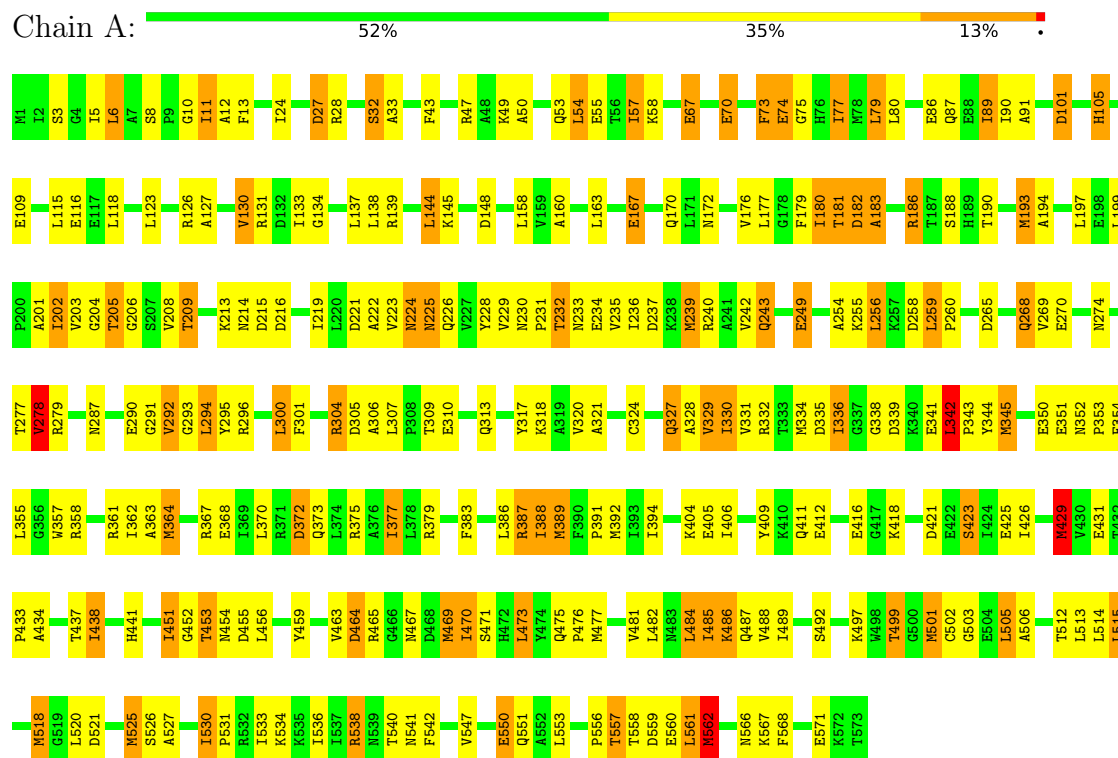
Mol	Chain	Residues	Atoms						Trace
1	A	573	Total	C	H	N	O	S	0
			8956	2790	4514	757	874	21	
1	B	573	Total	C	H	N	O	S	0
			8956	2790	4514	757	874	21	

4 Residue-property plots [i](#)

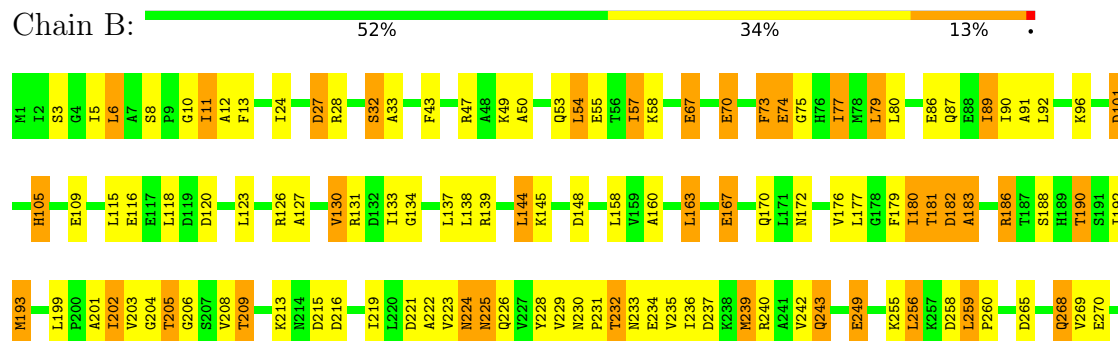
4.1 Average score per residue in the NMR ensemble

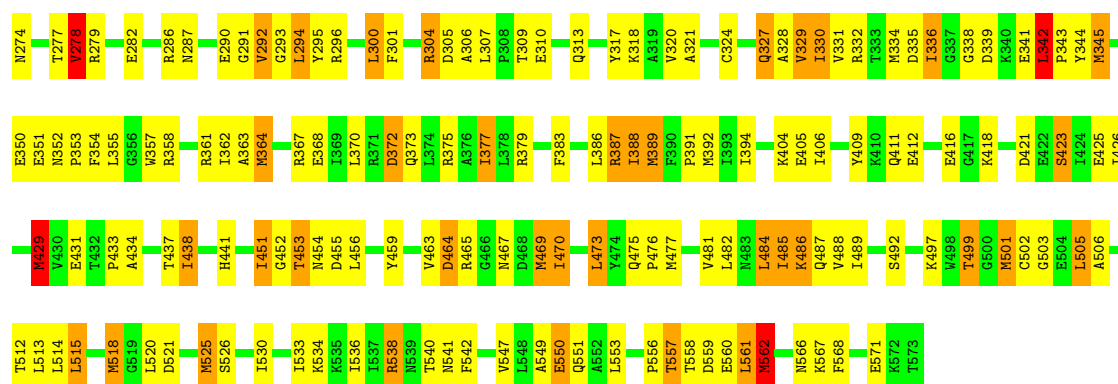
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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



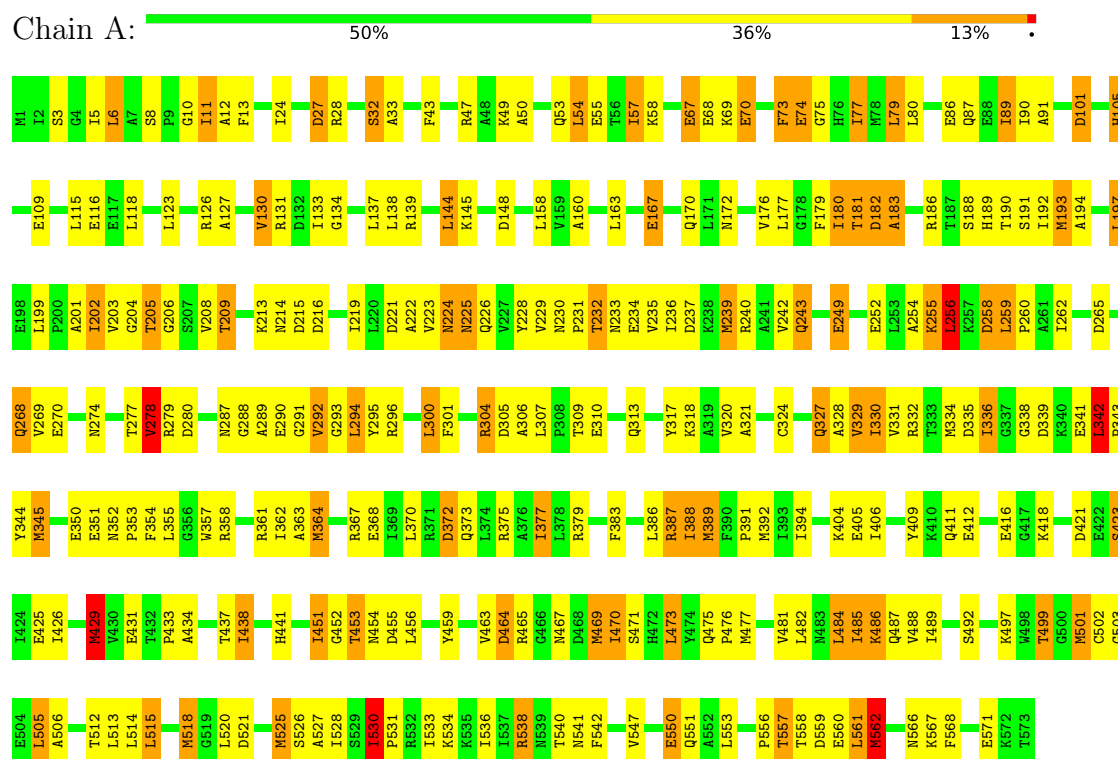


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

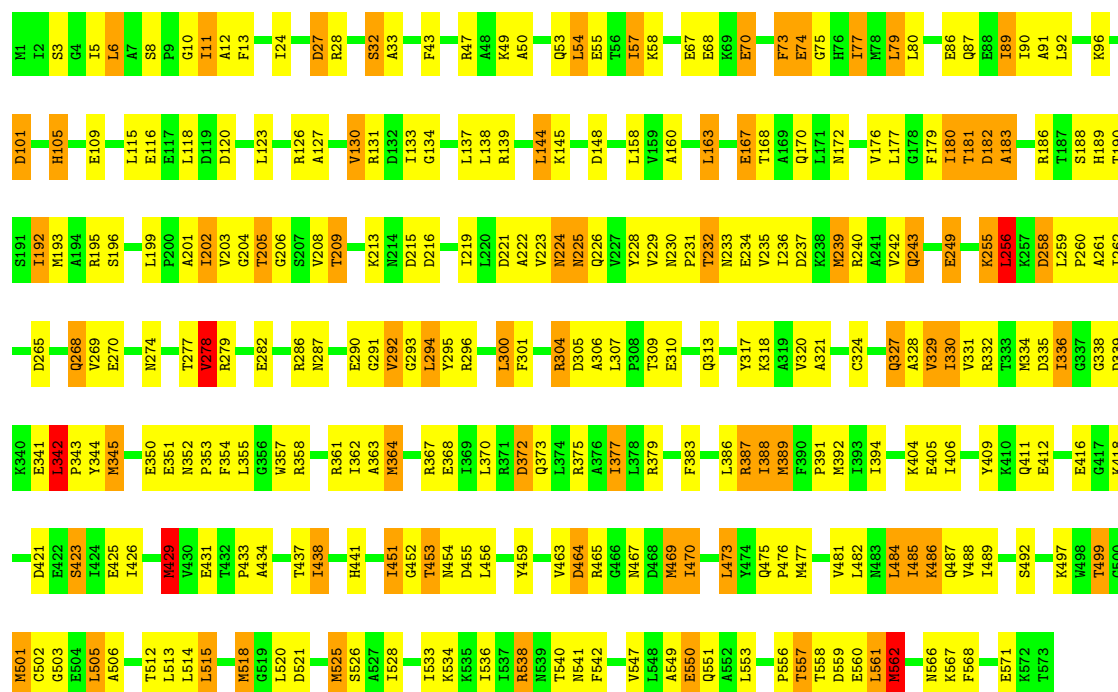
4.2.1 Score per residue for model 1

- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase



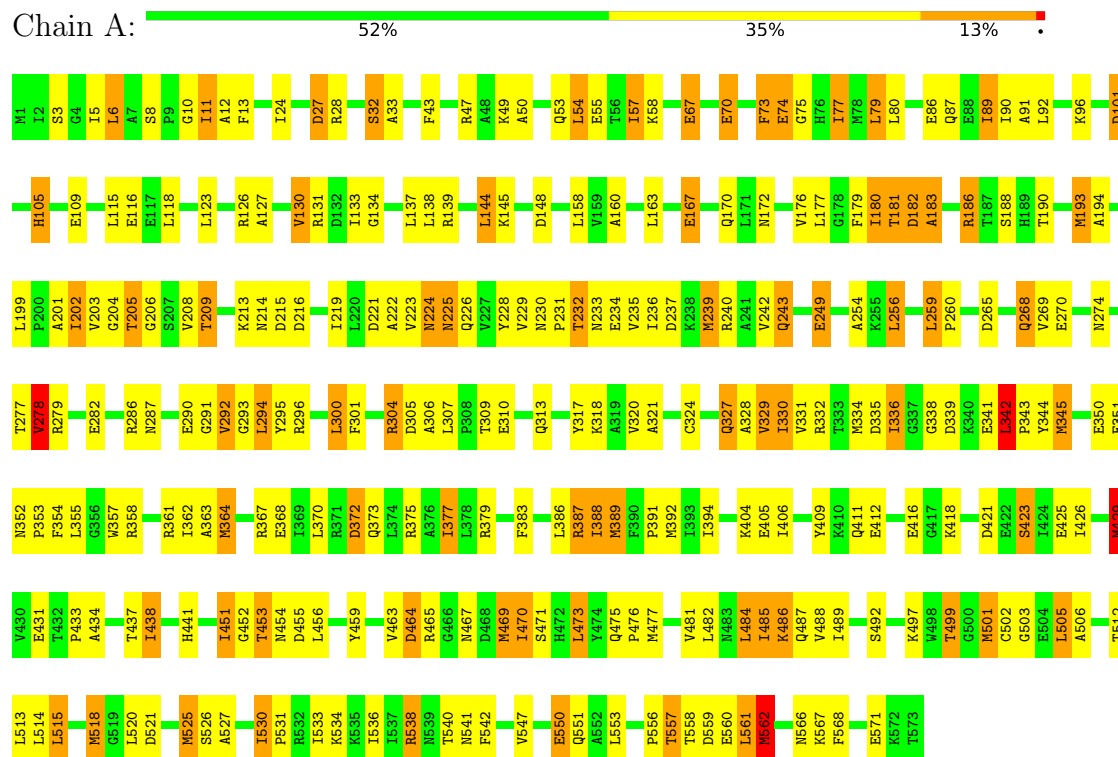
- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase





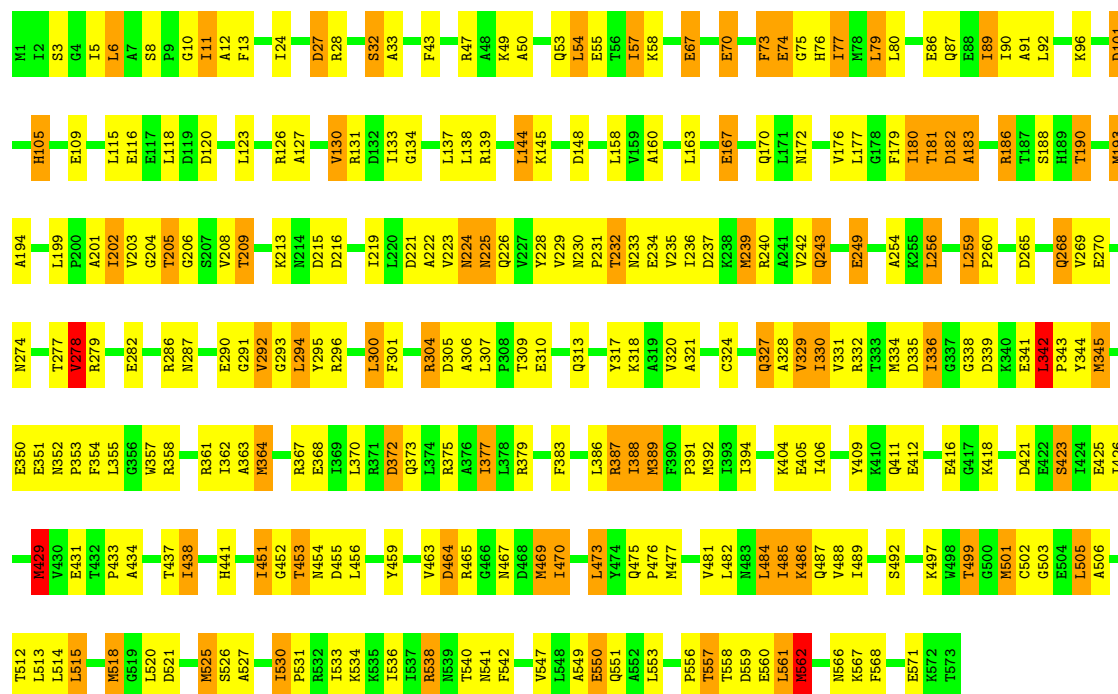
4.2.2 Score per residue for model 2

- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase



- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase

Chain B: 



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

6.1 Standard geometry

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	1.37±0.00	21±0/4495 (0.5± 0.0%)	1.17±0.00	10±0/6061 (0.2± 0.0%)
1	B	1.37±0.00	22±0/4495 (0.5± 0.0%)	1.17±0.00	9±0/6061 (0.1± 0.0%)
All	All	1.37	86/17980 (0.5%)	1.17	37/24244 (0.2%)

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	A	345	MET	SD-CE	13.99	2.14	1.79	1	2
1	B	345	MET	SD-CE	13.99	2.14	1.79	1	2
1	B	469	MET	SD-CE	13.78	2.14	1.79	1	2
1	A	469	MET	SD-CE	13.78	2.13	1.79	1	2
1	A	364	MET	SD-CE	10.61	2.06	1.79	1	2
1	B	364	MET	SD-CE	10.60	2.06	1.79	1	2
1	B	562	MET	SD-CE	8.83	2.01	1.79	1	2
1	A	562	MET	SD-CE	8.70	2.01	1.79	1	2
1	B	562	MET	CG-SD	7.56	1.99	1.80	1	2
1	A	562	MET	CG-SD	7.54	1.99	1.80	1	2
1	A	239	MET	SD-CE	7.25	1.97	1.79	2	2
1	B	239	MET	SD-CE	7.16	1.97	1.79	1	2
1	B	364	MET	CG-SD	6.82	1.97	1.80	1	2
1	A	364	MET	CG-SD	6.80	1.97	1.80	1	2
1	B	475	GLN	CA-C	-6.62	1.45	1.52	1	2
1	A	475	GLN	CA-C	-6.60	1.45	1.52	1	2
1	A	525	MET	SD-CE	6.47	1.95	1.79	1	2
1	A	345	MET	CG-SD	6.46	1.97	1.80	1	2
1	B	525	MET	SD-CE	6.45	1.95	1.79	1	2
1	B	345	MET	CG-SD	6.42	1.96	1.80	1	2
1	A	334	MET	CG-SD	6.12	1.96	1.80	1	2
1	B	501	MET	CG-SD	6.12	1.96	1.80	1	2
1	B	334	MET	CG-SD	6.12	1.96	1.80	1	2
1	A	501	MET	CG-SD	6.09	1.96	1.80	1	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	389	MET	SD-CE	5.96	1.94	1.79	1	2
1	A	389	MET	SD-CE	5.93	1.94	1.79	1	2
1	A	239	MET	CG-SD	5.80	1.95	1.80	1	2
1	B	475	GLN	C-O	-5.76	1.19	1.24	1	2
1	A	475	GLN	C-O	-5.75	1.19	1.24	1	2
1	B	239	MET	CG-SD	5.71	1.95	1.80	2	2
1	A	477	MET	SD-CE	5.50	1.93	1.79	1	2
1	B	120	ASP	N-CA	5.49	1.52	1.46	2	2
1	B	477	MET	SD-CE	5.41	1.93	1.79	1	2
1	B	429	MET	SD-CE	5.28	1.92	1.79	1	2
1	A	429	MET	SD-CE	5.23	1.92	1.79	1	2
1	B	334	MET	SD-CE	5.18	1.92	1.79	1	2
1	A	334	MET	SD-CE	5.14	1.92	1.79	1	2
1	A	525	MET	CG-SD	5.09	1.93	1.80	1	2
1	A	550	GLU	N-CA	-5.05	1.40	1.46	1	2
1	B	525	MET	CG-SD	5.05	1.93	1.80	1	2
1	A	469	MET	CG-SD	5.03	1.93	1.80	1	2
1	B	469	MET	CG-SD	5.03	1.93	1.80	1	2
1	B	550	GLU	N-CA	-5.01	1.40	1.46	1	2

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	530	ILE	N-CA-CB	8.43	117.03	110.45	1	1
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	278	VAL	CB-CA-C	-6.25	101.05	111.29	1	2
1	B	278	VAL	CB-CA-C	-6.24	101.06	111.29	1	2
1	B	487	GLN	N-CA-C	-5.79	105.11	111.82	1	2
1	A	487	GLN	N-CA-C	-5.74	105.16	111.82	1	2
1	A	224	ASN	N-CA-C	-5.36	106.42	113.17	1	2
1	B	338	GLY	N-CA-C	-5.35	100.51	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	-5.29	106.50	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	B	73	PHE	CA-CB-CG	-5.15	108.65	113.80	1	2
1	A	73	PHE	CA-CB-CG	-5.09	108.71	113.80	2	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
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.

There are no planarity outliers.

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	4442	4514	4506	420±0
1	B	4442	4514	4506	416±5
All	All	17768	18056	18024	1635

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 46.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:562:MET:SD	1:B:562:MET:CE	1.48	2.01	1	2
1:B:364:MET:SD	1:B:364:MET:CE	1.43	2.06	1	2
1:A:364:MET:SD	1:A:364:MET:CE	1.42	2.06	1	2
1:A:469:MET:SD	1:A:469:MET:CE	1.36	2.14	1	2
1:B:469:MET:CE	1:B:469:MET:SD	1.36	2.14	1	2
1:B:345:MET:SD	1:B:345:MET:CE	1.35	2.14	1	2
1:A:345:MET:SD	1:A:345:MET:CE	1.35	2.14	1	2
1:B:54:LEU:O	1:B:54:LEU:HD22	1.25	1.27	2	2
1:A:54:LEU:O	1:A:54:LEU:HD22	1.24	1.28	1	2
1:A:54:LEU:HD22	1:A:54:LEU:C	1.21	1.60	1	2
1:B:54:LEU:HD13	1:B:55:GLU:N	1.20	1.52	1	2
1:A:54:LEU:HD13	1:A:55:GLU:N	1.19	1.52	1	2
1:B:527:ALA:O	1:B:530:ILE:CG2	1.18	1.92	2	1
1:A:527:ALA:O	1:A:530:ILE:CG2	1.17	1.92	2	2
1:B:54:LEU:HD22	1:B:54:LEU:C	1.17	1.61	1	2
1:A:301:PHE:O	1:A:304:ARG:NE	1.14	1.79	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:301:PHE:O	1:B:304:ARG:NE	1.14	1.80	1	2
1:B:144:LEU:HD13	1:B:144:LEU:O	1.11	1.46	2	2
1:A:144:LEU:HD13	1:A:144:LEU:O	1.07	1.46	1	2
1:B:291:GLY:HA2	1:B:327:GLN:CG	1.07	1.79	1	2
1:A:291:GLY:HA2	1:A:327:GLN:CG	1.06	1.79	1	2
1:B:11:ILE:HD12	1:B:12:ALA:N	1.04	1.67	2	2
1:A:527:ALA:O	1:A:530:ILE:HG22	1.04	1.52	1	2
1:A:11:ILE:HD12	1:A:12:ALA:N	1.02	1.67	1	2
1:A:77:ILE:HD13	1:A:77:ILE:N	1.02	1.68	1	2
1:B:77:ILE:HD13	1:B:77:ILE:N	1.02	1.68	2	2
1:A:291:GLY:HA2	1:A:327:GLN:HG3	1.00	1.03	1	2
1:B:232:THR:CG2	1:B:233:ASN:H	1.00	1.69	2	2
1:A:221:ASP:HA	1:A:239:MET:CE	0.99	1.87	2	2
1:A:232:THR:CG2	1:A:233:ASN:H	0.99	1.69	2	2
1:B:291:GLY:HA2	1:B:327:GLN:HG3	0.99	1.02	1	2
1:B:221:ASP:HA	1:B:239:MET:CE	0.98	1.87	1	2
1:A:232:THR:CG2	1:A:233:ASN:N	0.98	2.26	2	2
1:A:232:THR:HG22	1:A:233:ASN:N	0.98	1.71	2	2
1:B:232:THR:HG22	1:B:233:ASN:N	0.98	1.71	2	2
1:B:232:THR:CG2	1:B:233:ASN:N	0.97	2.26	2	2
1:B:304:ARG:NE	1:B:304:ARG:O	0.96	1.97	1	2
1:A:54:LEU:C	1:A:54:LEU:CD2	0.96	2.37	1	2
1:A:304:ARG:NE	1:A:304:ARG:O	0.96	1.98	1	2
1:B:527:ALA:O	1:B:530:ILE:HG22	0.94	1.58	2	1
1:B:527:ALA:O	1:B:530:ILE:HG23	0.94	1.61	2	1
1:A:527:ALA:O	1:A:530:ILE:HG23	0.93	1.61	2	1
1:B:221:ASP:HA	1:B:239:MET:HE2	0.92	1.41	2	2
1:A:11:ILE:HG21	1:A:243:GLN:CA	0.92	1.95	1	2
1:A:484:LEU:HD23	1:A:485:ILE:N	0.92	1.80	1	2
1:B:11:ILE:HG21	1:B:243:GLN:HA	0.91	1.42	2	2
1:A:160:ALA:O	1:A:181:THR:HG22	0.91	1.65	1	2
1:B:144:LEU:C	1:B:144:LEU:HD22	0.91	1.91	1	2
1:B:54:LEU:C	1:B:54:LEU:CD2	0.91	2.37	2	2
1:B:484:LEU:HD23	1:B:485:ILE:N	0.91	1.80	1	2
1:B:11:ILE:HG21	1:B:243:GLN:CA	0.91	1.95	2	2
1:B:160:ALA:O	1:B:181:THR:HG22	0.91	1.65	1	2
1:A:481:VAL:O	1:A:485:ILE:HG23	0.90	1.66	1	2
1:A:144:LEU:C	1:A:144:LEU:HD22	0.90	1.91	1	2
1:A:221:ASP:HA	1:A:239:MET:HE2	0.89	1.41	1	2
1:A:11:ILE:HG21	1:A:243:GLN:HA	0.89	1.42	1	2
1:A:456:LEU:HD13	1:A:484:LEU:HD21	0.89	1.45	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:228:TYR:HB3	1:B:231:PRO:HG3	0.88	1.45	2	2
1:A:228:TYR:HB3	1:A:231:PRO:HG3	0.88	1.46	1	2
1:A:11:ILE:HD12	1:A:12:ALA:H	0.87	1.27	2	2
1:B:481:VAL:O	1:B:485:ILE:HG23	0.87	1.66	1	2
1:A:388:ILE:HD12	1:A:389:MET:N	0.87	1.83	1	2
1:B:456:LEU:HD13	1:B:484:LEU:HD21	0.87	1.45	1	2
1:A:180:ILE:HD11	1:A:208:VAL:HG11	0.86	1.47	2	2
1:B:225:ASN:O	1:B:225:ASN:CG	0.86	2.19	2	2
1:B:388:ILE:HD12	1:B:389:MET:N	0.86	1.86	1	2
1:A:225:ASN:CG	1:A:225:ASN:O	0.85	2.19	1	2
1:B:518:MET:SD	1:B:553:LEU:HD11	0.84	2.13	1	2
1:A:518:MET:SD	1:A:553:LEU:HD11	0.83	2.13	1	2
1:B:11:ILE:HD12	1:B:12:ALA:H	0.83	1.27	1	2
1:A:473:LEU:HD12	1:B:394:ILE:HD11	0.82	1.51	1	2
1:A:54:LEU:O	1:A:54:LEU:CD2	0.81	2.23	1	2
1:B:291:GLY:CA	1:B:327:GLN:HG3	0.81	1.98	1	2
1:A:556:PRO:HB3	1:B:441:HIS:ND1	0.81	1.89	1	2
1:B:429:MET:SD	1:B:431:GLU:HG3	0.81	2.16	1	2
1:B:77:ILE:N	1:B:77:ILE:CD1	0.81	2.44	2	2
1:A:372:ASP:C	1:A:372:ASP:OD1	0.81	2.24	1	2
1:B:180:ILE:HD11	1:B:208:VAL:HG11	0.81	1.51	2	2
1:A:77:ILE:N	1:A:77:ILE:CD1	0.80	2.43	2	2
1:A:429:MET:SD	1:A:431:GLU:HG3	0.80	2.16	1	2
1:A:330:ILE:HD12	1:A:330:ILE:C	0.80	2.02	1	2
1:A:291:GLY:CA	1:A:327:GLN:HG3	0.79	1.99	1	2
1:B:372:ASP:OD1	1:B:372:ASP:C	0.79	2.24	1	2
1:B:330:ILE:C	1:B:330:ILE:HD12	0.79	2.02	1	2
1:A:189:HIS:O	1:A:192:ILE:HG22	0.79	1.77	1	1
1:A:11:ILE:HD11	1:A:13:PHE:CZ	0.79	2.13	2	2
1:B:54:LEU:O	1:B:54:LEU:CD2	0.79	2.23	1	2
1:B:163:LEU:HB3	1:B:190:THR:HG21	0.79	1.53	1	1
1:B:11:ILE:HD11	1:B:13:PHE:CZ	0.78	2.13	1	2
1:B:482:LEU:O	1:B:485:ILE:HG12	0.78	1.79	1	2
1:B:139:ARG:HB3	1:B:144:LEU:HG	0.78	1.55	1	2
1:A:139:ARG:HB3	1:A:144:LEU:HG	0.77	1.56	2	2
1:B:13:PHE:CZ	1:B:240:ARG:HD2	0.77	2.15	1	2
1:A:13:PHE:CZ	1:A:240:ARG:HD2	0.77	2.15	2	2
1:B:54:LEU:CD1	1:B:55:GLU:N	0.76	2.44	2	2
1:A:144:LEU:O	1:A:144:LEU:CD1	0.76	2.32	1	2
1:A:464:ASP:CG	1:B:355:LEU:O	0.76	2.29	1	2
1:A:482:LEU:O	1:A:485:ILE:HG12	0.76	1.79	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:505:LEU:HD13	1:A:506:ALA:H	0.76	1.41	1	2
1:A:394:ILE:HD11	1:B:473:LEU:HD12	0.76	1.58	1	2
1:B:530:ILE:HD12	1:B:530:ILE:O	0.76	1.81	2	1
1:A:530:ILE:C	1:A:530:ILE:HD12	0.75	2.07	2	1
1:A:530:ILE:HD12	1:A:530:ILE:O	0.74	1.80	2	1
1:B:505:LEU:CD1	1:B:505:LEU:N	0.74	2.50	1	2
1:A:54:LEU:CD1	1:A:55:GLU:N	0.74	2.44	1	2
1:B:144:LEU:CD2	1:B:145:LYS:O	0.74	2.35	2	2
1:A:11:ILE:CG2	1:A:243:GLN:HA	0.74	2.13	1	2
1:A:144:LEU:CD2	1:A:145:LYS:O	0.74	2.35	1	2
1:B:144:LEU:O	1:B:144:LEU:CD1	0.74	2.32	2	2
1:A:54:LEU:HD21	1:A:77:ILE:HG13	0.74	1.60	2	2
1:B:11:ILE:CG2	1:B:243:GLN:HA	0.74	2.13	1	2
1:B:429:MET:SD	1:B:431:GLU:CG	0.74	2.76	1	2
1:A:429:MET:SD	1:A:431:GLU:CG	0.73	2.76	1	2
1:A:505:LEU:CD1	1:A:505:LEU:N	0.73	2.50	1	2
1:A:193:MET:SD	1:A:197:LEU:HD22	0.73	2.24	1	1
1:A:228:TYR:CD1	1:A:235:VAL:HG11	0.73	2.19	2	2
1:B:294:LEU:HD12	1:B:502:CYS:SG	0.73	2.23	1	2
1:B:456:LEU:HD22	1:B:484:LEU:HD11	0.73	1.60	1	2
1:B:530:ILE:HD12	1:B:530:ILE:C	0.73	2.08	2	1
1:B:228:TYR:CB	1:B:231:PRO:HG3	0.73	2.14	2	2
1:B:168:THR:CG2	1:B:193:MET:SD	0.73	2.76	1	1
1:A:228:TYR:CB	1:A:231:PRO:HG3	0.73	2.14	1	2
1:A:73:PHE:O	1:A:77:ILE:HG12	0.73	1.84	1	2
1:A:294:LEU:HD12	1:A:502:CYS:SG	0.72	2.24	1	2
1:B:202:ILE:O	1:B:202:ILE:HD13	0.72	1.84	2	2
1:A:291:GLY:CA	1:A:327:GLN:CG	0.72	2.65	1	2
1:B:505:LEU:HD13	1:B:506:ALA:H	0.72	1.42	1	2
1:A:232:THR:O	1:A:236:ILE:HG13	0.72	1.84	1	2
1:A:202:ILE:HD13	1:A:202:ILE:O	0.72	1.85	2	2
1:A:441:HIS:ND1	1:B:556:PRO:HB3	0.72	1.99	1	2
1:B:11:ILE:CD1	1:B:12:ALA:N	0.72	2.51	1	2
1:B:73:PHE:O	1:B:77:ILE:HG12	0.72	1.84	2	2
1:B:232:THR:O	1:B:236:ILE:HG13	0.72	1.84	1	2
1:B:54:LEU:HD21	1:B:77:ILE:HG13	0.71	1.61	1	2
1:B:228:TYR:CD1	1:B:235:VAL:HG11	0.71	2.19	1	2
1:A:130:VAL:O	1:A:133:ILE:HG22	0.71	1.85	2	2
1:A:530:ILE:HG23	1:A:531:PRO:HD3	0.71	1.61	1	2
1:B:130:VAL:O	1:B:133:ILE:HG22	0.71	1.85	1	2
1:A:11:ILE:CD1	1:A:12:ALA:N	0.71	2.51	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:219:ILE:HD11	1:A:236:ILE:HG12	0.70	1.62	1	2
1:A:301:PHE:CD1	1:A:342:LEU:HD13	0.70	2.21	1	2
1:B:287:ASN:O	1:B:530:ILE:HG12	0.70	1.86	2	1
1:A:567:LYS:O	1:A:571:GLU:HG3	0.70	1.87	1	2
1:B:321:ALA:O	1:B:324:CYS:SG	0.70	2.49	1	2
1:A:433:PRO:O	1:A:437:THR:HG23	0.70	1.85	1	2
1:A:287:ASN:O	1:A:530:ILE:HG12	0.70	1.86	2	1
1:A:321:ALA:O	1:A:324:CYS:SG	0.70	2.49	1	2
1:B:224:ASN:O	1:B:225:ASN:OD1	0.70	2.09	2	2
1:A:11:ILE:HD11	1:A:13:PHE:CE1	0.70	2.22	1	2
1:B:287:ASN:O	1:B:530:ILE:CG1	0.70	2.40	2	1
1:A:180:ILE:HD11	1:A:208:VAL:CG1	0.70	2.16	1	2
1:A:392:MET:N	1:A:429:MET:SD	0.70	2.64	1	2
1:B:11:ILE:HD11	1:B:13:PHE:CE1	0.70	2.22	2	2
1:B:219:ILE:HD11	1:B:236:ILE:HG12	0.70	1.62	2	2
1:B:179:PHE:CZ	1:B:181:THR:OG1	0.69	2.45	1	2
1:B:567:LYS:O	1:B:571:GLU:HG3	0.69	1.87	1	2
1:B:13:PHE:CE2	1:B:240:ARG:HD2	0.69	2.23	1	2
1:B:392:MET:N	1:B:429:MET:SD	0.69	2.64	1	2
1:A:456:LEU:HD22	1:A:484:LEU:HD11	0.69	1.62	1	2
1:B:291:GLY:CA	1:B:327:GLN:CG	0.69	2.65	1	2
1:B:301:PHE:CD1	1:B:342:LEU:HD13	0.69	2.22	1	2
1:A:224:ASN:O	1:A:225:ASN:OD1	0.69	2.10	1	2
1:A:287:ASN:O	1:A:530:ILE:CG1	0.69	2.40	2	1
1:A:13:PHE:CE2	1:A:240:ARG:HD2	0.69	2.23	1	2
1:A:317:TYR:CE2	1:A:377:ILE:HD13	0.69	2.23	1	2
1:A:355:LEU:O	1:B:464:ASP:CG	0.69	2.36	1	2
1:B:228:TYR:CG	1:B:235:VAL:HG11	0.69	2.23	1	2
1:B:144:LEU:HD22	1:B:145:LYS:O	0.69	1.88	2	2
1:A:556:PRO:HB3	1:B:441:HIS:CG	0.69	2.23	1	2
1:A:144:LEU:HD22	1:A:145:LYS:O	0.68	1.88	1	2
1:B:274:ASN:ND2	1:B:526:SER:N	0.68	2.42	1	2
1:B:429:MET:O	1:B:429:MET:HG3	0.68	1.88	1	2
1:A:54:LEU:HD13	1:A:55:GLU:H	0.68	1.46	2	2
1:A:429:MET:O	1:A:429:MET:HG3	0.68	1.88	1	2
1:B:317:TYR:CE2	1:B:377:ILE:HD13	0.68	2.22	1	2
1:A:228:TYR:CG	1:A:235:VAL:HG11	0.68	2.22	2	2
1:A:431:GLU:CD	1:A:452:GLY:HA3	0.68	2.13	1	2
1:A:431:GLU:HA	1:A:456:LEU:HG	0.68	1.65	1	2
1:B:304:ARG:CD	1:B:306:ALA:O	0.68	2.42	1	2
1:B:431:GLU:HA	1:B:456:LEU:HG	0.68	1.66	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:139:ARG:HB3	1:B:144:LEU:CG	0.68	2.18	2	2
1:B:54:LEU:HD13	1:B:54:LEU:C	0.68	2.14	2	2
1:B:431:GLU:CD	1:B:452:GLY:HA3	0.68	2.14	1	2
1:B:434:ALA:O	1:B:437:THR:OG1	0.68	2.11	1	2
1:A:464:ASP:N	1:A:464:ASP:OD1	0.68	2.27	1	2
1:B:433:PRO:O	1:B:437:THR:HG23	0.68	1.89	1	2
1:A:139:ARG:HB3	1:A:144:LEU:CG	0.67	2.18	1	2
1:B:464:ASP:OD1	1:B:464:ASP:N	0.67	2.27	1	2
1:A:232:THR:HG23	1:A:233:ASN:H	0.67	1.47	1	2
1:A:274:ASN:ND2	1:A:526:SER:N	0.67	2.41	1	2
1:B:13:PHE:CG	1:B:240:ARG:NH1	0.67	2.63	2	2
1:A:54:LEU:C	1:A:54:LEU:HD13	0.67	2.15	1	2
1:A:304:ARG:CD	1:A:306:ALA:O	0.67	2.43	1	2
1:A:13:PHE:CG	1:A:240:ARG:NH1	0.67	2.63	2	2
1:A:179:PHE:CZ	1:A:181:THR:OG1	0.67	2.46	1	2
1:B:232:THR:HG23	1:B:233:ASN:H	0.67	1.48	1	2
1:B:505:LEU:N	1:B:505:LEU:HD13	0.67	2.04	1	2
1:A:232:THR:HG22	1:A:234:GLU:H	0.66	1.51	1	2
1:B:54:LEU:HD13	1:B:55:GLU:H	0.66	1.47	2	2
1:B:144:LEU:HD13	1:B:144:LEU:C	0.66	2.10	2	2
1:A:434:ALA:O	1:A:437:THR:OG1	0.66	2.12	1	2
1:B:304:ARG:O	1:B:304:ARG:CZ	0.66	2.43	1	2
1:A:505:LEU:HD13	1:A:505:LEU:N	0.66	2.05	1	2
1:B:180:ILE:HD11	1:B:208:VAL:CG1	0.66	2.21	1	2
1:A:144:LEU:HD13	1:A:144:LEU:C	0.66	2.10	2	2
1:A:127:ALA:O	1:A:130:VAL:HG22	0.66	1.90	2	2
1:A:230:ASN:N	1:A:231:PRO:CD	0.66	2.59	1	2
1:A:160:ALA:O	1:A:181:THR:CG2	0.65	2.44	2	2
1:A:230:ASN:N	1:A:231:PRO:HD3	0.65	2.07	1	2
1:A:375:ARG:HH11	1:A:379:ARG:HH21	0.65	1.33	1	2
1:A:301:PHE:O	1:A:304:ARG:CD	0.65	2.44	1	2
1:A:304:ARG:O	1:A:304:ARG:CZ	0.65	2.44	1	2
1:B:160:ALA:O	1:B:181:THR:CG2	0.65	2.43	2	2
1:B:438:ILE:O	1:B:438:ILE:HG23	0.65	1.91	1	2
1:A:10:GLY:O	1:A:222:ALA:HB3	0.65	1.92	1	2
1:A:221:ASP:HA	1:A:239:MET:HE1	0.65	1.66	2	2
1:A:406:ILE:HD13	1:A:426:ILE:HD13	0.65	1.68	1	2
1:B:232:THR:HG22	1:B:234:GLU:H	0.65	1.51	1	2
1:B:406:ILE:HD13	1:B:426:ILE:HD13	0.65	1.68	1	2
1:A:180:ILE:CD1	1:A:208:VAL:HG11	0.65	2.21	1	2
1:A:258:ASP:OD1	1:A:258:ASP:N	0.65	2.30	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:230:ASN:N	1:B:231:PRO:CD	0.65	2.59	1	2
1:B:232:THR:HG22	1:B:233:ASN:H	0.65	1.34	1	2
1:B:456:LEU:CD2	1:B:484:LEU:HD11	0.65	2.22	1	2
1:B:230:ASN:N	1:B:231:PRO:HD3	0.64	2.07	1	2
1:B:193:MET:SD	1:B:193:MET:C	0.64	2.80	2	1
1:A:321:ALA:C	1:A:324:CYS:SG	0.64	2.80	1	2
1:B:74:GLU:CD	1:B:74:GLU:C	0.64	2.64	1	2
1:B:505:LEU:HD22	1:B:506:ALA:N	0.64	2.07	1	2
1:A:74:GLU:C	1:A:74:GLU:CD	0.64	2.65	1	2
1:A:373:GLN:O	1:A:377:ILE:HG12	0.64	1.92	1	2
1:B:301:PHE:O	1:B:304:ARG:CD	0.64	2.45	1	2
1:B:375:ARG:HH11	1:B:379:ARG:HH21	0.64	1.34	1	2
1:A:438:ILE:HG23	1:A:438:ILE:O	0.64	1.91	1	2
1:A:259:LEU:CB	1:A:260:PRO:CD	0.64	2.75	1	1
1:B:10:GLY:O	1:B:222:ALA:HB3	0.64	1.92	1	2
1:B:221:ASP:HA	1:B:239:MET:HE1	0.64	1.66	2	2
1:B:321:ALA:C	1:B:324:CYS:SG	0.64	2.81	1	2
1:B:127:ALA:O	1:B:130:VAL:HG22	0.63	1.93	2	2
1:B:373:GLN:O	1:B:377:ILE:HG12	0.63	1.93	1	2
1:A:505:LEU:HD22	1:A:506:ALA:N	0.63	2.08	1	2
1:A:193:MET:SD	1:A:193:MET:C	0.63	2.81	2	1
1:B:304:ARG:HD2	1:B:306:ALA:O	0.63	1.94	1	2
1:B:484:LEU:HD23	1:B:484:LEU:C	0.63	2.18	1	2
1:A:456:LEU:CD2	1:A:484:LEU:HD11	0.63	2.24	1	2
1:B:54:LEU:CD2	1:B:77:ILE:HG13	0.63	2.24	2	2
1:A:441:HIS:CG	1:B:556:PRO:HB3	0.62	2.28	1	2
1:B:180:ILE:CD1	1:B:208:VAL:HG11	0.62	2.25	1	2
1:B:505:LEU:CD1	1:B:505:LEU:H	0.62	2.07	1	2
1:A:484:LEU:HD23	1:A:484:LEU:C	0.62	2.19	1	2
1:A:505:LEU:CD1	1:A:505:LEU:H	0.62	2.07	1	2
1:A:228:TYR:HB3	1:A:231:PRO:CG	0.62	2.25	1	2
1:A:501:MET:SD	1:A:520:LEU:HD22	0.62	2.35	1	2
1:A:301:PHE:O	1:A:304:ARG:CZ	0.62	2.47	1	2
1:B:205:THR:CG2	1:B:208:VAL:H	0.62	2.08	1	2
1:A:54:LEU:CD2	1:A:77:ILE:HG13	0.61	2.24	1	2
1:A:304:ARG:HD2	1:A:306:ALA:O	0.61	1.94	1	2
1:B:533:ILE:O	1:B:536:ILE:HG22	0.61	1.95	2	2
1:A:205:THR:CG2	1:A:208:VAL:H	0.61	2.08	2	2
1:A:489:ILE:O	1:A:492:SER:HB2	0.61	1.95	1	2
1:A:391:PRO:HA	1:A:429:MET:HG2	0.61	1.73	1	2
1:A:431:GLU:HG2	1:A:452:GLY:H	0.61	1.54	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:139:ARG:HB3	1:B:144:LEU:CD1	0.61	2.25	1	2
1:A:533:ILE:O	1:A:536:ILE:HG22	0.61	1.96	2	2
1:A:139:ARG:HB3	1:A:144:LEU:CD1	0.61	2.26	2	2
1:B:501:MET:SD	1:B:520:LEU:HD22	0.61	2.36	1	2
1:B:296:ARG:NE	1:B:332:ARG:NH2	0.61	2.49	1	2
1:B:391:PRO:HA	1:B:429:MET:HG2	0.61	1.72	1	2
1:B:330:ILE:C	1:B:330:ILE:CD1	0.60	2.72	1	2
1:A:90:ILE:HD12	1:A:91:ALA:N	0.60	2.11	1	2
1:A:193:MET:HG3	1:A:194:ALA:N	0.60	2.11	2	2
1:B:228:TYR:HB3	1:B:231:PRO:CG	0.60	2.25	2	2
1:A:287:ASN:HB3	1:A:530:ILE:HG23	0.60	1.72	1	2
1:A:391:PRO:CA	1:A:429:MET:HE3	0.60	2.26	1	2
1:B:90:ILE:HD12	1:B:91:ALA:N	0.60	2.10	1	2
1:B:489:ILE:O	1:B:492:SER:HB2	0.60	1.95	1	2
1:A:375:ARG:NH2	1:A:416:GLU:OE1	0.60	2.35	1	2
1:B:193:MET:HG3	1:B:194:ALA:N	0.60	2.10	2	1
1:A:296:ARG:NE	1:A:332:ARG:NH2	0.60	2.49	1	2
1:B:387:ARG:HH21	1:B:425:GLU:H	0.60	1.40	1	2
1:A:67:GLU:CD	1:A:67:GLU:H	0.60	2.05	2	2
1:B:301:PHE:O	1:B:304:ARG:CZ	0.60	2.48	1	2
1:B:530:ILE:C	1:B:530:ILE:CD1	0.60	2.72	2	1
1:A:193:MET:SD	1:A:197:LEU:CD2	0.59	2.90	1	1
1:B:67:GLU:H	1:B:67:GLU:CD	0.59	2.04	2	1
1:B:79:LEU:HD13	1:B:79:LEU:O	0.59	1.98	2	2
1:A:310:GLU:N	1:A:372:ASP:OD2	0.59	2.34	1	2
1:B:431:GLU:HG2	1:B:452:GLY:H	0.59	1.54	1	2
1:A:79:LEU:HD13	1:A:79:LEU:O	0.59	1.98	1	2
1:A:144:LEU:HD22	1:A:145:LYS:C	0.59	2.22	1	2
1:A:54:LEU:O	1:A:57:ILE:HG12	0.59	1.98	1	2
1:A:505:LEU:HD13	1:A:506:ALA:N	0.59	2.12	1	2
1:B:144:LEU:HD22	1:B:145:LYS:C	0.59	2.22	2	2
1:B:391:PRO:CA	1:B:429:MET:HE3	0.59	2.27	1	2
1:B:54:LEU:C	1:B:54:LEU:CD1	0.58	2.76	2	2
1:B:375:ARG:NH2	1:B:416:GLU:OE1	0.58	2.36	1	2
1:B:268:GLN:H	1:B:268:GLN:CD	0.58	2.06	1	2
1:A:387:ARG:HH21	1:A:425:GLU:H	0.58	1.40	1	2
1:B:225:ASN:O	1:B:225:ASN:ND2	0.58	2.37	2	2
1:A:388:ILE:HD12	1:A:388:ILE:C	0.58	2.23	1	2
1:A:562:MET:SD	1:A:566:ASN:ND2	0.58	2.77	1	2
1:B:310:GLU:N	1:B:372:ASP:OD2	0.58	2.36	1	2
1:A:421:ASP:OD1	1:A:423:SER:HB2	0.58	1.99	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:514:LEU:O	1:B:518:MET:CG	0.58	2.52	1	2
1:A:268:GLN:CD	1:A:268:GLN:H	0.58	2.06	1	2
1:B:144:LEU:C	1:B:144:LEU:CD2	0.58	2.63	2	2
1:B:421:ASP:OD1	1:B:423:SER:HB2	0.58	1.99	1	2
1:A:89:ILE:HD13	1:A:89:ILE:O	0.58	1.99	1	2
1:A:54:LEU:C	1:A:54:LEU:CD1	0.57	2.77	2	2
1:A:481:VAL:O	1:A:485:ILE:CG2	0.57	2.48	1	2
1:B:54:LEU:HG	1:B:77:ILE:HD12	0.57	1.76	1	2
1:B:182:ASP:OD1	1:B:182:ASP:N	0.57	2.38	2	2
1:B:481:VAL:O	1:B:485:ILE:CG2	0.57	2.48	1	2
1:B:562:MET:SD	1:B:566:ASN:ND2	0.57	2.78	1	2
1:A:309:THR:C	1:A:372:ASP:OD2	0.57	2.48	1	2
1:B:54:LEU:HG	1:B:77:ILE:CD1	0.57	2.29	1	2
1:B:451:ILE:CD1	1:B:451:ILE:N	0.57	2.68	1	2
1:B:505:LEU:HD13	1:B:506:ALA:N	0.57	2.13	1	2
1:A:514:LEU:O	1:A:518:MET:CG	0.57	2.52	1	2
1:A:530:ILE:C	1:A:530:ILE:CD1	0.57	2.72	2	1
1:A:225:ASN:O	1:A:225:ASN:ND2	0.57	2.37	1	2
1:B:54:LEU:O	1:B:57:ILE:HG12	0.57	1.99	1	2
1:B:176:VAL:HG13	1:B:176:VAL:O	0.57	1.99	2	2
1:A:11:ILE:HG21	1:A:243:GLN:CB	0.57	2.30	1	2
1:A:89:ILE:CG2	1:A:90:ILE:N	0.57	2.68	2	2
1:A:287:ASN:HB3	1:A:530:ILE:CG2	0.57	2.30	1	1
1:A:13:PHE:CD2	1:A:240:ARG:NH1	0.57	2.73	1	2
1:A:451:ILE:N	1:A:451:ILE:CD1	0.57	2.68	1	2
1:B:309:THR:C	1:B:372:ASP:OD2	0.57	2.48	1	2
1:A:133:ILE:CG2	1:A:134:GLY:N	0.57	2.67	2	2
1:B:229:VAL:C	1:B:231:PRO:HD3	0.57	2.25	2	2
1:A:274:ASN:ND2	1:A:525:MET:C	0.56	2.63	1	2
1:A:179:PHE:CE2	1:A:190:THR:OG1	0.56	2.51	2	1
1:B:179:PHE:CE2	1:B:190:THR:OG1	0.56	2.51	2	1
1:A:54:LEU:HG	1:A:77:ILE:HD12	0.56	1.76	2	2
1:A:176:VAL:HG13	1:A:176:VAL:O	0.56	2.00	2	2
1:A:292:VAL:HG12	1:A:327:GLN:NE2	0.56	2.15	1	2
1:A:486:LYS:HD2	1:A:553:LEU:HD13	0.56	1.76	1	2
1:A:182:ASP:OD1	1:A:182:ASP:N	0.56	2.37	2	2
1:B:13:PHE:CD2	1:B:240:ARG:NH1	0.56	2.73	2	2
1:B:89:ILE:CG2	1:B:90:ILE:N	0.56	2.68	2	2
1:B:133:ILE:CG2	1:B:134:GLY:N	0.56	2.67	2	2
1:B:223:VAL:HG23	1:B:224:ASN:N	0.56	2.16	1	2
1:B:294:LEU:CB	1:B:502:CYS:SG	0.56	2.94	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:321:ALA:HA	1:B:324:CYS:SG	0.56	2.40	1	2
1:B:486:LYS:HD2	1:B:553:LEU:HD13	0.56	1.75	1	2
1:A:391:PRO:HA	1:A:429:MET:HE3	0.56	1.77	1	2
1:B:485:ILE:CG1	1:B:486:LYS:N	0.56	2.68	1	2
1:A:74:GLU:HG3	1:A:75:GLY:N	0.56	2.16	2	2
1:A:229:VAL:C	1:A:231:PRO:HD3	0.56	2.25	2	2
1:A:464:ASP:OD1	1:B:355:LEU:O	0.56	2.23	1	2
1:A:54:LEU:HG	1:A:77:ILE:CD1	0.56	2.31	1	2
1:B:89:ILE:HD13	1:B:89:ILE:O	0.56	1.99	2	2
1:B:274:ASN:ND2	1:B:525:MET:C	0.56	2.64	1	2
1:B:278:VAL:HG23	1:B:279:ARG:N	0.56	2.16	1	2
1:A:485:ILE:CG1	1:A:486:LYS:N	0.56	2.68	1	2
1:B:412:GLU:O	1:B:416:GLU:HG3	0.56	2.01	1	2
1:A:77:ILE:HD13	1:A:77:ILE:H	0.56	1.57	2	2
1:A:294:LEU:CB	1:A:502:CYS:SG	0.56	2.93	1	2
1:B:202:ILE:HD13	1:B:202:ILE:C	0.56	2.26	1	2
1:A:321:ALA:HA	1:A:324:CYS:SG	0.56	2.41	1	2
1:B:11:ILE:HG21	1:B:243:GLN:CB	0.56	2.30	1	2
1:B:292:VAL:HG12	1:B:327:GLN:NE2	0.56	2.15	1	2
1:B:505:LEU:H	1:B:505:LEU:HD12	0.56	1.61	1	2
1:A:223:VAL:HG23	1:A:224:ASN:N	0.55	2.16	2	2
1:A:412:GLU:O	1:A:416:GLU:HG3	0.55	2.01	1	2
1:B:388:ILE:HD12	1:B:388:ILE:C	0.55	2.26	1	2
1:A:249:GLU:C	1:A:249:GLU:CD	0.55	2.74	1	2
1:A:324:CYS:CB	1:A:327:GLN:NE2	0.55	2.70	1	2
1:B:221:ASP:OD2	1:B:226:GLN:HB2	0.55	2.02	1	2
1:A:105:HIS:CE1	1:A:109:GLU:OE1	0.55	2.60	1	2
1:A:278:VAL:HG23	1:A:279:ARG:N	0.55	2.16	1	2
1:A:221:ASP:OD2	1:A:226:GLN:HB2	0.55	2.02	1	2
1:B:13:PHE:N	1:B:13:PHE:CD1	0.55	2.74	2	2
1:B:105:HIS:CE1	1:B:109:GLU:OE1	0.55	2.60	1	2
1:B:249:GLU:C	1:B:249:GLU:CD	0.55	2.74	1	2
1:A:505:LEU:H	1:A:505:LEU:HD12	0.55	1.61	1	2
1:B:179:PHE:CE2	1:B:181:THR:OG1	0.55	2.60	1	2
1:A:252:GLU:O	1:A:255:LYS:HG2	0.54	2.02	1	1
1:B:391:PRO:HA	1:B:429:MET:HE3	0.54	1.78	1	2
1:A:13:PHE:CD1	1:A:13:PHE:N	0.54	2.74	1	2
1:A:221:ASP:CA	1:A:239:MET:CE	0.54	2.78	1	2
1:A:259:LEU:HB3	1:A:260:PRO:CD	0.54	2.31	1	1
1:B:330:ILE:O	1:B:330:ILE:CG1	0.54	2.55	1	2
1:A:330:ILE:O	1:A:330:ILE:CG1	0.54	2.55	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:PHE:CE2	1:A:181:THR:OG1	0.54	2.61	1	2
1:A:294:LEU:CD1	1:A:502:CYS:SG	0.54	2.95	1	2
1:A:105:HIS:NE2	1:A:109:GLU:CD	0.54	2.66	1	2
1:A:405:GLU:HG3	1:A:409:TYR:CE2	0.54	2.38	1	2
1:B:324:CYS:CB	1:B:327:GLN:NE2	0.54	2.71	1	2
1:A:202:ILE:HD13	1:A:202:ILE:C	0.54	2.27	2	2
1:B:256:LEU:CD1	1:B:256:LEU:C	0.54	2.80	1	1
1:B:105:HIS:NE2	1:B:109:GLU:CD	0.54	2.66	2	2
1:A:243:GLN:C	1:A:243:GLN:CD	0.54	2.76	1	2
1:B:513:LEU:CD2	1:B:568:PHE:CE1	0.54	2.91	1	2
1:B:193:MET:CG	1:B:194:ALA:N	0.54	2.71	2	1
1:A:513:LEU:CD2	1:A:568:PHE:CE1	0.53	2.92	1	2
1:B:74:GLU:HG3	1:B:75:GLY:N	0.53	2.17	2	2
1:B:221:ASP:OD2	1:B:224:ASN:ND2	0.53	2.41	2	2
1:B:294:LEU:CD1	1:B:502:CYS:SG	0.53	2.94	1	2
1:B:331:VAL:HG11	1:B:377:ILE:HD12	0.53	1.80	1	2
1:A:202:ILE:HD11	1:A:205:THR:HB	0.53	1.79	2	2
1:A:221:ASP:OD2	1:A:224:ASN:ND2	0.53	2.41	1	2
1:A:473:LEU:N	1:A:473:LEU:CD2	0.53	2.71	1	2
1:B:243:GLN:C	1:B:243:GLN:CD	0.53	2.76	1	2
1:B:350:GLU:OE1	1:B:350:GLU:N	0.53	2.41	1	2
1:A:355:LEU:O	1:B:464:ASP:OD1	0.53	2.25	1	2
1:B:54:LEU:CG	1:B:77:ILE:HG13	0.53	2.33	1	2
1:B:144:LEU:HD22	1:B:145:LYS:N	0.53	2.19	2	2
1:B:405:GLU:HG3	1:B:409:TYR:CE2	0.53	2.38	1	2
1:A:73:PHE:O	1:A:77:ILE:CG1	0.53	2.57	1	2
1:B:202:ILE:HD11	1:B:205:THR:HB	0.53	1.80	2	2
1:B:265:ASP:OD2	1:B:541:ASN:ND2	0.53	2.42	1	2
1:B:473:LEU:CD2	1:B:473:LEU:N	0.53	2.72	1	2
1:A:278:VAL:CG2	1:A:279:ARG:N	0.53	2.72	1	2
1:B:429:MET:CE	1:B:431:GLU:CD	0.53	2.82	1	2
1:A:375:ARG:NH1	1:A:379:ARG:NH2	0.53	2.57	1	2
1:A:388:ILE:C	1:A:388:ILE:CD1	0.53	2.81	1	2
1:B:73:PHE:O	1:B:77:ILE:CG1	0.53	2.57	1	2
1:B:294:LEU:HA	1:B:330:ILE:HG13	0.53	1.81	1	2
1:B:453:THR:OG1	1:B:505:LEU:CD1	0.52	2.58	1	2
1:A:54:LEU:HD21	1:A:77:ILE:CG1	0.52	2.33	1	2
1:A:265:ASP:OD2	1:A:541:ASN:ND2	0.52	2.42	1	2
1:A:350:GLU:N	1:A:350:GLU:OE1	0.52	2.42	1	2
1:B:451:ILE:HD13	1:B:499:THR:HG23	0.52	1.81	1	2
1:A:193:MET:CG	1:A:194:ALA:N	0.52	2.71	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:438:ILE:O	1:B:438:ILE:CG2	0.52	2.57	1	2
1:A:324:CYS:HB2	1:A:327:GLN:CD	0.52	2.30	1	2
1:B:54:LEU:HD13	1:B:55:GLU:CA	0.52	2.32	1	2
1:A:438:ILE:O	1:A:438:ILE:CG2	0.52	2.58	1	2
1:A:514:LEU:O	1:A:518:MET:HG3	0.52	2.05	1	2
1:B:221:ASP:C	1:B:223:VAL:N	0.52	2.66	1	2
1:B:388:ILE:C	1:B:388:ILE:CD1	0.52	2.83	1	2
1:A:144:LEU:C	1:A:144:LEU:CD2	0.52	2.63	1	2
1:A:205:THR:HG21	1:A:208:VAL:HG12	0.52	1.81	2	2
1:A:451:ILE:HD13	1:A:499:THR:HG23	0.52	1.81	1	2
1:A:453:THR:OG1	1:A:505:LEU:CD1	0.52	2.57	1	2
1:A:463:VAL:CG1	1:B:361:ARG:NH1	0.52	2.73	1	2
1:B:202:ILE:C	1:B:202:ILE:CD1	0.52	2.83	2	2
1:A:221:ASP:C	1:A:223:VAL:N	0.52	2.66	1	2
1:A:330:ILE:C	1:A:330:ILE:CD1	0.52	2.72	1	2
1:A:331:VAL:HG11	1:A:377:ILE:HD12	0.52	1.80	1	2
1:A:429:MET:CE	1:A:431:GLU:CD	0.52	2.83	1	2
1:B:278:VAL:CG2	1:B:279:ARG:N	0.52	2.72	1	2
1:B:375:ARG:NH1	1:B:379:ARG:NH2	0.52	2.58	1	2
1:B:54:LEU:HD21	1:B:77:ILE:CG1	0.52	2.33	1	2
1:B:68:GLU:CB	1:B:279:ARG:HH21	0.52	2.18	1	1
1:B:86:GLU:O	1:B:90:ILE:CG1	0.52	2.58	2	2
1:B:274:ASN:HD22	1:B:525:MET:C	0.52	2.13	1	2
1:B:292:VAL:HG22	1:B:329:VAL:HA	0.52	1.82	1	2
1:B:324:CYS:HB2	1:B:327:GLN:CD	0.52	2.30	1	2
1:A:54:LEU:CG	1:A:77:ILE:HG13	0.52	2.34	1	2
1:A:205:THR:CG2	1:A:206:GLY:N	0.52	2.73	1	2
1:A:254:ALA:O	1:A:255:LYS:C	0.52	2.53	1	1
1:A:321:ALA:CA	1:A:324:CYS:SG	0.52	2.98	1	2
1:B:321:ALA:CA	1:B:324:CYS:SG	0.52	2.98	1	2
1:B:327:GLN:C	1:B:327:GLN:OE1	0.52	2.53	1	2
1:B:514:LEU:O	1:B:518:MET:HG3	0.52	2.05	1	2
1:B:542:PHE:C	1:B:542:PHE:CD1	0.52	2.88	1	2
1:A:86:GLU:O	1:A:90:ILE:CG1	0.51	2.58	1	2
1:A:327:GLN:C	1:A:327:GLN:OE1	0.51	2.52	1	2
1:A:515:LEU:CD1	1:A:515:LEU:N	0.51	2.74	1	2
1:B:292:VAL:O	1:B:330:ILE:HG23	0.51	2.05	1	2
1:A:221:ASP:OD1	1:A:239:MET:SD	0.51	2.68	1	2
1:A:3:SER:OG	1:A:225:ASN:ND2	0.51	2.43	1	2
1:A:144:LEU:HD22	1:A:145:LYS:N	0.51	2.19	1	2
1:A:202:ILE:C	1:A:202:ILE:CD1	0.51	2.84	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:205:THR:CG2	1:B:206:GLY:N	0.51	2.73	2	2
1:B:221:ASP:OD1	1:B:239:MET:SD	0.51	2.69	1	2
1:B:255:LYS:NZ	1:B:258:ASP:OD2	0.51	2.40	1	1
1:B:557:THR:HB	1:B:560:GLU:OE1	0.51	2.05	1	2
1:A:294:LEU:HA	1:A:330:ILE:HG13	0.51	1.81	1	2
1:B:77:ILE:HD13	1:B:77:ILE:H	0.51	1.58	1	2
1:A:542:PHE:CD1	1:A:542:PHE:C	0.51	2.88	1	2
1:B:168:THR:HG21	1:B:193:MET:SD	0.51	2.45	1	1
1:A:274:ASN:HD22	1:A:525:MET:C	0.51	2.13	1	2
1:A:292:VAL:HG22	1:A:329:VAL:HA	0.51	1.81	1	2
1:B:3:SER:OG	1:B:225:ASN:ND2	0.51	2.43	2	2
1:A:219:ILE:CD1	1:A:236:ILE:HG12	0.51	2.36	2	2
1:A:292:VAL:O	1:A:330:ILE:HG23	0.51	2.04	1	2
1:A:324:CYS:HB2	1:A:327:GLN:NE2	0.51	2.21	1	2
1:B:431:GLU:HG2	1:B:452:GLY:N	0.51	2.21	1	2
1:A:451:ILE:N	1:A:451:ILE:HD12	0.50	2.20	1	2
1:B:221:ASP:CA	1:B:239:MET:CE	0.50	2.78	1	2
1:B:219:ILE:CD1	1:B:236:ILE:HG12	0.50	2.36	1	2
1:B:451:ILE:N	1:B:451:ILE:HD12	0.50	2.20	1	2
1:B:205:THR:HG22	1:B:206:GLY:N	0.50	2.21	1	2
1:B:375:ARG:HH11	1:B:379:ARG:NH2	0.50	2.04	1	2
1:A:172:ASN:O	1:A:176:VAL:HG12	0.50	2.06	2	2
1:B:144:LEU:O	1:B:144:LEU:HD22	0.50	2.07	1	2
1:B:324:CYS:HB2	1:B:327:GLN:NE2	0.50	2.22	1	2
1:A:294:LEU:HB2	1:A:502:CYS:SG	0.50	2.46	1	2
1:A:375:ARG:HH11	1:A:379:ARG:NH2	0.50	2.03	1	2
1:A:556:PRO:HB3	1:B:441:HIS:CE1	0.50	2.41	1	2
1:B:205:THR:HG21	1:B:208:VAL:HG12	0.50	1.83	2	2
1:B:386:LEU:O	1:B:387:ARG:CZ	0.50	2.59	1	2
1:B:456:LEU:HD22	1:B:484:LEU:CD1	0.50	2.36	1	2
1:B:53:GLN:O	1:B:57:ILE:HG23	0.50	2.06	1	2
1:B:221:ASP:O	1:B:223:VAL:HG13	0.50	2.06	2	2
1:B:294:LEU:HB2	1:B:502:CYS:SG	0.50	2.47	1	2
1:A:144:LEU:O	1:A:144:LEU:HD22	0.50	2.07	1	2
1:A:431:GLU:HG2	1:A:452:GLY:N	0.50	2.21	1	2
1:A:557:THR:HB	1:A:560:GLU:OE1	0.50	2.05	1	2
1:B:144:LEU:C	1:B:144:LEU:CD1	0.50	2.78	2	2
1:A:205:THR:HG22	1:A:206:GLY:N	0.49	2.22	1	2
1:A:293:GLY:O	1:A:330:ILE:HG12	0.49	2.07	1	2
1:A:330:ILE:HD12	1:A:330:ILE:O	0.49	2.06	1	2
1:B:515:LEU:CD1	1:B:515:LEU:N	0.49	2.74	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:GLN:O	1:A:57:ILE:HG23	0.49	2.06	1	2
1:A:459:TYR:HB3	1:B:459:TYR:O	0.49	2.07	1	2
1:A:80:LEU:HD13	1:A:137:LEU:HD11	0.49	1.84	2	2
1:A:386:LEU:O	1:A:387:ARG:CZ	0.49	2.59	1	2
1:B:224:ASN:OD1	1:B:224:ASN:C	0.49	2.55	2	2
1:A:224:ASN:C	1:A:224:ASN:OD1	0.49	2.56	2	2
1:A:293:GLY:O	1:A:330:ILE:CG1	0.49	2.61	1	2
1:B:158:LEU:O	1:B:180:ILE:HG23	0.49	2.07	1	2
1:A:182:ASP:OD2	1:A:209:THR:CG2	0.49	2.61	1	2
1:A:252:GLU:O	1:A:255:LYS:CG	0.49	2.61	1	1
1:A:233:ASN:O	1:A:237:ASP:OD2	0.49	2.31	2	2
1:B:57:ILE:CG1	1:B:58:LYS:N	0.49	2.76	1	2
1:B:80:LEU:HD13	1:B:137:LEU:HD11	0.49	1.84	1	2
1:B:182:ASP:OD2	1:B:209:THR:CG2	0.49	2.60	1	2
1:B:233:ASN:O	1:B:237:ASP:OD2	0.49	2.31	1	2
1:B:363:ALA:HB1	1:B:370:LEU:HB2	0.49	1.85	1	2
1:A:144:LEU:C	1:A:144:LEU:CD1	0.49	2.78	2	2
1:A:221:ASP:O	1:A:223:VAL:HG13	0.49	2.08	1	2
1:B:330:ILE:HD12	1:B:330:ILE:O	0.49	2.06	1	2
1:B:330:ILE:O	1:B:330:ILE:HG13	0.49	2.08	1	2
1:A:538:ARG:HE	1:A:538:ARG:C	0.49	2.16	1	2
1:B:341:GLU:OE1	1:B:343:PRO:N	0.49	2.46	1	2
1:A:431:GLU:CA	1:A:456:LEU:HG	0.48	2.37	1	2
1:B:293:GLY:O	1:B:330:ILE:CG1	0.48	2.61	1	2
1:A:74:GLU:CG	1:A:75:GLY:N	0.48	2.76	1	2
1:A:101:ASP:OD1	1:A:101:ASP:N	0.48	2.45	2	2
1:A:557:THR:HG22	1:A:560:GLU:H	0.48	1.69	1	2
1:B:274:ASN:OD1	1:B:274:ASN:C	0.48	2.57	1	2
1:A:105:HIS:HE2	1:A:109:GLU:CD	0.48	2.17	2	1
1:A:341:GLU:OE1	1:A:343:PRO:N	0.48	2.47	1	2
1:B:74:GLU:CG	1:B:75:GLY:N	0.48	2.76	1	2
1:B:144:LEU:CD1	1:B:144:LEU:N	0.48	2.77	2	2
1:B:172:ASN:O	1:B:176:VAL:HG12	0.48	2.08	1	2
1:B:293:GLY:O	1:B:330:ILE:HG12	0.48	2.08	1	2
1:A:8:SER:OG	1:A:199:LEU:O	0.48	2.28	2	2
1:B:538:ARG:HE	1:B:538:ARG:C	0.48	2.17	1	2
1:A:49:LYS:O	1:A:50:ALA:C	0.48	2.57	2	2
1:A:139:ARG:CB	1:A:144:LEU:CD1	0.48	2.92	2	2
1:A:270:GLU:N	1:A:270:GLU:OE1	0.48	2.47	1	2
1:B:49:LYS:O	1:B:50:ALA:C	0.48	2.57	2	2
1:B:139:ARG:CB	1:B:144:LEU:CD1	0.48	2.92	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:GLY:O	1:A:221:ASP:O	0.48	2.32	2	2
1:B:10:GLY:O	1:B:221:ASP:O	0.48	2.32	1	2
1:B:301:PHE:O	1:B:301:PHE:HD1	0.48	1.92	1	2
1:B:282:GLU:O	1:B:286:ARG:HG2	0.48	2.09	2	1
1:A:54:LEU:HD13	1:A:55:GLU:CA	0.47	2.33	1	2
1:A:268:GLN:CD	1:A:268:GLN:N	0.47	2.72	1	2
1:A:330:ILE:O	1:A:330:ILE:HG13	0.47	2.08	1	2
1:A:363:ALA:HB1	1:A:370:LEU:HB2	0.47	1.85	1	2
1:B:320:VAL:O	1:B:324:CYS:SG	0.47	2.61	1	2
1:B:557:THR:HG22	1:B:560:GLU:H	0.47	1.69	1	2
1:A:274:ASN:OD1	1:A:274:ASN:C	0.47	2.57	1	2
1:B:221:ASP:O	1:B:223:VAL:N	0.47	2.48	1	2
1:B:530:ILE:HG23	1:B:531:PRO:HD3	0.47	1.85	2	1
1:A:144:LEU:CD1	1:A:144:LEU:N	0.47	2.77	2	2
1:A:335:ASP:OD1	1:A:335:ASP:O	0.47	2.33	1	2
1:A:429:MET:HE2	1:A:431:GLU:OE2	0.47	2.10	1	2
1:B:391:PRO:CA	1:B:429:MET:HG2	0.47	2.38	1	2
1:A:126:ARG:O	1:A:130:VAL:HG13	0.47	2.10	1	2
1:A:330:ILE:O	1:A:330:ILE:CD1	0.47	2.62	1	2
1:A:358:ARG:NH1	1:A:392:MET:SD	0.47	2.87	1	2
1:A:538:ARG:O	1:A:538:ARG:NE	0.47	2.45	1	2
1:B:11:ILE:CD1	1:B:13:PHE:CZ	0.47	2.94	2	2
1:B:268:GLN:CD	1:B:268:GLN:N	0.47	2.72	1	2
1:A:294:LEU:C	1:A:294:LEU:CD2	0.47	2.88	1	2
1:A:304:ARG:CD	1:A:304:ARG:C	0.47	2.88	1	2
1:A:341:GLU:CD	1:A:342:LEU:C	0.47	2.82	1	2
1:B:68:GLU:HB2	1:B:279:ARG:HH21	0.47	1.69	1	1
1:B:123:LEU:N	1:B:123:LEU:HD12	0.47	2.24	2	2
1:B:270:GLU:OE1	1:B:270:GLU:N	0.47	2.48	1	2
1:B:330:ILE:CD1	1:B:330:ILE:O	0.47	2.62	1	2
1:B:335:ASP:OD1	1:B:335:ASP:O	0.47	2.33	1	2
1:B:341:GLU:CD	1:B:342:LEU:C	0.47	2.82	1	2
1:B:451:ILE:HG23	1:B:456:LEU:HD12	0.47	1.86	1	2
1:B:562:MET:CE	1:B:562:MET:CG	0.47	2.92	1	2
1:A:11:ILE:CG2	1:A:243:GLN:HB2	0.47	2.40	1	2
1:A:451:ILE:HG23	1:A:456:LEU:HD12	0.47	1.86	1	2
1:B:8:SER:OG	1:B:199:LEU:O	0.47	2.28	1	2
1:B:27:ASP:OD1	1:B:27:ASP:N	0.47	2.48	2	2
1:B:294:LEU:C	1:B:294:LEU:CD2	0.47	2.88	1	2
1:A:57:ILE:CG1	1:A:58:LYS:N	0.47	2.76	2	2
1:A:221:ASP:O	1:A:223:VAL:N	0.47	2.48	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:PHE:CZ	1:B:47:ARG:NE	0.47	2.83	1	2
1:B:431:GLU:CA	1:B:456:LEU:HG	0.47	2.37	1	2
1:A:123:LEU:HD12	1:A:123:LEU:N	0.47	2.24	1	2
1:A:300:LEU:HD12	1:A:313:GLN:HE22	0.47	1.70	1	2
1:A:339:ASP:OD1	1:B:351:GLU:OE1	0.47	2.33	1	2
1:A:391:PRO:CA	1:A:429:MET:HG2	0.47	2.39	1	2
1:B:304:ARG:CD	1:B:304:ARG:C	0.47	2.88	1	2
1:A:11:ILE:CD1	1:A:13:PHE:CZ	0.46	2.94	1	2
1:A:27:ASP:OD1	1:A:27:ASP:N	0.46	2.48	1	2
1:A:130:VAL:CG2	1:A:131:ARG:N	0.46	2.77	2	2
1:A:377:ILE:HG22	1:A:386:LEU:CD2	0.46	2.40	1	2
1:A:292:VAL:CG1	1:A:327:GLN:NE2	0.46	2.79	1	2
1:B:11:ILE:CG2	1:B:243:GLN:HB2	0.46	2.40	2	2
1:B:313:GLN:OE1	1:B:317:TYR:OH	0.46	2.28	1	2
1:B:377:ILE:HG22	1:B:386:LEU:CD2	0.46	2.40	1	2
1:B:429:MET:SD	1:B:431:GLU:HB2	0.46	2.49	1	2
1:B:429:MET:HE2	1:B:431:GLU:OE2	0.46	2.10	1	2
1:A:282:GLU:O	1:A:286:ARG:HG2	0.46	2.10	2	1
1:A:67:GLU:N	1:A:67:GLU:OE1	0.46	2.48	1	1
1:A:301:PHE:O	1:A:301:PHE:HD1	0.46	1.92	1	2
1:B:223:VAL:CG2	1:B:224:ASN:N	0.46	2.79	1	2
1:A:361:ARG:NH2	1:A:394:ILE:HG21	0.46	2.25	1	2
1:B:123:LEU:N	1:B:123:LEU:CD1	0.46	2.79	2	2
1:B:358:ARG:NH1	1:B:392:MET:SD	0.46	2.87	1	2
1:A:43:PHE:CZ	1:A:47:ARG:NE	0.46	2.83	2	2
1:A:429:MET:SD	1:A:431:GLU:HB2	0.46	2.49	1	2
1:A:459:TYR:O	1:B:459:TYR:HB3	0.46	2.10	1	2
1:B:105:HIS:HE2	1:B:109:GLU:CD	0.46	2.17	1	1
1:B:202:ILE:HG12	1:B:203:VAL:N	0.46	2.26	1	2
1:A:256:LEU:O	1:A:259:LEU:HD21	0.46	2.11	1	1
1:B:300:LEU:HD12	1:B:313:GLN:HE22	0.46	1.69	1	2
1:A:288:GLY:C	1:A:530:ILE:CD1	0.46	2.88	1	1
1:A:318:LYS:NZ	1:A:383:PHE:CE2	0.46	2.80	1	2
1:B:512:THR:CB	1:B:536:ILE:HG21	0.46	2.41	1	2
1:A:256:LEU:HD23	1:A:256:LEU:H	0.46	1.71	2	1
1:A:294:LEU:HD23	1:A:295:TYR:N	0.46	2.26	1	2
1:A:512:THR:CB	1:A:536:ILE:HG21	0.46	2.41	1	2
1:B:11:ILE:CG2	1:B:243:GLN:CA	0.46	2.82	2	2
1:B:221:ASP:C	1:B:223:VAL:H	0.46	2.19	2	2
1:B:318:LYS:NZ	1:B:383:PHE:CE2	0.46	2.81	1	2
1:A:463:VAL:CG1	1:B:361:ARG:HH12	0.46	2.24	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:5:ILE:O	1:B:6:LEU:O	0.46	2.34	2	2
1:B:361:ARG:NH2	1:B:394:ILE:HG21	0.46	2.26	1	2
1:B:375:ARG:HH22	1:B:418:LYS:HZ2	0.46	1.52	1	2
1:A:188:SER:O	1:A:191:SER:OG	0.46	2.34	1	1
1:A:265:ASP:CG	1:A:541:ASN:ND2	0.46	2.74	1	2
1:A:391:PRO:CB	1:A:429:MET:HE3	0.46	2.40	1	2
1:B:521:ASP:OD1	1:B:521:ASP:O	0.46	2.34	1	2
1:A:54:LEU:CD2	1:A:77:ILE:CG1	0.45	2.94	1	2
1:B:54:LEU:CD2	1:B:77:ILE:CG1	0.45	2.94	2	2
1:B:87:GLN:O	1:B:90:ILE:HG13	0.45	2.11	1	2
1:B:204:GLY:O	1:B:205:THR:C	0.45	2.60	1	2
1:A:5:ILE:O	1:A:6:LEU:O	0.45	2.34	2	2
1:A:158:LEU:O	1:A:180:ILE:HG23	0.45	2.11	1	2
1:A:190:THR:O	1:A:193:MET:HG3	0.45	2.11	1	2
1:A:221:ASP:C	1:A:223:VAL:H	0.45	2.19	2	2
1:A:223:VAL:CG2	1:A:224:ASN:N	0.45	2.79	2	2
1:A:255:LYS:O	1:A:256:LEU:HG	0.45	2.11	1	1
1:A:562:MET:CE	1:A:566:ASN:HD21	0.45	2.24	1	2
1:B:290:GLU:O	1:B:290:GLU:OE1	0.45	2.34	1	2
1:A:118:LEU:N	1:A:118:LEU:CD2	0.45	2.80	2	2
1:A:133:ILE:HG23	1:A:134:GLY:N	0.45	2.25	2	2
1:A:202:ILE:HG12	1:A:203:VAL:N	0.45	2.26	2	2
1:A:454:ASN:CG	1:A:455:ASP:N	0.45	2.74	1	2
1:A:484:LEU:C	1:A:484:LEU:CD2	0.45	2.86	1	2
1:B:130:VAL:CG2	1:B:131:ARG:N	0.45	2.79	2	2
1:B:186:ARG:C	1:B:188:SER:H	0.45	2.19	1	2
1:B:292:VAL:CG1	1:B:327:GLN:NE2	0.45	2.79	1	2
1:B:391:PRO:CB	1:B:429:MET:HE3	0.45	2.41	1	2
1:A:367:ARG:O	1:A:368:GLU:C	0.45	2.60	1	2
1:B:101:ASP:N	1:B:101:ASP:OD1	0.45	2.47	2	1
1:B:256:LEU:H	1:B:256:LEU:HD23	0.45	1.72	2	1
1:A:68:GLU:OE1	1:A:69:LYS:NZ	0.45	2.35	1	1
1:A:123:LEU:N	1:A:123:LEU:CD1	0.45	2.79	1	2
1:A:186:ARG:C	1:A:188:SER:H	0.45	2.20	2	2
1:B:101:ASP:OD1	1:B:101:ASP:N	0.45	2.47	1	1
1:B:265:ASP:CG	1:B:541:ASN:ND2	0.45	2.74	1	2
1:B:294:LEU:HD23	1:B:295:TYR:N	0.45	2.26	1	2
1:A:265:ASP:OD2	1:A:541:ASN:OD1	0.45	2.34	1	2
1:A:361:ARG:NH1	1:B:463:VAL:CG1	0.45	2.79	1	2
1:B:118:LEU:N	1:B:118:LEU:CD2	0.45	2.79	1	2
1:B:133:ILE:HG23	1:B:134:GLY:N	0.45	2.25	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:ARG:HH11	1:A:186:ARG:CG	0.45	2.25	2	1
1:B:195:ARG:O	1:B:195:ARG:NH1	0.45	2.50	1	1
1:A:205:THR:HG23	1:A:208:VAL:H	0.45	1.71	2	2
1:A:290:GLU:OE1	1:A:290:GLU:O	0.45	2.35	1	2
1:B:367:ARG:O	1:B:368:GLU:C	0.45	2.60	1	2
1:B:562:MET:CE	1:B:566:ASN:HD21	0.45	2.25	1	2
1:B:186:ARG:HH11	1:B:186:ARG:CG	0.45	2.25	2	1
1:B:89:ILE:HD13	1:B:89:ILE:C	0.45	2.37	1	2
1:B:126:ARG:O	1:B:130:VAL:HG13	0.45	2.12	1	2
1:B:189:HIS:O	1:B:192:ILE:HG22	0.45	2.12	1	1
1:B:454:ASN:CG	1:B:455:ASP:N	0.45	2.75	1	2
1:B:221:ASP:CA	1:B:239:MET:HE2	0.45	2.30	2	1
1:A:274:ASN:OD1	1:A:274:ASN:O	0.44	2.35	1	2
1:A:521:ASP:O	1:A:521:ASP:OD1	0.44	2.35	1	2
1:A:86:GLU:OE1	1:A:87:GLN:NE2	0.44	2.50	2	2
1:A:177:LEU:N	1:A:177:LEU:CD2	0.44	2.80	1	2
1:A:289:ALA:N	1:A:530:ILE:HD13	0.44	2.28	1	1
1:A:341:GLU:OE2	1:A:342:LEU:C	0.44	2.60	1	2
1:B:57:ILE:HD11	1:B:73:PHE:CD1	0.44	2.48	1	2
1:A:50:ALA:O	1:A:54:LEU:HB3	0.44	2.11	1	2
1:A:87:GLN:O	1:A:90:ILE:HG13	0.44	2.12	1	2
1:A:204:GLY:O	1:A:205:THR:C	0.44	2.60	2	2
1:A:351:GLU:OE1	1:B:339:ASP:OD1	0.44	2.35	1	2
1:B:341:GLU:OE2	1:B:342:LEU:C	0.44	2.61	1	2
1:B:484:LEU:O	1:B:488:VAL:HG23	0.44	2.12	1	2
1:A:473:LEU:N	1:A:473:LEU:HD22	0.44	2.28	1	2
1:B:163:LEU:CB	1:B:190:THR:HG21	0.44	2.35	1	1
1:B:177:LEU:N	1:B:177:LEU:CD2	0.44	2.80	1	2
1:B:274:ASN:OD1	1:B:274:ASN:O	0.44	2.35	1	2
1:B:327:GLN:HG2	1:B:328:ALA:N	0.44	2.27	1	2
1:A:484:LEU:O	1:A:488:VAL:HG23	0.44	2.12	1	2
1:B:50:ALA:O	1:B:54:LEU:HB3	0.44	2.12	2	2
1:A:138:LEU:N	1:A:138:LEU:CD2	0.44	2.80	1	2
1:A:391:PRO:HA	1:A:429:MET:CG	0.44	2.42	1	2
1:B:86:GLU:OE1	1:B:87:GLN:NE2	0.44	2.51	1	2
1:B:92:LEU:O	1:B:96:LYS:N	0.44	2.50	1	2
1:B:304:ARG:NE	1:B:304:ARG:C	0.44	2.72	1	2
1:B:388:ILE:O	1:B:388:ILE:HG13	0.44	2.13	1	2
1:A:327:GLN:HG2	1:A:328:ALA:N	0.44	2.27	1	2
1:A:429:MET:SD	1:A:431:GLU:CB	0.44	3.06	1	2
1:B:11:ILE:HD12	1:B:11:ILE:C	0.44	2.35	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:305:ASP:O	1:B:344:TYR:CD1	0.44	2.71	1	2
1:A:11:ILE:CG2	1:A:243:GLN:CA	0.44	2.82	2	2
1:A:224:ASN:OD1	1:A:226:GLN:N	0.44	2.51	1	2
1:A:304:ARG:NE	1:A:304:ARG:C	0.44	2.73	1	2
1:A:305:ASP:O	1:A:344:TYR:CD1	0.44	2.70	1	2
1:A:324:CYS:HB3	1:A:327:GLN:HE22	0.44	1.73	1	2
1:B:265:ASP:OD2	1:B:541:ASN:OD1	0.44	2.35	1	2
1:B:324:CYS:HB3	1:B:327:GLN:HE22	0.44	1.73	1	2
1:B:527:ALA:C	1:B:530:ILE:HG22	0.44	2.35	2	1
1:A:57:ILE:HD11	1:A:73:PHE:CD1	0.43	2.48	2	2
1:B:260:PRO:C	1:B:262:ILE:H	0.43	2.20	1	1
1:B:301:PHE:CZ	1:B:307:LEU:HA	0.43	2.48	1	2
1:B:287:ASN:O	1:B:530:ILE:HG13	0.43	2.11	2	1
1:A:89:ILE:HD13	1:A:89:ILE:C	0.43	2.38	2	2
1:A:558:THR:O	1:A:559:ASP:C	0.43	2.62	1	2
1:B:538:ARG:O	1:B:538:ARG:NE	0.43	2.45	1	2
1:A:301:PHE:CZ	1:A:307:LEU:HA	0.43	2.49	1	2
1:B:11:ILE:CD1	1:B:11:ILE:C	0.43	2.91	1	2
1:B:224:ASN:OD1	1:B:226:GLN:N	0.43	2.51	1	2
1:A:182:ASP:O	1:A:183:ALA:O	0.43	2.37	1	2
1:A:336:ILE:HG23	1:A:362:ILE:HD12	0.43	1.89	1	2
1:B:429:MET:SD	1:B:431:GLU:CB	0.43	3.06	1	2
1:A:92:LEU:O	1:A:96:LYS:N	0.43	2.50	2	1
1:A:361:ARG:HH22	1:A:394:ILE:HG21	0.43	1.73	1	2
1:B:57:ILE:HG12	1:B:58:LYS:N	0.43	2.28	1	2
1:B:503:GLY:C	1:B:505:LEU:CD1	0.43	2.92	1	2
1:A:503:GLY:C	1:A:505:LEU:CD1	0.43	2.92	1	2
1:B:186:ARG:C	1:B:188:SER:N	0.43	2.76	2	2
1:B:336:ILE:HG23	1:B:362:ILE:HD12	0.43	1.89	1	2
1:A:24:ILE:CG1	1:A:139:ARG:HH11	0.43	2.27	2	2
1:A:260:PRO:C	1:A:262:ILE:H	0.43	2.22	1	1
1:A:464:ASP:CG	1:A:467:ASN:CB	0.43	2.91	1	2
1:B:138:LEU:N	1:B:138:LEU:CD2	0.43	2.81	1	2
1:B:484:LEU:C	1:B:484:LEU:CD2	0.43	2.86	1	2
1:B:208:VAL:CG1	1:B:209:THR:N	0.43	2.82	1	2
1:B:429:MET:HE2	1:B:431:GLU:CD	0.43	2.38	1	2
1:B:186:ARG:CG	1:B:186:ARG:NH1	0.43	2.81	2	1
1:A:305:ASP:O	1:A:344:TYR:CE1	0.43	2.72	1	2
1:B:547:VAL:O	1:B:551:GLN:HG3	0.43	2.14	1	2
1:A:70:GLU:OE1	1:A:70:GLU:C	0.42	2.62	1	2
1:A:116:GLU:C	1:A:116:GLU:CD	0.42	2.87	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:208:VAL:CG1	1:A:209:THR:N	0.42	2.82	2	2
1:B:182:ASP:O	1:B:183:ALA:O	0.42	2.37	2	2
1:B:277:THR:O	1:B:278:VAL:C	0.42	2.62	1	2
1:A:86:GLU:C	1:A:86:GLU:CD	0.42	2.88	2	2
1:A:341:GLU:OE2	1:A:342:LEU:O	0.42	2.37	1	2
1:A:441:HIS:CE1	1:B:556:PRO:HB3	0.42	2.48	1	2
1:A:287:ASN:O	1:A:530:ILE:HG13	0.42	2.10	2	1
1:B:287:ASN:HB3	1:B:530:ILE:HG23	0.42	1.90	2	1
1:A:221:ASP:CB	1:A:224:ASN:OD1	0.42	2.68	2	2
1:B:181:THR:O	1:B:203:VAL:C	0.42	2.63	1	2
1:B:205:THR:HG23	1:B:208:VAL:H	0.42	1.72	1	2
1:B:287:ASN:HD21	1:B:528:ILE:HD13	0.42	1.73	1	1
1:A:282:GLU:OE2	1:A:286:ARG:NH2	0.42	2.52	2	1
1:A:181:THR:O	1:A:203:VAL:C	0.42	2.63	1	2
1:A:186:ARG:C	1:A:188:SER:N	0.42	2.76	2	2
1:B:8:SER:CB	1:B:199:LEU:O	0.42	2.67	1	2
1:A:186:ARG:CG	1:A:186:ARG:NH1	0.42	2.82	2	1
1:A:259:LEU:N	1:A:260:PRO:HD2	0.42	2.29	2	1
1:A:8:SER:CB	1:A:199:LEU:O	0.42	2.68	1	2
1:A:277:THR:N	1:A:280:ASP:OD2	0.42	2.52	1	1
1:A:375:ARG:HH22	1:A:418:LYS:NZ	0.42	2.12	1	2
1:A:429:MET:HE2	1:A:431:GLU:CD	0.42	2.39	1	2
1:A:513:LEU:HD22	1:A:568:PHE:CD1	0.42	2.50	1	2
1:B:282:GLU:OE1	1:B:286:ARG:NH2	0.42	2.52	1	1
1:B:330:ILE:HD13	1:B:389:MET:HB2	0.42	1.91	1	2
1:B:361:ARG:HH22	1:B:394:ILE:HG21	0.42	1.74	1	2
1:B:386:LEU:HD23	1:B:387:ARG:C	0.42	2.39	1	2
1:A:301:PHE:O	1:A:301:PHE:CD1	0.42	2.73	1	2
1:B:86:GLU:C	1:B:86:GLU:CD	0.42	2.87	1	2
1:B:221:ASP:CB	1:B:224:ASN:OD1	0.42	2.67	1	2
1:A:547:VAL:O	1:A:551:GLN:HG3	0.42	2.14	1	2
1:B:32:SER:OG	1:B:33:ALA:N	0.42	2.52	1	2
1:B:89:ILE:C	1:B:89:ILE:CD1	0.42	2.93	1	2
1:B:89:ILE:HG23	1:B:90:ILE:N	0.42	2.30	1	2
1:B:167:GLU:N	1:B:167:GLU:OE1	0.42	2.52	2	2
1:B:392:MET:H	1:B:429:MET:CE	0.42	2.27	1	2
1:A:57:ILE:HG12	1:A:58:LYS:N	0.42	2.29	1	2
1:A:179:PHE:O	1:A:201:ALA:HB1	0.42	2.15	1	2
1:B:304:ARG:HD3	1:B:306:ALA:O	0.42	2.15	1	2
1:B:305:ASP:O	1:B:344:TYR:CE1	0.42	2.73	1	2
1:B:259:LEU:N	1:B:260:PRO:HD2	0.42	2.29	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:550:GLU:O	1:A:551:GLN:C	0.42	2.62	1	2
1:B:116:GLU:C	1:B:116:GLU:CD	0.42	2.87	2	2
1:B:179:PHE:O	1:B:201:ALA:HB1	0.42	2.15	2	2
1:A:232:THR:HG22	1:A:234:GLU:N	0.41	2.27	2	2
1:A:330:ILE:HD13	1:A:389:MET:HB2	0.41	1.92	1	2
1:B:115:LEU:O	1:B:118:LEU:HB2	0.41	2.15	1	2
1:A:214:ASN:OD1	1:A:214:ASN:O	0.41	2.38	1	2
1:B:24:ILE:CG1	1:B:139:ARG:HH11	0.41	2.27	1	2
1:B:301:PHE:O	1:B:301:PHE:CD1	0.41	2.73	1	2
1:A:11:ILE:CG2	1:A:243:GLN:CB	0.41	2.99	2	2
1:A:167:GLU:OE1	1:A:167:GLU:N	0.41	2.53	1	2
1:A:320:VAL:O	1:A:324:CYS:SG	0.41	2.61	1	2
1:A:388:ILE:O	1:A:388:ILE:HG13	0.41	2.14	1	2
1:B:464:ASP:CG	1:B:467:ASN:CB	0.41	2.93	1	2
1:B:513:LEU:HD22	1:B:568:PHE:CD1	0.41	2.49	1	2
1:B:558:THR:O	1:B:559:ASP:C	0.41	2.61	1	2
1:A:89:ILE:HG23	1:A:90:ILE:N	0.41	2.31	2	2
1:A:115:LEU:O	1:A:118:LEU:HB2	0.41	2.15	2	2
1:A:180:ILE:O	1:A:180:ILE:HG12	0.41	2.15	1	2
1:A:277:THR:O	1:A:278:VAL:C	0.41	2.62	1	2
1:A:327:GLN:OE1	1:A:327:GLN:O	0.41	2.38	1	2
1:B:70:GLU:C	1:B:70:GLU:OE1	0.41	2.63	1	2
1:B:352:ASN:O	1:B:353:PRO:C	0.41	2.64	1	2
1:B:549:ALA:O	1:B:550:GLU:C	0.41	2.63	1	2
1:A:387:ARG:CD	1:A:387:ARG:N	0.41	2.83	1	2
1:A:392:MET:H	1:A:429:MET:CE	0.41	2.28	1	2
1:B:375:ARG:HH22	1:B:418:LYS:NZ	0.41	2.13	1	2
1:B:473:LEU:N	1:B:473:LEU:HD22	0.41	2.30	1	2
1:B:190:THR:O	1:B:193:MET:HG3	0.41	2.15	2	1
1:A:89:ILE:C	1:A:89:ILE:CD1	0.41	2.94	2	2
1:B:391:PRO:HA	1:B:429:MET:CG	0.41	2.41	1	2
1:B:405:GLU:O	1:B:406:ILE:C	0.41	2.62	1	2
1:A:32:SER:OG	1:A:33:ALA:N	0.41	2.52	2	2
1:A:177:LEU:N	1:A:177:LEU:HD22	0.41	2.31	1	2
1:A:386:LEU:HD23	1:A:387:ARG:C	0.41	2.40	1	2
1:B:327:GLN:OE1	1:B:327:GLN:O	0.41	2.38	1	2
1:A:176:VAL:O	1:A:176:VAL:CG1	0.41	2.69	1	2
1:A:313:GLN:OE1	1:A:317:TYR:OH	0.41	2.29	1	2
1:A:470:ILE:O	1:A:471:SER:C	0.41	2.64	1	2
1:B:11:ILE:CG2	1:B:243:GLN:CB	0.41	2.99	1	2
1:B:176:VAL:O	1:B:176:VAL:CG1	0.41	2.68	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:341:GLU:OE2	1:B:342:LEU:O	0.41	2.38	1	2
1:B:470:ILE:O	1:B:470:ILE:HG23	0.41	2.16	1	2
1:B:282:GLU:OE2	1:B:286:ARG:NH2	0.41	2.52	2	1
1:A:292:VAL:O	1:A:330:ILE:CG2	0.41	2.69	1	2
1:A:327:GLN:OE1	1:A:328:ALA:C	0.41	2.64	1	2
1:A:456:LEU:HD22	1:A:484:LEU:CD1	0.41	2.38	1	2
1:B:11:ILE:CD1	1:B:13:PHE:CE1	0.41	3.01	1	2
1:A:130:VAL:HG23	1:A:131:ARG:N	0.40	2.31	1	2
1:A:205:THR:HG21	1:A:208:VAL:CG1	0.40	2.46	1	2
1:A:295:TYR:HB3	1:A:331:VAL:HA	0.40	1.94	1	2
1:A:352:ASN:O	1:A:353:PRO:C	0.40	2.63	1	2
1:B:86:GLU:O	1:B:90:ILE:HG12	0.40	2.15	1	2
1:B:235:VAL:C	1:B:237:ASP:N	0.40	2.79	1	1
1:B:181:THR:H	1:B:202:ILE:HD13	0.40	1.76	1	1
1:B:76:HIS:C	1:B:77:ILE:HD13	0.40	2.37	2	1
1:B:292:VAL:O	1:B:330:ILE:CG2	0.40	2.69	1	2
1:B:295:TYR:HB3	1:B:331:VAL:HA	0.40	1.93	1	2
1:B:485:ILE:HG13	1:B:486:LYS:N	0.40	2.32	1	2
1:A:324:CYS:HB3	1:A:327:GLN:NE2	0.40	2.31	1	2
1:A:405:GLU:O	1:A:406:ILE:C	0.40	2.62	1	2
1:A:456:LEU:HD23	1:A:456:LEU:HA	0.40	1.80	1	2
1:A:470:ILE:O	1:A:470:ILE:HG23	0.40	2.16	1	2

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%)	536±0 (94±0%)	28±0 (5±0%)	7±0 (1±0%)	13	61
1	B	571/573 (100%)	536±0 (94±0%)	27±1 (5±0%)	8±0 (1±0%)	12	60
All	All	2284/2292 (100%)	2146 (94%)	109 (5%)	29 (1%)	12	60

All 19 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	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	278	VAL	2
1	A	255	LYS	1
1	A	256	LEU	1
1	B	255	LYS	1
1	B	256	LEU	1
1	B	261	ALA	1
1	A	254	ALA	1
1	A	259	LEU	1
1	B	254	ALA	1
1	B	259	LEU	1

6.3.2 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 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%)	394±2 (83±0%)	80±2 (17±0%)	4	38
1	B	474/474 (100%)	395±0 (83±0%)	79±0 (17±0%)	4	39
All	All	1896/1896 (100%)	1579 (83%)	317 (17%)	4	39

All 165 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	11	ILE	2
1	A	27	ASP	2
1	A	28	ARG	2
1	A	32	SER	2
1	A	54	LEU	2
1	A	57	ILE	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	67	GLU	2
1	A	70	GLU	2
1	A	74	GLU	2
1	A	77	ILE	2
1	A	79	LEU	2
1	A	89	ILE	2
1	A	101	ASP	2
1	A	105	HIS	2
1	A	130	VAL	2
1	A	144	LEU	2
1	A	163	LEU	2
1	A	167	GLU	2
1	A	170	GLN	2
1	A	180	ILE	2
1	A	181	THR	2
1	A	182	ASP	2
1	A	193	MET	2
1	A	202	ILE	2
1	A	205	THR	2
1	A	209	THR	2
1	A	213	LYS	2
1	A	215	ASP	2
1	A	216	ASP	2
1	A	225	ASN	2
1	A	242	VAL	2
1	A	243	GLN	2
1	A	249	GLU	2
1	A	256	LEU	2
1	A	268	GLN	2
1	A	269	VAL	2
1	A	292	VAL	2
1	A	294	LEU	2
1	A	300	LEU	2
1	A	304	ARG	2
1	A	327	GLN	2
1	A	329	VAL	2
1	A	330	ILE	2
1	A	336	ILE	2
1	A	342	LEU	2
1	A	354	PHE	2
1	A	357	TRP	2
1	A	372	ASP	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	377	ILE	2
1	A	387	ARG	2
1	A	388	ILE	2
1	A	404	LYS	2
1	A	411	GLN	2
1	A	423	SER	2
1	A	429	MET	2
1	A	438	ILE	2
1	A	451	ILE	2
1	A	453	THR	2
1	A	464	ASP	2
1	A	465	ARG	2
1	A	470	ILE	2
1	A	473	LEU	2
1	A	484	LEU	2
1	A	485	ILE	2
1	A	486	LYS	2
1	A	497	LYS	2
1	A	499	THR	2
1	A	505	LEU	2
1	A	515	LEU	2
1	A	518	MET	2
1	A	530	ILE	2
1	A	534	LYS	2
1	A	538	ARG	2
1	A	540	THR	2
1	A	557	THR	2
1	A	561	LEU	2
1	A	562	MET	2
1	B	11	ILE	2
1	B	27	ASP	2
1	B	28	ARG	2
1	B	32	SER	2
1	B	54	LEU	2
1	B	57	ILE	2
1	B	67	GLU	2
1	B	70	GLU	2
1	B	74	GLU	2
1	B	77	ILE	2
1	B	79	LEU	2
1	B	89	ILE	2
1	B	101	ASP	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	105	HIS	2
1	B	130	VAL	2
1	B	144	LEU	2
1	B	163	LEU	2
1	B	167	GLU	2
1	B	170	GLN	2
1	B	180	ILE	2
1	B	181	THR	2
1	B	182	ASP	2
1	B	202	ILE	2
1	B	205	THR	2
1	B	209	THR	2
1	B	213	LYS	2
1	B	215	ASP	2
1	B	216	ASP	2
1	B	225	ASN	2
1	B	242	VAL	2
1	B	243	GLN	2
1	B	249	GLU	2
1	B	256	LEU	2
1	B	268	GLN	2
1	B	269	VAL	2
1	B	292	VAL	2
1	B	294	LEU	2
1	B	300	LEU	2
1	B	304	ARG	2
1	B	327	GLN	2
1	B	329	VAL	2
1	B	330	ILE	2
1	B	336	ILE	2
1	B	342	LEU	2
1	B	354	PHE	2
1	B	357	TRP	2
1	B	372	ASP	2
1	B	377	ILE	2
1	B	387	ARG	2
1	B	388	ILE	2
1	B	404	LYS	2
1	B	411	GLN	2
1	B	423	SER	2
1	B	429	MET	2
1	B	438	ILE	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	451	ILE	2
1	B	453	THR	2
1	B	464	ASP	2
1	B	465	ARG	2
1	B	470	ILE	2
1	B	473	LEU	2
1	B	484	LEU	2
1	B	485	ILE	2
1	B	486	LYS	2
1	B	497	LYS	2
1	B	499	THR	2
1	B	505	LEU	2
1	B	515	LEU	2
1	B	518	MET	2
1	B	534	LYS	2
1	B	538	ARG	2
1	B	540	THR	2
1	B	557	THR	2
1	B	561	LEU	2
1	B	562	MET	2
1	A	197	LEU	1
1	A	258	ASP	1
1	A	259	LEU	1
1	A	528	ILE	1
1	B	192	ILE	1
1	B	196	SER	1
1	B	258	ASP	1
1	B	259	LEU	1
1	A	186	ARG	1
1	B	186	ARG	1
1	B	190	THR	1
1	B	193	MET	1
1	B	530	ILE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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