



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:06 AM UTC

PDB ID : 1L6O / pdb_00001l6o
Title : XENOPUS DISHEVELLED PDZ DOMAIN
Authors : Cheyette, B.N.R.; Waxman, J.S.; Miller, J.R.; Takemaru, K.-I.; Sheldahl, L.C.;
Khlebtsova, N.; Fox, E.P.; Earnest, T.; Moon, R.T.
Deposited on : 2002-03-11
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

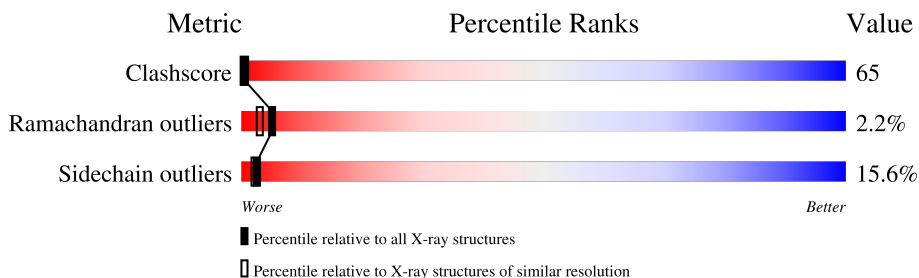
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	95	8% 45% 37% 9%
1	B	95	7% 29% 46% 15% .
1	C	95	9% 48% 34% 5% .
2	D	8	12% 25% 50% 12%
2	E	8	12% 25% 38% 25%
2	F	8	12% 25% 25% 38%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2328 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Segment polarity protein dishevelled homolog DVL-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	95	Total	C	N	O	Se	0	0	0
			724	453	128	138	5			
1	B	93	Total	C	N	O	Se	0	0	0
			703	441	122	135	5			
1	C	92	Total	C	N	O	Se	0	0	0
			693	435	119	134	5			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	MSE	-	SEE REMARK 999	UNP P51142
A	259	MSE	MET	modified residue	UNP P51142
A	287	MSE	MET	modified residue	UNP P51142
A	303	MSE	MET	modified residue	UNP P51142
A	315	MSE	MET	modified residue	UNP P51142
A	341	LEU	-	expression tag	UNP P51142
A	342	GLU	-	expression tag	UNP P51142
A	343	HIS	-	expression tag	UNP P51142
A	344	HIS	-	expression tag	UNP P51142
A	345	HIS	-	expression tag	UNP P51142
B	251	MSE	-	SEE REMARK 999	UNP P51142
B	259	MSE	MET	modified residue	UNP P51142
B	287	MSE	MET	modified residue	UNP P51142
B	303	MSE	MET	modified residue	UNP P51142
B	315	MSE	MET	modified residue	UNP P51142
B	341	LEU	-	expression tag	UNP P51142
B	342	GLU	-	expression tag	UNP P51142
B	343	HIS	-	expression tag	UNP P51142
B	344	HIS	-	expression tag	UNP P51142
B	345	HIS	-	expression tag	UNP P51142
C	251	MSE	-	SEE REMARK 999	UNP P51142
C	259	MSE	MET	modified residue	UNP P51142
C	287	MSE	MET	modified residue	UNP P51142

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Chain	Residue	Modelled	Actual	Comment	Reference
C	303	MSE	MET	modified residue	UNP P51142
C	315	MSE	MET	modified residue	UNP P51142
C	341	LEU	-	expression tag	UNP P51142
C	342	GLU	-	expression tag	UNP P51142
C	343	HIS	-	expression tag	UNP P51142
C	344	HIS	-	expression tag	UNP P51142
C	345	HIS	-	expression tag	UNP P51142

- Molecule 2 is a protein called Dapper 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	8	Total	C	N	O	S	0	0	0
			61	39	9	12	1			
2	E	8	Total	C	N	O	S	0	0	0
			61	39	9	12	1			
2	F	8	Total	C	N	O	S	0	0	0
			61	39	9	12	1			

- Molecule 3 is water.

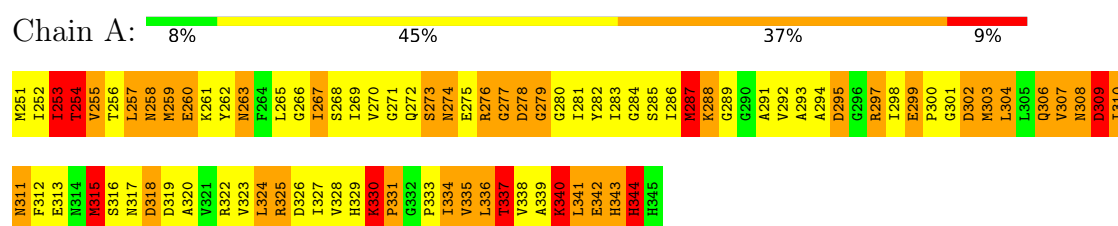
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	3	Total	O	0	0
			3	3		
3	C	4	Total	O	0	0
			4	4		
3	E	1	Total	O	0	0
			1	1		
3	F	1	Total	O	0	0
			1	1		

3 Residue-property plots

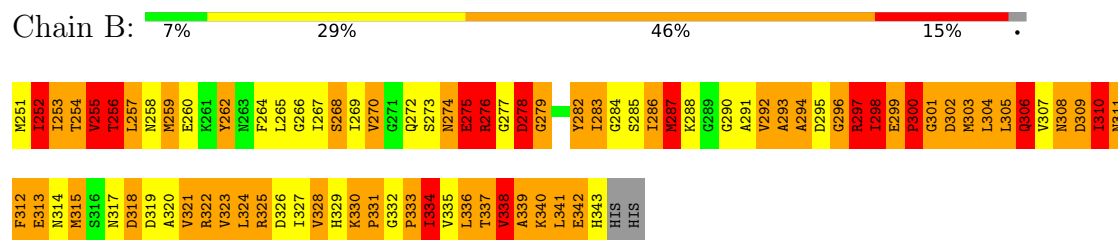
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

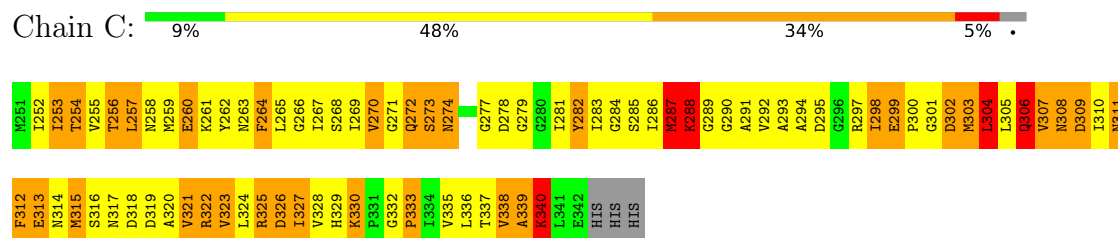
- Molecule 1: Segment polarity protein dishevelled homolog DVL-2



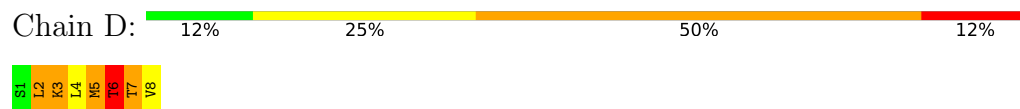
- Molecule 1: Segment polarity protein dishevelled homolog DVL-2



- Molecule 1: Segment polarity protein dishevelled homolog DVL-2



- Molecule 2: Dapper 1



- Molecule 2: Dapper 1





● Molecule 2: Dapper 1



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.73Å 84.73Å 123.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.23 – 2.20	Depositor
% Data completeness (in resolution range)	96.0 (54.23-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.277 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2328	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

5 Model quality ⓘ

5.1 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 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	4.20	146/730 (20.0%)	2.81	74/977 (7.6%)
1	B	3.95	110/707 (15.6%)	3.10	108/947 (11.4%)
1	C	3.61	101/696 (14.5%)	2.87	60/932 (6.4%)
2	D	5.06	11/60 (18.3%)	2.88	8/78 (10.3%)
2	E	5.08	9/60 (15.0%)	2.98	7/78 (9.0%)
2	F	5.32	12/60 (20.0%)	3.18	8/78 (10.3%)
All	All	4.04	389/2313 (16.8%)	2.93	265/3090 (8.6%)

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 outliers	#Planarity outliers
1	B	0	3
2	D	0	1
2	F	0	1
All	All	0	5

All (389) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	MSE	SE-CE	-27.11	1.14	1.95
2	D	5	MET	SD-CE	-24.34	1.18	1.79
1	B	315	MSE	SE-CE	-23.68	1.24	1.95
2	E	5	MET	SD-CE	-22.39	1.23	1.79
1	C	286	ILE	C-O	-20.29	1.02	1.24
2	F	6	THR	CA-CB	20.27	1.84	1.53
1	B	336	LEU	CA-C	-19.21	1.29	1.52
1	A	283	ILE	CA-C	18.43	1.74	1.52
1	B	303	MSE	CA-C	17.44	1.74	1.52
1	A	311	ASN	C-O	-16.73	1.03	1.24
1	C	283	ILE	CA-CB	-15.73	1.34	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	MET	N-CA	14.97	1.65	1.46
2	E	6	THR	CA-CB	14.80	1.76	1.53
1	B	321	VAL	C-O	14.52	1.40	1.24
1	A	284	GLY	C-O	-14.50	1.04	1.23
1	B	319	ASP	CA-C	-14.45	1.34	1.52
1	B	270	VAL	N-CA	-14.32	1.29	1.46
1	A	331	PRO	CA-C	-13.90	1.36	1.52
1	B	334	ILE	CA-C	-13.66	1.35	1.52
1	B	269	ILE	C-O	-13.47	1.10	1.24
1	A	280	GLY	C-O	13.39	1.35	1.23
1	C	270	VAL	CA-CB	13.09	1.70	1.54
1	B	338	VAL	CA-C	-12.99	1.36	1.52
1	C	311	ASN	C-O	-12.80	1.08	1.24
2	F	6	THR	CB-CG2	-12.69	1.10	1.52
1	C	323	VAL	CA-C	-12.64	1.36	1.52
2	D	5	MET	N-CA	12.60	1.62	1.46
1	B	283	ILE	CA-C	12.50	1.67	1.52
1	A	292	VAL	CA-C	-12.42	1.36	1.52
1	B	272	GLN	CA-C	-12.26	1.37	1.52
1	A	281	ILE	N-CA	-12.14	1.31	1.46
1	C	328	VAL	C-O	-11.88	1.10	1.24
1	A	311	ASN	CA-CB	11.80	1.70	1.53
1	B	339	ALA	CA-C	11.72	1.67	1.52
1	B	286	ILE	C-O	-11.58	1.11	1.24
1	B	337	THR	N-CA	-11.55	1.31	1.46
1	A	307	VAL	N-CA	-11.51	1.32	1.46
1	C	305	LEU	CA-C	11.38	1.67	1.53
1	A	267	ILE	C-O	-11.29	1.12	1.24
1	B	306	GLN	C-O	11.21	1.37	1.23
2	D	7	THR	CA-CB	10.97	1.74	1.53
1	B	259	MSE	SE-CE	-10.91	1.62	1.95
1	A	315	MSE	SE-CE	-10.90	1.62	1.95
1	C	288	LYS	C-N	-10.86	1.18	1.33
1	A	255	VAL	CA-CB	10.79	1.69	1.54
1	B	338	VAL	CB-CG2	-10.79	1.17	1.52
1	A	338	VAL	C-O	-10.78	1.12	1.23
1	A	293	ALA	CA-CB	10.71	1.71	1.53
2	F	4	LEU	N-CA	-10.64	1.32	1.46
1	C	306	GLN	N-CA	-10.61	1.33	1.46
1	B	292	VAL	CA-CB	-10.53	1.40	1.54
1	B	335	VAL	N-CA	-10.46	1.33	1.46
1	C	267	ILE	C-O	-10.29	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	VAL	CA-CB	-10.22	1.42	1.54
2	F	2	LEU	CA-C	-10.22	1.39	1.52
1	A	327	ILE	CA-CB	-10.13	1.40	1.54
1	A	262	TYR	C-O	-10.12	1.11	1.23
1	A	298	ILE	N-CA	-10.01	1.34	1.46
1	A	306	GLN	CA-C	9.96	1.65	1.52
1	A	269	ILE	C-O	-9.92	1.13	1.24
2	E	6	THR	C-O	-9.91	1.13	1.24
1	A	334	ILE	CA-CB	-9.90	1.41	1.54
1	A	306	GLN	C-O	-9.86	1.10	1.23
1	B	286	ILE	CA-C	-9.83	1.39	1.52
1	C	338	VAL	CA-C	-9.82	1.41	1.52
1	C	322	ARG	N-CA	9.74	1.58	1.46
1	A	336	LEU	N-CA	-9.71	1.33	1.46
1	A	270	VAL	C-O	-9.71	1.13	1.24
1	C	269	ILE	CA-C	-9.71	1.40	1.52
1	C	321	VAL	C-O	9.70	1.35	1.24
1	A	287	MSE	SE-CE	-9.68	1.66	1.95
1	A	260	GLU	CA-C	-9.64	1.43	1.53
1	B	254	THR	C-O	-9.62	1.11	1.23
1	A	254	THR	CA-CB	-9.56	1.39	1.53
1	C	288	LYS	CB-CG	-9.46	1.24	1.52
1	B	322	ARG	N-CA	9.44	1.58	1.46
2	D	4	LEU	N-CA	-9.42	1.34	1.46
1	C	283	ILE	CA-C	-9.37	1.42	1.53
1	B	327	ILE	CA-C	-9.36	1.39	1.52
1	A	261	LYS	N-CA	-9.35	1.34	1.46
1	B	254	THR	N-CA	-9.21	1.33	1.45
1	A	272	GLN	CA-CB	-9.16	1.40	1.53
2	E	3	LYS	CD-CE	9.03	1.79	1.52
1	A	265	LEU	CA-C	-8.97	1.40	1.52
1	A	286	ILE	CA-C	8.92	1.64	1.52
1	B	309	ASP	C-O	-8.90	1.11	1.23
1	C	333	PRO	CB-CG	8.90	1.94	1.49
1	B	303	MSE	CA-CB	-8.85	1.41	1.53
1	B	252	ILE	N-CA	-8.80	1.35	1.46
1	A	265	LEU	C-O	-8.79	1.12	1.24
1	B	333	PRO	C-O	8.79	1.35	1.24
1	C	319	ASP	C-O	-8.74	1.13	1.24
1	C	321	VAL	CA-CB	8.68	1.64	1.54
1	A	330	LYS	CA-C	-8.66	1.42	1.52
1	C	294	ALA	C-O	-8.66	1.12	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	318	ASP	CA-CB	-8.65	1.39	1.53
1	C	273	SER	N-CA	-8.63	1.35	1.46
1	C	269	ILE	CA-CB	8.59	1.65	1.54
2	F	4	LEU	CG-CD1	8.58	1.80	1.52
1	A	270	VAL	CA-C	8.57	1.62	1.52
1	B	303	MSE	SE-CE	-8.52	1.69	1.95
1	A	318	ASP	CA-C	8.50	1.63	1.52
1	B	268	SER	N-CA	8.49	1.55	1.45
1	B	326	ASP	C-O	-8.48	1.14	1.24
1	A	327	ILE	C-O	-8.45	1.12	1.24
1	B	320	ALA	CA-C	-8.45	1.41	1.52
1	B	311	ASN	CB-CG	8.43	1.73	1.52
1	C	288	LYS	CA-CB	-8.40	1.40	1.53
1	B	270	VAL	CA-CB	8.37	1.66	1.54
1	A	252	ILE	CA-CB	-8.35	1.44	1.54
1	A	319	ASP	CA-CB	8.31	1.66	1.53
1	B	323	VAL	CA-C	-8.26	1.42	1.52
1	A	302	ASP	CG-OD1	8.25	1.41	1.25
1	C	292	VAL	C-O	-8.24	1.14	1.24
1	C	322	ARG	C-O	8.21	1.34	1.24
2	D	6	THR	CB-CG2	-8.16	1.25	1.52
1	C	325	ARG	CG-CD	8.15	1.76	1.52
1	C	314	ASN	CB-CG	8.12	1.72	1.52
1	B	270	VAL	C-O	-8.12	1.16	1.24
1	A	281	ILE	CA-CB	8.08	1.66	1.54
1	A	252	ILE	N-CA	-8.02	1.36	1.46
1	A	253	ILE	CG1-CD1	8.00	1.82	1.51
1	B	255	VAL	N-CA	-8.00	1.36	1.46
1	C	264	PHE	CA-C	-7.99	1.42	1.52
2	D	7	THR	CA-C	-7.97	1.42	1.52
1	C	264	PHE	N-CA	-7.95	1.35	1.45
1	A	257	LEU	CA-C	-7.95	1.43	1.52
1	B	309	ASP	CA-C	-7.93	1.40	1.52
1	A	322	ARG	NE-CZ	-7.92	1.24	1.33
2	F	2	LEU	CA-CB	-7.91	1.41	1.53
1	A	268	SER	CA-C	7.86	1.63	1.52
1	B	282	TYR	CA-C	-7.85	1.43	1.52
1	C	301	GLY	CA-C	7.84	1.62	1.51
1	B	269	ILE	CA-CB	7.83	1.65	1.54
1	B	306	GLN	CA-C	-7.82	1.43	1.52
1	A	307	VAL	CA-C	7.82	1.62	1.52
1	C	312	PHE	N-CA	7.69	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	304	LEU	C-O	7.69	1.33	1.24
1	C	264	PHE	CB-CG	-7.68	1.32	1.50
1	C	293	ALA	C-O	-7.67	1.14	1.24
1	B	272	GLN	CG-CD	7.67	1.71	1.52
1	C	321	VAL	N-CA	-7.66	1.37	1.46
1	B	325	ARG	CA-C	-7.65	1.43	1.52
1	C	300	PRO	C-O	-7.63	1.14	1.23
1	A	279	GLY	C-O	-7.63	1.14	1.23
2	F	2	LEU	C-O	-7.50	1.14	1.23
1	C	328	VAL	CA-CB	7.46	1.63	1.54
1	B	324	LEU	CG-CD1	7.44	1.77	1.52
1	B	293	ALA	CA-CB	-7.41	1.41	1.53
1	A	292	VAL	C-N	7.39	1.43	1.34
1	B	318	ASP	CA-C	-7.38	1.43	1.52
1	B	312	PHE	CB-CG	-7.38	1.33	1.50
1	A	262	TYR	CG-CD1	-7.37	1.23	1.39
1	A	320	ALA	CA-C	7.37	1.62	1.52
1	A	336	LEU	CA-C	-7.33	1.43	1.52
1	A	253	ILE	CB-CG2	7.32	1.76	1.52
1	A	254	THR	CB-OG1	-7.30	1.32	1.43
1	B	308	ASN	CA-C	7.29	1.62	1.53
1	A	323	VAL	N-CA	-7.28	1.37	1.46
1	A	280	GLY	N-CA	7.21	1.53	1.45
2	E	5	MET	C-O	-7.20	1.13	1.23
2	E	5	MET	N-CA	7.19	1.55	1.46
1	B	253	ILE	N-CA	-7.18	1.37	1.46
1	A	287	MSE	CA-C	-7.16	1.43	1.52
1	C	295	ASP	N-CA	7.16	1.55	1.46
1	B	302	ASP	N-CA	7.15	1.55	1.46
1	C	330	LYS	CD-CE	7.14	1.73	1.52
1	B	259	MSE	CA-C	-7.13	1.40	1.52
2	E	7	THR	CA-C	-7.12	1.43	1.52
1	C	281	ILE	CA-CB	7.08	1.65	1.55
1	A	337	THR	CA-CB	7.07	1.71	1.53
1	A	306	GLN	CB-CG	-7.03	1.31	1.52
1	C	269	ILE	N-CA	7.03	1.54	1.46
2	F	5	MET	C-N	6.99	1.42	1.33
1	A	339	ALA	CA-C	-6.99	1.44	1.52
1	A	297	ARG	NE-CZ	-6.99	1.25	1.33
1	B	321	VAL	CA-CB	6.97	1.62	1.54
1	B	294	ALA	CA-C	-6.93	1.43	1.52
1	C	336	LEU	CA-C	-6.89	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	ASN	CA-C	6.88	1.62	1.52
1	B	337	THR	CA-C	6.87	1.60	1.52
1	A	263	ASN	C-O	-6.86	1.14	1.23
1	C	333	PRO	C-O	-6.85	1.15	1.23
1	A	257	LEU	CA-CB	-6.83	1.43	1.53
2	E	6	THR	N-CA	6.83	1.54	1.46
1	C	309	ASP	CA-C	-6.82	1.42	1.52
1	C	287	MSE	SE-CE	6.79	2.15	1.95
1	B	319	ASP	N-CA	6.78	1.54	1.46
1	A	281	ILE	C-O	-6.77	1.17	1.24
1	A	316	SER	CA-C	6.75	1.61	1.52
1	B	312	PHE	N-CA	-6.74	1.37	1.46
1	A	300	PRO	C-O	-6.71	1.16	1.23
1	A	287	MSE	CA-CB	-6.68	1.43	1.53
1	B	305	LEU	CG-CD2	-6.68	1.30	1.52
1	C	317	ASN	CA-CB	6.67	1.64	1.53
1	C	340	LYS	CA-C	-6.67	1.44	1.52
1	A	270	VAL	N-CA	-6.67	1.38	1.46
1	C	252	ILE	N-CA	-6.67	1.37	1.46
1	A	310	ILE	CB-CG2	6.65	1.74	1.52
1	B	311	ASN	CA-CB	-6.63	1.43	1.53
1	A	268	SER	N-CA	-6.62	1.37	1.45
2	E	4	LEU	CG-CD1	6.62	1.74	1.52
1	A	315	MSE	CG-SE	6.61	2.15	1.95
1	A	299	GLU	N-CA	6.61	1.51	1.45
2	D	6	THR	C-O	-6.61	1.17	1.24
1	A	324	LEU	CA-C	6.59	1.61	1.52
1	B	310	ILE	C-O	6.58	1.31	1.24
1	A	283	ILE	C-O	-6.56	1.17	1.24
1	A	255	VAL	CB-CG2	-6.52	1.31	1.52
1	C	337	THR	C-N	-6.49	1.25	1.33
1	B	288	LYS	CA-CB	-6.48	1.43	1.53
1	C	297	ARG	NE-CZ	6.47	1.40	1.33
1	C	319	ASP	CA-C	-6.44	1.44	1.52
1	A	330	LYS	CA-CB	-6.44	1.43	1.53
1	A	304	LEU	N-CA	-6.43	1.38	1.46
1	C	307	VAL	CA-CB	-6.42	1.46	1.54
1	C	321	VAL	CA-C	6.42	1.60	1.52
1	B	342	GLU	CA-C	6.40	1.61	1.52
1	C	310	ILE	CA-CB	-6.39	1.46	1.54
1	B	335	VAL	CA-C	6.38	1.60	1.52
1	B	319	ASP	C-N	6.37	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	298	ILE	N-CA	6.36	1.53	1.46
2	D	4	LEU	CG-CD2	6.36	1.73	1.52
1	C	322	ARG	CA-CB	-6.30	1.42	1.53
1	A	329	HIS	C-O	-6.29	1.15	1.24
1	B	301	GLY	CA-C	6.27	1.60	1.51
1	C	260	GLU	CA-C	-6.26	1.44	1.52
1	A	285	SER	CA-C	-6.26	1.44	1.52
1	C	295	ASP	C-O	-6.25	1.15	1.23
1	B	325	ARG	C-O	-6.24	1.16	1.24
1	C	323	VAL	C-O	6.23	1.31	1.24
1	B	309	ASP	N-CA	6.22	1.54	1.46
1	B	318	ASP	C-O	6.22	1.31	1.24
1	C	289	GLY	N-CA	6.21	1.56	1.44
1	A	268	SER	C-O	-6.19	1.16	1.23
1	C	317	ASN	C-O	6.17	1.31	1.24
1	A	266	GLY	N-CA	6.17	1.53	1.45
2	D	8	VAL	CB-CG1	-6.16	1.32	1.52
1	A	304	LEU	CB-CG	-6.15	1.41	1.53
1	C	299	GLU	C-O	-6.15	1.19	1.24
1	A	281	ILE	CB-CG1	-6.15	1.41	1.53
1	B	325	ARG	NE-CZ	-6.14	1.26	1.33
1	A	311	ASN	CG-OD1	-6.13	1.11	1.23
1	B	306	GLN	CB-CG	6.13	1.70	1.52
1	A	259	MSE	SE-CE	6.12	2.13	1.95
1	C	330	LYS	CG-CD	6.12	1.70	1.52
1	A	322	ARG	CA-C	6.11	1.61	1.52
1	B	252	ILE	CA-C	-6.11	1.45	1.52
1	C	282	TYR	N-CA	6.10	1.53	1.45
1	A	285	SER	C-N	-6.09	1.25	1.33
1	A	315	MSE	CB-CG	-6.09	1.34	1.52
1	A	274	ASN	CA-C	-6.07	1.44	1.53
1	A	307	VAL	C-N	-6.07	1.25	1.33
1	B	279	GLY	CA-C	-6.06	1.43	1.51
1	A	310	ILE	CA-CB	-6.06	1.46	1.54
1	A	317	ASN	N-CA	-6.05	1.39	1.46
1	C	299	GLU	CA-C	-6.05	1.46	1.52
1	B	337	THR	CA-CB	-6.04	1.43	1.53
1	C	329	HIS	N-CA	-6.03	1.38	1.46
1	B	267	ILE	CB-CG2	6.03	1.72	1.52
1	B	270	VAL	CB-CG1	-6.03	1.32	1.52
1	C	320	ALA	C-O	-6.03	1.17	1.24
1	A	323	VAL	CA-CB	6.03	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	324	LEU	CG-CD2	6.01	1.72	1.52
1	A	253	ILE	C-O	6.01	1.30	1.23
2	F	5	MET	CA-C	-5.98	1.45	1.53
1	A	283	ILE	N-CA	-5.97	1.39	1.46
1	A	344	HIS	CA-C	-5.95	1.44	1.52
1	A	292	VAL	CA-CB	5.92	1.62	1.54
1	A	258	ASN	C-O	5.92	1.31	1.23
2	D	3	LYS	C-N	-5.92	1.25	1.33
1	A	287	MSE	C-N	-5.90	1.25	1.33
1	C	326	ASP	CG-OD1	5.88	1.36	1.25
1	B	259	MSE	CG-SE	5.88	2.13	1.95
2	F	7	THR	CA-CB	-5.88	1.39	1.54
1	A	331	PRO	CA-CB	5.83	1.61	1.53
1	B	297	ARG	CD-NE	-5.82	1.38	1.46
1	B	302	ASP	CB-CG	5.82	1.66	1.52
1	A	324	LEU	C-N	-5.81	1.26	1.33
1	A	327	ILE	CB-CG1	-5.81	1.41	1.53
1	A	288	LYS	C-O	-5.81	1.17	1.23
1	A	325	ARG	CB-CG	5.80	1.69	1.52
1	C	302	ASP	CA-C	5.79	1.60	1.52
1	C	309	ASP	CA-CB	-5.79	1.46	1.54
1	C	283	ILE	C-O	-5.79	1.18	1.23
1	C	272	GLN	CD-NE2	5.79	1.45	1.33
1	C	322	ARG	CA-C	-5.77	1.45	1.52
1	A	266	GLY	CA-C	5.76	1.59	1.51
1	B	328	VAL	CA-C	-5.74	1.44	1.52
1	C	281	ILE	CA-C	5.72	1.59	1.52
1	A	326	ASP	C-O	-5.71	1.16	1.24
1	A	286	ILE	C-O	-5.71	1.18	1.24
1	B	252	ILE	CG1-CD1	-5.71	1.29	1.51
1	B	318	ASP	CB-CG	-5.70	1.37	1.52
1	C	290	GLY	CA-C	-5.69	1.45	1.52
1	A	324	LEU	C-O	-5.69	1.17	1.24
2	D	3	LYS	CA-CB	-5.69	1.43	1.53
1	B	309	ASP	CG-OD2	5.69	1.36	1.25
1	A	343	HIS	C-O	-5.68	1.16	1.24
1	A	319	ASP	C-O	-5.65	1.17	1.24
1	B	304	LEU	CA-C	5.65	1.60	1.52
1	B	256	THR	CA-CB	5.65	1.61	1.53
1	A	313	GLU	N-CA	5.64	1.53	1.46
1	C	339	ALA	C-O	5.63	1.30	1.24
1	C	271	GLY	CA-C	5.62	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	329	HIS	CA-C	5.62	1.60	1.52
1	B	299	GLU	N-CA	5.61	1.50	1.46
1	B	310	ILE	CB-CG1	-5.60	1.42	1.53
1	A	288	LYS	C-N	-5.59	1.26	1.34
1	A	255	VAL	C-O	-5.59	1.18	1.24
1	C	256	THR	C-O	-5.59	1.17	1.24
1	B	267	ILE	CA-C	-5.58	1.46	1.52
1	B	335	VAL	CB-CG2	5.58	1.71	1.52
1	B	266	GLY	C-O	5.56	1.31	1.23
1	A	269	ILE	N-CA	-5.54	1.38	1.46
1	C	268	SER	CA-C	-5.53	1.45	1.52
1	C	340	LYS	C-O	-5.53	1.17	1.23
1	A	341	LEU	C-N	-5.53	1.25	1.33
1	C	303	MSE	SE-CE	-5.53	1.78	1.95
1	A	339	ALA	CA-CB	-5.52	1.45	1.53
1	C	266	GLY	N-CA	5.52	1.53	1.45
1	A	282	TYR	CA-CB	5.52	1.65	1.54
1	A	278	ASP	CB-CG	5.52	1.65	1.52
1	B	322	ARG	C-O	5.52	1.30	1.24
1	B	318	ASP	N-CA	5.51	1.53	1.46
1	C	316	SER	CA-C	5.50	1.60	1.52
1	A	295	ASP	CB-CG	-5.50	1.38	1.52
1	C	315	MSE	CA-C	-5.50	1.45	1.53
1	B	305	LEU	CA-C	5.49	1.59	1.52
1	A	312	PHE	C-N	-5.48	1.26	1.34
1	C	292	VAL	CA-C	5.46	1.59	1.52
1	A	309	ASP	CG-OD2	5.45	1.35	1.25
1	A	303	MSE	CA-C	5.45	1.59	1.52
1	A	299	GLU	CA-C	-5.43	1.47	1.52
1	A	267	ILE	CA-CB	-5.41	1.47	1.54
1	A	336	LEU	C-O	5.39	1.30	1.23
1	A	289	GLY	CA-C	5.39	1.59	1.52
1	B	335	VAL	C-O	5.38	1.30	1.24
1	C	326	ASP	CG-OD2	5.38	1.35	1.25
1	A	301	GLY	N-CA	-5.38	1.36	1.44
1	C	337	THR	C-O	-5.36	1.18	1.24
1	A	336	LEU	CG-CD1	5.35	1.70	1.52
2	F	4	LEU	CA-CB	5.34	1.60	1.53
1	A	267	ILE	N-CA	-5.32	1.40	1.46
1	C	324	LEU	C-O	-5.32	1.17	1.24
1	C	322	ARG	CG-CD	5.32	1.68	1.52
1	B	313	GLU	CA-C	-5.31	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	330	LYS	C-N	-5.31	1.26	1.33
1	B	290	GLY	CA-C	-5.31	1.47	1.52
1	C	328	VAL	CA-C	-5.31	1.46	1.52
1	C	315	MSE	C-O	-5.31	1.16	1.23
1	B	341	LEU	CA-C	5.30	1.59	1.52
1	A	252	ILE	CA-C	-5.29	1.46	1.52
1	B	298	ILE	N-CA	5.26	1.52	1.46
1	A	294	ALA	CA-CB	-5.25	1.44	1.53
1	A	253	ILE	CB-CG1	-5.24	1.43	1.53
1	B	317	ASN	CG-OD1	5.23	1.33	1.23
1	B	278	ASP	CA-C	5.23	1.59	1.52
1	C	313	GLU	CA-C	-5.23	1.45	1.52
1	B	297	ARG	CZ-NH1	-5.21	1.25	1.32
1	A	339	ALA	N-CA	-5.20	1.39	1.46
1	C	325	ARG	CA-C	-5.19	1.46	1.52
1	A	330	LYS	CD-CE	5.17	1.68	1.52
1	B	324	LEU	C-O	5.17	1.30	1.24
1	C	286	ILE	CB-CG1	-5.16	1.43	1.53
1	B	312	PHE	CG-CD2	-5.14	1.28	1.38
1	A	273	SER	N-CA	-5.14	1.40	1.46
1	A	315	MSE	N-CA	5.13	1.52	1.45
1	B	287	MSE	C-O	-5.13	1.17	1.23
1	A	291	ALA	CA-CB	-5.12	1.45	1.53
1	C	320	ALA	CA-C	5.11	1.59	1.52
1	A	312	PHE	CA-CB	5.09	1.61	1.53
1	C	292	VAL	CB-CG1	-5.09	1.35	1.52
1	C	285	SER	CB-OG	5.09	1.52	1.42
1	C	332	GLY	C-O	-5.09	1.17	1.24
1	B	306	GLN	CA-CB	5.09	1.62	1.53
1	B	267	ILE	C-O	5.08	1.29	1.23
1	A	297	ARG	CG-CD	5.08	1.67	1.52
1	A	294	ALA	C-O	-5.07	1.17	1.24
1	B	322	ARG	CA-CB	-5.06	1.45	1.53
1	B	317	ASN	CA-C	-5.05	1.46	1.52
1	A	263	ASN	CG-ND2	5.03	1.43	1.33
1	A	274	ASN	C-O	5.02	1.29	1.24
1	A	252	ILE	C-O	-5.02	1.17	1.24
1	B	254	THR	CB-OG1	5.01	1.51	1.43
1	A	273	SER	C-O	5.01	1.30	1.23
1	B	325	ARG	CB-CG	-5.01	1.37	1.52
1	C	339	ALA	CA-C	5.00	1.58	1.52
1	A	256	THR	CA-C	-5.00	1.46	1.52

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	288	LYS	CA-C-N	-19.17	93.22	123.31
1	C	288	LYS	C-N-CA	-19.17	93.22	123.31
1	C	288	LYS	N-CA-CB	17.50	134.09	110.29
1	B	334	ILE	CB-CA-C	-11.76	92.01	111.29
1	C	288	LYS	O-C-N	-11.50	109.11	122.68
1	A	297	ARG	N-CA-C	11.46	123.52	111.14
1	C	303	MSE	CA-C-N	-11.41	107.07	123.05
1	C	303	MSE	C-N-CA	-11.41	107.07	123.05
1	C	268	SER	CA-C-N	-11.15	107.49	122.99
1	C	268	SER	C-N-CA	-11.15	107.49	122.99
1	A	308	ASN	CA-C-N	-10.94	100.64	121.54
1	A	308	ASN	C-N-CA	-10.94	100.64	121.54
1	B	254	THR	N-CA-CB	-10.84	94.20	111.43
1	A	256	THR	N-CA-C	10.62	125.83	108.52
1	C	337	THR	CA-C-O	10.60	131.64	120.30
2	E	6	THR	OG1-CB-CG2	-10.52	88.26	109.30
1	C	287	MSE	CA-C-N	-10.43	102.39	120.95
1	C	287	MSE	C-N-CA	-10.43	102.39	120.95
2	F	7	THR	CA-CB-OG1	-10.30	94.15	109.60
1	B	274	ASN	N-CA-C	-9.82	96.09	109.54
1	A	315	MSE	CG-SE-CE	-9.81	77.35	98.92
1	B	309	ASP	CA-C-N	-9.66	108.18	122.68
1	B	309	ASP	C-N-CA	-9.66	108.18	122.68
1	B	290	GLY	N-CA-C	-9.51	96.28	112.06
1	B	286	ILE	CA-C-O	-9.49	111.01	120.31
1	B	340	LYS	CA-C-O	9.42	131.43	120.69
1	B	310	ILE	CB-CA-C	-9.41	95.80	110.95
2	D	7	THR	OG1-CB-CG2	-9.30	90.69	109.30
1	B	336	LEU	N-CA-C	-9.27	94.89	109.72
1	B	313	GLU	CA-C-N	-9.25	108.18	122.60
1	B	313	GLU	C-N-CA	-9.25	108.18	122.60
1	C	268	SER	CA-CB-OG	-8.96	93.18	111.10
1	A	292	VAL	N-CA-C	8.94	119.75	110.72
1	C	288	LYS	CA-C-O	8.81	131.99	122.03
1	C	287	MSE	N-CA-C	8.81	122.54	109.59
1	B	321	VAL	N-CA-C	8.79	118.86	110.42
1	B	255	VAL	CA-C-N	-8.72	110.68	122.72
1	B	255	VAL	C-N-CA	-8.72	110.68	122.72
1	C	337	THR	O-C-N	-8.72	113.15	123.27
1	B	276	ARG	N-CA-C	-8.63	99.84	110.88
1	A	313	GLU	N-CA-C	8.44	121.41	111.71
2	D	7	THR	CA-CB-OG1	-8.41	96.98	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	322	ARG	CA-C-N	-8.23	108.73	120.42
1	C	322	ARG	C-N-CA	-8.23	108.73	120.42
1	B	318	ASP	N-CA-C	8.16	120.18	111.28
2	F	6	THR	CB-CA-C	-8.13	95.68	111.78
1	A	343	HIS	N-CA-C	8.10	128.05	110.80
1	A	335	VAL	CB-CA-C	-8.08	99.85	110.84
1	A	336	LEU	CA-C-N	-7.99	109.79	122.73
1	A	336	LEU	C-N-CA	-7.99	109.79	122.73
1	B	319	ASP	N-CA-C	-7.98	102.66	111.36
1	B	294	ALA	CA-C-N	-7.97	106.85	121.52
1	B	294	ALA	C-N-CA	-7.97	106.85	121.52
1	B	317	ASN	N-CA-C	7.95	119.94	111.28
1	A	342	GLU	CB-CA-C	-7.94	94.31	111.78
1	A	273	SER	CA-C-O	7.89	129.75	120.43
1	B	343	HIS	CA-C-O	7.87	134.19	120.80
1	A	309	ASP	N-CA-C	7.77	127.35	110.80
1	B	334	ILE	CA-C-O	-7.75	111.09	120.78
1	B	254	THR	CA-C-N	-7.63	108.23	121.97
1	B	254	THR	C-N-CA	-7.63	108.23	121.97
1	C	295	ASP	N-CA-C	-7.63	104.50	113.88
1	B	254	THR	O-C-N	-7.62	112.50	122.94
1	C	265	LEU	N-CA-C	-7.58	103.02	111.82
1	C	337	THR	CA-C-N	-7.58	111.92	122.69
1	C	337	THR	C-N-CA	-7.58	111.92	122.69
1	A	283	ILE	CB-CA-C	-7.58	102.22	111.08
1	B	324	LEU	CB-CG-CD2	-7.53	88.11	110.70
1	B	334	ILE	N-CA-C	-7.52	93.71	109.34
1	B	297	ARG	NE-CZ-NH1	-7.51	113.99	121.50
1	B	334	ILE	CG1-CB-CG2	-7.34	88.68	110.70
1	A	337	THR	OG1-CB-CG2	-7.24	94.82	109.30
1	B	319	ASP	N-CA-CB	-7.18	99.54	110.16
1	B	314	ASN	N-CA-CB	-7.15	99.65	110.73
1	C	310	ILE	CB-CG1-CD1	-7.07	98.95	113.80
1	A	262	TYR	CA-C-O	-7.05	112.90	121.36
1	A	291	ALA	CA-C-O	-7.05	112.14	120.10
1	A	325	ARG	CA-C-N	-7.04	108.82	121.14
1	A	325	ARG	C-N-CA	-7.04	108.82	121.14
1	B	252	ILE	CA-C-N	-7.02	109.34	121.97
1	B	252	ILE	C-N-CA	-7.02	109.34	121.97
1	A	304	LEU	CB-CG-CD1	7.00	131.70	110.70
1	C	286	ILE	N-CA-C	6.99	117.94	107.80
1	B	336	LEU	O-C-N	6.98	132.26	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	317	ASN	CA-C-O	6.96	127.92	120.55
1	C	260	GLU	N-CA-C	-6.92	103.18	111.69
2	D	6	THR	CB-CA-C	-6.91	97.73	112.78
1	A	289	GLY	CA-C-O	6.90	125.56	119.56
1	B	298	ILE	CB-CA-C	-6.88	101.42	111.68
1	A	311	ASN	CA-C-O	-6.88	112.94	120.43
1	A	297	ARG	NE-CZ-NH2	6.87	125.38	119.20
1	A	288	LYS	O-C-N	-6.82	114.48	122.87
1	A	255	VAL	N-CA-C	6.81	118.29	108.48
1	B	335	VAL	CA-C-O	6.80	129.28	120.78
1	C	269	ILE	CA-C-N	-6.77	114.28	123.14
1	C	269	ILE	C-N-CA	-6.77	114.28	123.14
1	A	342	GLU	N-CA-C	6.76	120.84	110.36
1	B	299	GLU	CB-CA-C	-6.72	101.16	110.37
1	C	330	LYS	CG-CD-CE	6.72	126.75	111.30
1	B	329	HIS	N-CA-C	6.70	119.41	111.71
2	F	5	MET	CG-SD-CE	-6.69	86.18	100.90
1	A	288	LYS	N-CA-CB	-6.66	99.77	109.83
1	A	253	ILE	CA-CB-CG2	6.61	121.74	110.50
1	B	262	TYR	N-CA-C	6.61	118.99	109.14
1	C	256	THR	OG1-CB-CG2	-6.60	96.09	109.30
1	B	335	VAL	CA-C-N	-6.60	112.45	122.81
1	B	335	VAL	C-N-CA	-6.60	112.45	122.81
1	A	297	ARG	CB-CA-C	6.56	121.27	110.90
1	B	300	PRO	CA-C-N	6.52	134.19	121.41
1	B	300	PRO	C-N-CA	6.52	134.19	121.41
1	A	265	LEU	CA-C-O	-6.52	112.10	119.79
1	C	283	ILE	N-CA-CB	-6.51	104.49	111.46
1	A	286	ILE	N-CA-CB	-6.50	103.19	111.64
2	F	2	LEU	CA-C-O	-6.50	113.45	120.92
1	A	254	THR	CA-C-N	-6.48	114.12	123.06
1	A	254	THR	C-N-CA	-6.48	114.12	123.06
1	C	257	LEU	N-CA-C	6.46	119.93	109.40
1	A	287	MSE	N-CA-C	6.44	120.00	109.76
1	C	313	GLU	CA-C-N	-6.44	111.84	122.08
1	C	313	GLU	C-N-CA	-6.44	111.84	122.08
1	B	288	LYS	N-CA-CB	-6.44	101.16	110.36
1	C	306	GLN	N-CA-C	6.42	119.73	108.75
1	B	252	ILE	N-CA-CB	-6.39	100.68	111.23
1	B	253	ILE	CA-C-O	-6.39	112.80	120.78
1	B	267	ILE	CA-C-N	-6.38	111.69	122.92
1	B	267	ILE	C-N-CA	-6.38	111.69	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	GLY	CA-C-O	6.34	125.76	119.04
1	B	334	ILE	CA-CB-CG1	6.33	121.17	110.40
1	C	278	ASP	N-CA-C	6.33	120.14	109.76
1	B	322	ARG	CA-C-N	-6.25	111.90	120.46
1	B	322	ARG	C-N-CA	-6.25	111.90	120.46
1	B	312	PHE	CB-CG-CD1	6.22	131.27	120.70
1	B	308	ASN	CA-C-N	-6.21	117.11	126.86
1	B	308	ASN	C-N-CA	-6.21	117.11	126.86
1	C	303	MSE	N-CA-C	6.21	119.94	109.76
2	F	8	VAL	CA-C-O	-6.21	102.38	121.00
1	A	335	VAL	N-CA-C	6.20	117.23	108.36
1	B	272	GLN	N-CA-C	-6.19	99.31	109.40
1	A	333	PRO	N-CD-CG	-6.18	93.92	103.20
2	D	4	LEU	N-CA-C	-6.17	100.71	109.96
1	C	290	GLY	CA-C-O	6.16	131.75	122.27
1	C	338	VAL	CB-CA-C	-6.14	99.92	110.30
1	B	282	TYR	CA-C-O	-6.14	114.28	121.46
1	C	285	SER	CA-C-N	6.13	131.09	123.12
1	C	285	SER	C-N-CA	6.13	131.09	123.12
1	C	291	ALA	N-CA-C	6.13	118.75	111.33
1	B	270	VAL	N-CA-C	6.13	117.59	108.46
2	F	6	THR	N-CA-C	-6.12	99.25	107.88
1	A	267	ILE	N-CA-C	6.11	117.28	108.48
1	B	338	VAL	CB-CA-C	-6.11	100.00	111.30
1	B	259	MSE	CG-SE-CE	-6.10	85.50	98.92
1	A	276	ARG	N-CA-C	-6.07	105.91	113.55
1	B	311	ASN	N-CA-CB	6.06	120.28	110.77
1	A	283	ILE	N-CA-CB	-6.04	104.19	110.95
1	C	253	ILE	CA-C-N	6.04	131.64	122.95
1	C	253	ILE	C-N-CA	6.04	131.64	122.95
1	B	312	PHE	CB-CG-CD2	-6.02	110.46	120.70
1	B	327	ILE	CA-C-N	-6.00	110.95	120.55
1	B	327	ILE	C-N-CA	-6.00	110.95	120.55
2	D	5	MET	N-CA-C	5.99	120.66	112.04
1	B	291	ALA	CA-C-N	-5.95	110.88	120.64
1	B	291	ALA	C-N-CA	-5.95	110.88	120.64
1	A	317	ASN	CA-C-O	-5.93	114.23	120.63
1	B	296	GLY	CA-C-N	-5.93	110.77	121.14
1	B	296	GLY	C-N-CA	-5.93	110.77	121.14
1	C	285	SER	CA-C-O	-5.92	114.94	121.33
1	A	298	ILE	CA-CB-CG1	-5.91	100.36	110.40
1	B	311	ASN	CA-C-O	5.89	126.49	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	VAL	CA-CB-CG2	-5.89	100.38	110.40
1	A	298	ILE	N-CA-CB	-5.89	100.18	110.49
1	A	343	HIS	N-CA-CB	-5.87	100.57	110.49
1	A	251	MSE	CG-SE-CE	-5.87	86.02	98.92
2	E	5	MET	CA-C-O	-5.87	112.15	120.07
1	A	292	VAL	CA-CB-CG1	5.84	120.33	110.40
1	C	318	ASP	CB-CA-C	-5.83	100.77	110.68
1	B	270	VAL	CB-CA-C	-5.82	101.53	110.50
1	A	297	ARG	NE-CZ-NH1	-5.82	115.68	121.50
1	C	304	LEU	N-CA-C	-5.81	99.05	108.52
2	E	7	THR	N-CA-CB	-5.79	100.51	111.00
1	A	259	MSE	CG-SE-CE	-5.79	86.18	98.92
1	B	318	ASP	CB-CA-C	-5.77	101.21	110.79
1	A	287	MSE	CA-C-O	5.75	127.25	120.69
1	B	254	THR	N-CA-C	5.72	118.10	109.41
1	B	299	GLU	N-CA-C	5.72	114.72	108.14
2	E	5	MET	CB-CG-SD	5.71	129.83	112.70
1	B	284	GLY	CA-C-N	-5.71	112.85	123.01
1	B	284	GLY	C-N-CA	-5.71	112.85	123.01
1	B	336	LEU	CA-C-O	-5.70	114.67	121.11
1	A	270	VAL	CA-C-N	5.69	127.36	122.29
1	A	270	VAL	C-N-CA	5.69	127.36	122.29
1	A	304	LEU	CB-CG-CD2	-5.69	93.64	110.70
1	A	256	THR	CB-CA-C	5.68	119.50	110.19
1	C	284	GLY	CA-C-O	-5.68	110.69	120.57
1	B	256	THR	O-C-N	-5.66	116.88	123.27
1	C	254	THR	CB-CA-C	-5.65	102.47	111.17
1	B	302	ASP	N-CA-C	-5.65	102.28	110.24
1	A	340	LYS	N-CA-CB	5.65	118.87	110.29
1	B	256	THR	CA-C-N	-5.63	114.09	123.33
1	B	256	THR	C-N-CA	-5.63	114.09	123.33
2	E	1	SER	N-CA-CB	-5.63	100.93	110.50
1	C	253	ILE	O-C-N	5.61	127.91	122.69
1	B	318	ASP	N-CA-CB	-5.61	101.88	110.12
1	A	302	ASP	CA-C-O	5.59	127.05	120.96
1	B	325	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	B	337	THR	CA-C-O	5.58	127.14	120.28
1	A	265	LEU	O-C-N	5.57	129.80	122.33
1	B	335	VAL	O-C-N	-5.57	115.61	122.57
1	C	311	ASN	N-CA-C	5.56	118.60	109.76
1	C	308	ASN	CA-C-N	-5.55	115.39	125.66
1	C	308	ASN	C-N-CA	-5.55	115.39	125.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	THR	CB-CA-C	5.54	118.89	109.75
1	B	251	MSE	CA-CB-CG	-5.52	103.06	114.10
1	C	298	ILE	CA-C-N	-5.50	116.03	123.96
1	C	298	ILE	C-N-CA	-5.50	116.03	123.96
1	A	304	LEU	CB-CA-C	-5.50	101.04	110.22
1	A	328	VAL	N-CA-C	-5.47	105.89	113.00
1	A	262	TYR	CA-C-N	5.47	131.56	122.54
1	A	262	TYR	C-N-CA	5.47	131.56	122.54
2	E	7	THR	N-CA-C	-5.44	100.16	109.24
1	B	313	GLU	N-CA-C	5.42	119.15	112.54
1	C	287	MSE	CA-CB-CG	-5.42	103.27	114.10
2	E	6	THR	O-C-N	-5.40	117.42	123.04
1	B	267	ILE	CB-CA-C	-5.40	101.05	110.71
1	B	318	ASP	CB-CG-OD1	-5.40	105.99	118.40
1	B	255	VAL	N-CA-C	5.39	120.55	109.34
1	B	318	ASP	CA-CB-CG	-5.36	107.24	112.60
1	B	314	ASN	N-CA-C	-5.36	105.97	112.88
1	A	288	LYS	CA-C-N	-5.33	117.10	123.44
1	A	288	LYS	C-N-CA	-5.33	117.10	123.44
1	A	306	GLN	N-CA-CB	-5.33	101.56	110.99
1	B	297	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	A	295	ASP	O-C-N	-5.31	114.82	122.36
1	A	308	ASN	CB-CA-C	-5.30	103.75	112.06
1	A	343	HIS	CB-CA-C	-5.28	99.92	110.42
1	B	257	LEU	CA-CB-CG	-5.28	97.83	116.30
1	B	342	GLU	N-CA-C	5.27	118.70	110.32
1	A	279	GLY	CA-C-O	-5.25	115.66	120.80
1	A	333	PRO	CA-CB-CG	-5.24	94.54	104.50
1	B	286	ILE	N-CA-CB	-5.24	105.39	112.10
1	A	267	ILE	CA-C-N	-5.23	113.13	122.07
1	A	267	ILE	C-N-CA	-5.23	113.13	122.07
1	C	300	PRO	O-C-N	-5.21	116.61	122.91
1	A	310	ILE	CB-CG1-CD1	5.19	124.70	113.80
1	A	311	ASN	CA-CB-CG	-5.18	107.42	112.60
1	B	319	ASP	CB-CG-OD2	5.17	130.30	118.40
1	A	254	THR	OG1-CB-CG2	-5.17	98.96	109.30
1	B	275	GLU	N-CA-C	-5.17	99.79	110.80
1	C	339	ALA	N-CA-C	5.16	117.14	108.73
1	B	331	PRO	CA-C-O	-5.14	114.90	122.31
1	C	306	GLN	CA-C-O	-5.14	114.22	120.54
2	D	2	LEU	CA-C-N	-5.11	112.91	121.75
2	D	2	LEU	C-N-CA	-5.11	112.91	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6	THR	CA-C-N	-5.07	114.71	122.62
2	F	6	THR	C-N-CA	-5.07	114.71	122.62
1	B	257	LEU	N-CA-C	5.07	118.44	107.49
2	D	2	LEU	CA-C-O	-5.07	115.30	121.28
1	C	257	LEU	N-CA-CB	-5.06	102.02	110.83
1	B	256	THR	N-CA-C	5.06	117.48	109.24
1	B	333	PRO	N-CA-C	-5.06	102.05	112.47
1	B	340	LYS	CB-CA-C	5.04	118.06	109.84
1	B	293	ALA	CA-C-O	-5.04	115.16	120.55
1	C	312	PHE	CA-C-O	5.04	125.37	119.28
1	C	274	ASN	CB-CA-C	-5.04	102.53	114.16
1	B	285	SER	N-CA-CB	-5.03	103.28	111.22
1	B	325	ARG	CA-C-O	-5.02	115.10	120.42

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	252	ILE	Mainchain
1	B	300	PRO	Peptide
1	B	310	ILE	Mainchain
2	D	6	THR	Mainchain
2	F	7	THR	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	724	0	727	99	0
1	B	703	0	713	93	0
1	C	693	0	705	79	0
2	D	61	0	74	18	0
2	E	61	0	74	12	0
2	F	61	0	74	17	0
3	A	16	0	0	17	0
3	B	3	0	0	2	0
3	C	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	1	0
All	All	2328	0	2367	303	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 65.

All (303) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ILE:CG2	1:A:310:ILE:CB	1.74	1.65
1:B:303:MSE:C	1:B:303:MSE:CA	1.74	1.60
1:B:324:LEU:CG	1:B:324:LEU:CD1	1.77	1.60
2:E:6:THR:CB	2:E:6:THR:CA	1.76	1.59
1:C:325:ARG:CD	1:C:325:ARG:CG	1.76	1.58
2:D:7:THR:CB	2:D:7:THR:CA	1.74	1.58
2:E:3:LYS:CD	2:E:3:LYS:CE	1.79	1.57
2:F:4:LEU:CG	2:F:4:LEU:CD1	1.80	1.57
1:A:253:ILE:CD1	1:A:253:ILE:CG1	1.82	1.56
1:A:253:ILE:CB	1:A:253:ILE:CG2	1.76	1.56
2:F:6:THR:CA	2:F:6:THR:CB	1.84	1.53
1:C:287:MSE:CE	1:C:287:MSE:SE	2.15	1.44
1:B:315:MSE:SE	1:B:315:MSE:CE	1.24	1.43
1:A:315:MSE:CG	1:A:315:MSE:SE	2.15	1.43
1:C:333:PRO:CB	1:C:333:PRO:CG	1.94	1.40
1:A:303:MSE:SE	1:A:303:MSE:CE	1.14	1.33
1:C:299:GLU:OE1	1:C:340:LYS:NZ	1.59	1.32
2:D:5:MET:SD	2:D:5:MET:CE	1.18	1.28
1:A:341:LEU:HA	3:A:12:HOH:O	1.11	1.27
1:B:274:ASN:HB3	1:B:279:GLY:N	1.50	1.25
1:A:337:THR:HB	3:A:25:HOH:O	1.33	1.24
1:A:311:ASN:HB2	3:A:23:HOH:O	1.37	1.23
1:B:274:ASN:CB	1:B:279:GLY:H	1.52	1.21
2:D:5:MET:SD	2:D:5:MET:HE2	1.76	1.15
1:B:315:MSE:SE	1:B:315:MSE:HE2	1.81	1.13
2:D:5:MET:SD	2:D:5:MET:HE3	1.76	1.13
1:B:315:MSE:SE	1:B:315:MSE:HE1	1.81	1.12
1:A:303:MSE:CE	1:A:303:MSE:CG	2.29	1.10
2:D:5:MET:SD	2:D:5:MET:HE1	1.76	1.08
1:A:308:ASN:O	1:A:309:ASP:HB2	1.26	1.06
1:B:315:MSE:SE	1:B:315:MSE:HE3	1.81	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:MSE:SE	1:A:303:MSE:HE2	1.72	1.04
1:A:308:ASN:O	1:A:309:ASP:CB	1.93	1.04
2:D:5:MET:CE	2:D:5:MET:CG	2.35	1.03
1:C:307:VAL:HG23	1:C:312:PHE:CZ	1.94	1.03
1:B:315:MSE:CE	1:B:315:MSE:CG	2.36	1.02
1:A:303:MSE:SE	1:A:303:MSE:HE1	1.72	1.02
1:A:303:MSE:SE	1:A:303:MSE:HE3	1.72	1.00
1:A:315:MSE:CG	1:A:315:MSE:CE	2.39	0.99
1:B:258:ASN:OD1	1:B:260:GLU:HB2	1.64	0.98
1:B:276:ARG:HA	1:B:276:ARG:HE	1.29	0.96
1:A:253:ILE:CD1	1:A:253:ILE:CG2	2.44	0.96
3:A:9:HOH:O	2:D:7:THR:HB	1.65	0.94
1:A:315:MSE:CE	1:A:315:MSE:CB	2.46	0.93
1:B:256:THR:O	1:B:257:LEU:HD23	1.69	0.93
2:F:5:MET:CA	2:F:5:MET:HE2	1.98	0.92
1:A:315:MSE:CE	1:A:315:MSE:HB3	2.01	0.91
1:A:341:LEU:HD12	3:A:12:HOH:O	1.71	0.90
1:A:315:MSE:CB	1:A:315:MSE:HE2	2.03	0.88
2:F:5:MET:HE2	2:F:5:MET:HA	1.55	0.88
1:B:324:LEU:O	1:B:328:VAL:HG23	1.72	0.88
1:C:307:VAL:HG23	1:C:312:PHE:CE1	2.08	0.88
1:A:311:ASN:CB	3:A:23:HOH:O	2.05	0.88
2:F:6:THR:CA	2:F:6:THR:CG2	2.47	0.88
1:A:306:GLN:HB3	1:A:337:THR:OG1	1.75	0.87
1:C:303:MSE:O	1:C:338:VAL:HG23	1.74	0.87
1:A:274:ASN:H	1:A:277:GLY:HA2	1.40	0.87
1:A:253:ILE:CG2	1:A:253:ILE:HD13	2.05	0.86
1:A:253:ILE:CG1	1:A:253:ILE:CG2	2.53	0.86
2:F:7:THR:O	2:F:7:THR:OG1	1.87	0.86
2:F:6:THR:CB	2:F:6:THR:C	2.48	0.86
1:A:253:ILE:CD1	1:A:253:ILE:HG21	2.06	0.85
1:C:338:VAL:HG22	1:C:339:ALA:N	1.89	0.85
1:C:311:ASN:OD1	1:C:313:GLU:HB2	1.78	0.84
2:D:7:THR:CA	2:D:7:THR:CG2	2.54	0.83
1:C:270:VAL:CG1	2:F:2:LEU:HD22	2.09	0.83
1:A:253:ILE:CD1	1:A:253:ILE:CB	2.57	0.82
1:C:272:GLN:HB2	3:F:16:HOH:O	1.79	0.82
2:F:5:MET:CA	2:F:5:MET:CE	2.59	0.81
2:E:6:THR:CB	2:E:6:THR:C	2.53	0.80
1:B:324:LEU:CD1	1:B:324:LEU:CD2	2.59	0.79
1:C:312:PHE:HD2	1:C:315:MSE:HE3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:MSE:C	1:B:303:MSE:CB	2.55	0.78
1:A:315:MSE:HB3	1:A:315:MSE:HE3	1.64	0.78
1:C:270:VAL:HG11	2:F:2:LEU:HD22	1.67	0.77
2:F:5:MET:HA	2:F:5:MET:CE	2.15	0.77
1:A:342:GLU:N	3:A:12:HOH:O	2.17	0.77
2:D:7:THR:CA	2:D:7:THR:OG1	2.34	0.76
1:B:274:ASN:HB3	1:B:279:GLY:H	0.65	0.76
1:B:254:THR:C	1:B:255:VAL:HG12	2.11	0.75
1:B:324:LEU:CD1	1:B:324:LEU:HG	2.10	0.75
1:B:307:VAL:HG22	1:B:336:LEU:HD23	1.68	0.75
1:B:287:MSE:N	1:B:287:MSE:HE2	2.02	0.74
1:B:318:ASP:OD1	1:B:318:ASP:N	2.20	0.74
1:B:255:VAL:CG2	1:B:257:LEU:HD21	2.16	0.74
1:B:274:ASN:OD1	1:B:274:ASN:N	2.20	0.73
1:A:310:ILE:CG2	1:A:310:ILE:CA	2.64	0.73
1:C:308:ASN:ND2	1:C:335:VAL:H	1.86	0.73
1:A:302:ASP:OD2	1:A:340:LYS:NZ	2.20	0.72
1:A:309:ASP:OD2	3:A:17:HOH:O	2.06	0.72
2:D:7:THR:CB	2:D:7:THR:N	2.53	0.72
1:C:307:VAL:CG2	1:C:312:PHE:CZ	2.72	0.72
2:E:7:THR:C	2:E:8:VAL:HG13	2.13	0.71
1:A:254:THR:OG1	1:A:337:THR:HG22	1.90	0.71
1:C:312:PHE:HA	1:C:315:MSE:HE3	1.74	0.70
1:A:308:ASN:ND2	1:A:335:VAL:H	1.88	0.70
1:A:315:MSE:HB3	1:A:315:MSE:HE2	1.70	0.70
1:A:260:GLU:OE2	1:A:260:GLU:HA	1.92	0.69
1:A:276:ARG:HG3	1:A:276:ARG:NH1	2.08	0.69
1:C:299:GLU:CD	1:C:340:LYS:HZ2	1.92	0.68
1:C:311:ASN:OD1	1:C:313:GLU:CB	2.42	0.68
1:A:263:ASN:HB3	3:A:20:HOH:O	1.93	0.68
1:A:311:ASN:CG	3:A:23:HOH:O	2.30	0.67
1:A:341:LEU:HD21	2:E:4:LEU:HB2	1.75	0.66
1:C:338:VAL:CG2	1:C:339:ALA:N	2.57	0.66
1:A:311:ASN:OD1	3:A:23:HOH:O	2.11	0.66
1:A:330:LYS:HB3	1:A:331:PRO:HD2	1.76	0.66
1:A:343:HIS:CG	1:A:344:HIS:N	2.62	0.66
1:C:272:GLN:CD	1:C:282:TYR:OH	2.39	0.65
2:E:6:THR:CA	2:E:6:THR:CG2	2.70	0.65
1:C:302:ASP:OD2	1:C:340:LYS:NZ	2.29	0.65
2:F:4:LEU:CD1	2:F:4:LEU:CD2	2.69	0.65
1:B:292:VAL:HG12	1:B:292:VAL:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3:LYS:CE	2:E:3:LYS:HB2	2.28	0.64
1:B:258:ASN:C	1:B:260:GLU:H	2.03	0.63
1:A:274:ASN:CG	1:A:275:GLU:H	2.06	0.63
1:C:258:ASN:ND2	1:C:260:GLU:H	1.96	0.62
1:A:330:LYS:CD	3:A:22:HOH:O	2.46	0.62
1:B:265:LEU:O	1:B:292:VAL:HG23	2.00	0.62
1:A:343:HIS:ND1	1:A:344:HIS:N	2.48	0.62
1:A:330:LYS:CB	1:A:331:PRO:HD2	2.29	0.62
1:B:287:MSE:HE2	1:B:287:MSE:H	1.64	0.61
1:C:307:VAL:CG2	1:C:312:PHE:HZ	2.13	0.61
1:B:293:ALA:O	1:B:296:GLY:N	2.33	0.61
1:C:259:MSE:N	1:C:259:MSE:HE2	2.14	0.61
1:C:272:GLN:HG2	1:C:282:TYR:HE1	1.64	0.61
1:C:299:GLU:OE1	1:C:340:LYS:CE	2.48	0.61
1:C:326:ASP:O	1:C:330:LYS:HD3	2.01	0.61
1:B:256:THR:C	1:B:257:LEU:HD23	2.25	0.61
1:C:312:PHE:HD2	1:C:315:MSE:CE	2.14	0.61
1:A:253:ILE:HD13	1:A:253:ILE:HG21	1.73	0.60
1:B:274:ASN:HB2	1:B:278:ASP:HA	1.83	0.60
2:E:7:THR:C	2:E:8:VAL:CG1	2.72	0.60
1:A:274:ASN:CG	1:A:275:GLU:N	2.59	0.60
1:A:310:ILE:CG2	1:A:310:ILE:CG1	2.72	0.60
1:A:343:HIS:O	1:A:344:HIS:C	2.45	0.59
1:B:293:ALA:N	3:B:6:HOH:O	2.35	0.59
1:B:321:VAL:HG21	2:E:5:MET:HG2	1.84	0.59
1:A:306:GLN:HB3	1:A:337:THR:HG1	1.67	0.59
1:C:272:GLN:CD	1:C:282:TYR:HH	2.11	0.58
1:B:338:VAL:HG22	1:B:339:ALA:N	2.16	0.58
1:A:253:ILE:HD13	1:A:253:ILE:HG23	1.85	0.58
1:B:282:TYR:CE2	1:B:303:MSE:HB2	2.38	0.58
1:C:272:GLN:HE21	1:C:279:GLY:HA3	1.67	0.58
1:C:261:LYS:HB3	1:C:262:TYR:CD1	2.39	0.58
1:A:273:SER:OG	1:A:277:GLY:HA2	2.03	0.58
1:C:288:LYS:N	1:C:288:LYS:HD3	2.17	0.57
1:B:302:ASP:OD1	1:B:340:LYS:HD3	2.05	0.57
1:B:315:MSE:HE2	1:B:315:MSE:HB3	1.85	0.57
1:B:338:VAL:O	1:B:338:VAL:CG1	2.50	0.57
1:C:254:THR:HG22	1:C:254:THR:O	2.05	0.57
1:B:255:VAL:HG23	1:B:257:LEU:HD21	1.85	0.56
1:C:258:ASN:ND2	1:C:260:GLU:HB2	2.19	0.56
1:C:258:ASN:C	1:C:259:MSE:HE2	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:ILE:HG13	3:C:11:HOH:O	2.04	0.56
1:C:308:ASN:O	1:C:309:ASP:HB2	2.05	0.56
1:A:325:ARG:HD2	2:D:6:THR:HG21	1.88	0.56
1:B:258:ASN:OD1	1:B:260:GLU:CB	2.46	0.56
1:B:342:GLU:O	2:D:3:LYS:HB2	2.06	0.55
1:A:273:SER:OG	1:A:277:GLY:CA	2.55	0.55
1:B:295:ASP:OD2	1:B:297:ARG:HB2	2.07	0.55
1:B:268:SER:HA	2:E:7:THR:HA	1.88	0.55
1:B:257:LEU:O	1:B:259:MSE:N	2.40	0.55
1:A:341:LEU:CA	3:A:12:HOH:O	1.95	0.55
1:C:287:MSE:O	1:C:288:LYS:C	2.40	0.55
1:C:325:ARG:HD2	2:F:6:THR:HG21	1.89	0.55
1:A:343:HIS:O	1:A:344:HIS:O	2.25	0.55
1:A:306:GLN:NE2	3:A:23:HOH:O	2.36	0.55
1:A:253:ILE:CG2	1:A:253:ILE:HB	2.19	0.54
2:D:7:THR:CG2	2:D:7:THR:N	2.70	0.54
2:D:7:THR:CB	2:D:7:THR:C	2.71	0.54
1:A:308:ASN:HD21	1:A:335:VAL:H	1.52	0.54
1:A:310:ILE:CG2	1:A:310:ILE:HB	2.17	0.54
1:A:315:MSE:CG	1:A:315:MSE:HE3	2.34	0.54
1:B:303:MSE:CA	1:B:304:LEU:N	2.58	0.54
1:C:299:GLU:OE2	1:C:340:LYS:HE2	2.07	0.54
1:A:273:SER:HA	1:A:277:GLY:HA2	1.89	0.53
1:C:257:LEU:HB3	1:C:259:MSE:HE1	1.90	0.53
1:B:264:PHE:CZ	1:C:260:GLU:HB3	2.44	0.53
1:B:286:ILE:CD1	1:B:300:PRO:HD3	2.38	0.53
1:B:264:PHE:CE2	1:C:260:GLU:HB3	2.43	0.53
1:C:323:VAL:O	1:C:327:ILE:HG13	2.09	0.53
1:A:315:MSE:CB	1:A:315:MSE:HE3	2.31	0.53
1:B:303:MSE:C	1:B:303:MSE:CG	2.82	0.53
1:C:308:ASN:HD21	1:C:335:VAL:H	1.55	0.53
1:B:258:ASN:C	1:B:260:GLU:N	2.67	0.52
1:B:311:ASN:ND2	1:B:313:GLU:H	2.07	0.52
1:A:330:LYS:CB	1:A:331:PRO:CD	2.86	0.52
1:A:330:LYS:HB3	1:A:331:PRO:CD	2.39	0.52
1:A:330:LYS:HD3	3:A:22:HOH:O	2.07	0.52
1:C:258:ASN:HD21	1:C:260:GLU:HB2	1.73	0.52
1:A:299:GLU:OE2	1:C:287:MSE:HB3	2.10	0.52
1:A:259:MSE:HG3	1:A:334:ILE:CD1	2.40	0.51
2:F:4:LEU:CD1	2:F:4:LEU:CB	2.78	0.51
1:B:283:ILE:CD1	1:B:304:LEU:HD21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ILE:HD12	1:B:300:PRO:HD3	1.93	0.51
1:C:272:GLN:HG3	1:C:279:GLY:HA3	1.91	0.51
1:C:302:ASP:HB3	1:C:338:VAL:HG21	1.93	0.51
1:C:322:ARG:O	1:C:323:VAL:C	2.49	0.51
1:C:325:ARG:CG	1:C:325:ARG:NE	2.68	0.51
1:B:274:ASN:CB	1:B:279:GLY:N	2.35	0.51
1:B:286:ILE:HD11	1:B:299:GLU:HA	1.93	0.51
1:A:287:MSE:HE2	1:A:287:MSE:HA	1.91	0.51
1:C:302:ASP:OD1	1:C:340:LYS:HA	2.10	0.51
1:A:303:MSE:CE	1:A:303:MSE:HG2	2.36	0.50
1:B:252:ILE:HG22	1:B:253:ILE:N	2.27	0.50
1:B:277:GLY:O	1:B:278:ASP:C	2.54	0.49
1:B:325:ARG:NH2	3:B:10:HOH:O	2.45	0.49
2:F:5:MET:CA	2:F:5:MET:HE3	2.40	0.49
1:C:261:LYS:HB3	1:C:262:TYR:CE1	2.47	0.49
1:C:253:ILE:HG22	1:C:254:THR:N	2.28	0.49
1:C:303:MSE:O	1:C:338:VAL:CG2	2.55	0.49
1:A:253:ILE:HG21	1:A:253:ILE:HD12	1.91	0.49
1:B:282:TYR:CD2	1:B:303:MSE:HB2	2.48	0.49
1:A:278:ASP:O	1:A:279:GLY:C	2.54	0.48
1:B:283:ILE:HD11	1:B:304:LEU:HD21	1.94	0.48
1:C:308:ASN:O	1:C:309:ASP:CB	2.57	0.48
1:B:303:MSE:C	1:B:303:MSE:HG2	2.38	0.48
1:A:259:MSE:HG3	1:A:334:ILE:HD12	1.94	0.48
1:C:253:ILE:HG21	1:C:253:ILE:HD13	1.45	0.48
1:A:276:ARG:HG3	1:A:276:ARG:HH11	1.75	0.48
1:B:338:VAL:O	1:B:338:VAL:HG13	2.12	0.47
1:B:315:MSE:HE2	1:B:315:MSE:CB	2.45	0.47
1:C:299:GLU:OE1	1:C:299:GLU:N	2.47	0.47
1:B:305:LEU:O	1:B:312:PHE:HB2	2.14	0.47
1:B:330:LYS:C	1:B:331:PRO:O	2.52	0.47
1:C:306:GLN:HB2	1:C:311:ASN:HA	1.97	0.47
1:A:340:LYS:HB3	1:A:340:LYS:HE3	1.63	0.47
1:B:292:VAL:O	1:B:292:VAL:CG1	2.63	0.47
1:B:341:LEU:HD11	2:D:3:LYS:HA	1.97	0.47
1:A:306:GLN:HG3	1:A:310:ILE:O	2.15	0.46
1:C:256:THR:O	1:C:256:THR:CG2	2.64	0.46
1:C:274:ASN:N	1:C:277:GLY:O	2.47	0.46
1:B:257:LEU:O	1:B:259:MSE:HG2	2.16	0.46
1:B:293:ALA:C	1:B:295:ASP:N	2.71	0.46
1:A:307:VAL:HG22	1:A:336:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ASN:OD1	1:C:313:GLU:HG3	2.16	0.46
1:A:315:MSE:HE2	1:A:315:MSE:HB2	1.92	0.46
1:B:306:GLN:HB2	1:B:311:ASN:HA	1.98	0.45
1:B:334:ILE:HG21	1:B:334:ILE:HD13	1.21	0.45
1:C:299:GLU:CD	1:C:340:LYS:HE2	2.41	0.45
1:B:311:ASN:HD22	1:B:313:GLU:H	1.62	0.45
1:C:272:GLN:HE21	1:C:279:GLY:CA	2.29	0.45
1:C:330:LYS:HD2	1:C:330:LYS:N	2.30	0.45
1:B:274:ASN:HB2	1:B:278:ASP:CA	2.44	0.45
1:B:332:GLY:C	1:B:333:PRO:O	2.56	0.45
1:A:288:LYS:HA	1:A:288:LYS:HD2	1.71	0.45
1:B:254:THR:C	1:B:255:VAL:CG1	2.73	0.45
1:B:274:ASN:O	1:B:275:GLU:C	2.57	0.45
1:A:340:LYS:HE2	1:C:287:MSE:HE2	1.98	0.45
1:B:257:LEU:O	1:B:258:ASN:C	2.60	0.44
1:B:305:LEU:HD11	1:B:339:ALA:HB2	1.98	0.44
1:A:318:ASP:N	3:A:7:HOH:O	2.40	0.44
1:C:303:MSE:CG	1:C:304:LEU:N	2.79	0.44
1:A:307:VAL:HG22	1:A:336:LEU:CD2	2.47	0.44
1:B:255:VAL:HG22	1:B:257:LEU:HD21	1.95	0.44
1:A:274:ASN:H	1:A:277:GLY:CA	2.21	0.44
1:A:307:VAL:O	1:A:308:ASN:C	2.61	0.44
1:A:297:ARG:HG3	2:F:7:THR:HG21	1.99	0.44
1:C:312:PHE:CD2	1:C:315:MSE:HE3	2.39	0.44
1:C:303:MSE:HG2	1:C:304:LEU:N	2.32	0.43
1:C:272:GLN:NE2	1:C:282:TYR:OH	2.51	0.43
1:A:276:ARG:HH11	1:A:276:ARG:CG	2.31	0.43
1:A:307:VAL:HG21	1:A:324:LEU:HD13	1.99	0.43
1:C:323:VAL:O	1:C:327:ILE:CG1	2.66	0.43
1:A:271:GLY:O	2:D:2:LEU:HA	2.19	0.43
2:D:7:THR:N	2:D:7:THR:HG23	2.33	0.43
1:B:254:THR:O	1:B:255:VAL:CB	2.57	0.43
1:B:274:ASN:O	1:B:275:GLU:O	2.36	0.43
1:B:298:ILE:HG22	1:B:299:GLU:N	2.32	0.43
1:B:259:MSE:SE	1:B:334:ILE:HD12	2.68	0.43
1:B:276:ARG:HE	1:B:276:ARG:CA	2.12	0.42
1:C:299:GLU:OE1	1:C:302:ASP:OD2	2.36	0.42
1:A:330:LYS:CE	3:A:22:HOH:O	2.67	0.42
1:B:310:ILE:HG22	1:B:311:ASN:N	2.33	0.42
1:C:299:GLU:N	1:C:302:ASP:OD2	2.34	0.42
1:B:256:THR:C	1:B:257:LEU:CD2	2.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:GLU:CD	1:C:340:LYS:CE	2.93	0.42
1:C:311:ASN:OD1	1:C:313:GLU:CG	2.67	0.42
1:B:312:PHE:HD2	1:B:312:PHE:HA	1.37	0.42
1:B:262:TYR:OH	1:B:294:ALA:CB	2.68	0.42
1:B:299:GLU:N	1:B:302:ASP:OD2	2.29	0.42
2:E:4:LEU:HG	2:E:5:MET:N	2.34	0.42
1:B:315:MSE:CE	1:B:315:MSE:CB	2.93	0.42
1:B:276:ARG:HA	1:B:276:ARG:NE	2.13	0.42
1:A:302:ASP:CG	1:A:340:LYS:HZ2	2.20	0.41
1:B:322:ARG:O	1:B:323:VAL:C	2.62	0.41
1:A:303:MSE:CG	1:A:303:MSE:HE2	2.28	0.41
1:A:343:HIS:HB3	1:A:344:HIS:H	1.11	0.41
1:C:264:PHE:C	1:C:264:PHE:CD1	2.95	0.41
1:A:287:MSE:H	1:A:287:MSE:HG2	1.67	0.41
2:E:6:THR:CA	2:E:6:THR:OG1	2.56	0.41
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.89	0.41
1:A:258:ASN:HD21	1:A:260:GLU:HB2	1.86	0.41
1:C:323:VAL:HG13	1:C:327:ILE:HD11	2.03	0.41
1:C:307:VAL:CG2	1:C:312:PHE:CE1	2.94	0.41
2:F:6:THR:CB	2:F:7:THR:N	2.84	0.41
1:B:308:ASN:O	1:B:309:ASP:HB2	2.21	0.40
1:A:253:ILE:O	1:A:337:THR:HA	2.22	0.40
1:A:343:HIS:CG	1:A:344:HIS:H	2.10	0.40
1:B:264:PHE:C	1:B:264:PHE:CD1	2.99	0.40
1:C:257:LEU:CB	1:C:259:MSE:HE1	2.51	0.40
2:D:6:THR:HB	2:D:7:THR:H	1.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	81/95 (85%)	75 (93%)	4 (5%)	2 (2%)	4	2
1	B	35/95 (37%)	28 (80%)	4 (11%)	3 (9%)	0	0
1	C	89/95 (94%)	81 (91%)	8 (9%)	0	100	100
2	D	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	E	6/8 (75%)	6 (100%)	0	0	100	100
2	F	6/8 (75%)	6 (100%)	0	0	100	100
All	All	223/309 (72%)	201 (90%)	17 (8%)	5 (2%)	5	3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	HIS
1	B	301	GLY
1	A	309	ASP
1	B	278	ASP
1	B	275	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	79/74 (107%)	67 (85%)	12 (15%)	3	2
1	B	77/74 (104%)	63 (82%)	14 (18%)	2	1
1	C	76/74 (103%)	67 (88%)	9 (12%)	5	5
2	D	8/8 (100%)	8 (100%)	0	100	100
2	E	8/8 (100%)	6 (75%)	2 (25%)	0	0
2	F	8/8 (100%)	5 (62%)	3 (38%)	0	0
All	All	256/246 (104%)	216 (84%)	40 (16%)	2	2

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ILE
1	A	254	THR
1	A	255	VAL
1	A	267	ILE
1	A	287	MSE
1	A	295	ASP
1	A	304	LEU
1	A	315	MSE
1	A	330	LYS
1	A	337	THR
1	A	340	LYS
1	A	344	HIS
1	B	255	VAL
1	B	256	THR
1	B	270	VAL
1	B	273	SER
1	B	276	ARG
1	B	278	ASP
1	B	287	MSE
1	B	297	ARG
1	B	298	ILE
1	B	306	GLN
1	B	330	LYS
1	B	334	ILE
1	B	337	THR
1	B	338	VAL
1	C	255	VAL
1	C	273	SER
1	C	287	MSE
1	C	288	LYS
1	C	304	LEU
1	C	306	GLN
1	C	321	VAL
1	C	327	ILE
1	C	340	LYS
2	E	3	LYS
2	E	5	MET
2	F	1	SER
2	F	5	MET
2	F	6	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	GLN
1	A	308	ASN
1	A	329	HIS
1	A	344	HIS
1	B	263	ASN
1	B	308	ASN
1	B	311	ASN
1	C	258	ASN
1	C	272	GLN
1	C	306	GLN
1	C	308	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	288:LYS	C	289:GLY	N	1.18

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.