



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:37 PM GMT

PDB ID : 1L6O
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

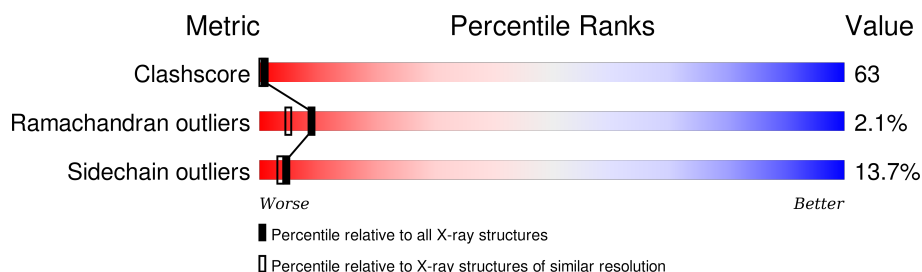
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

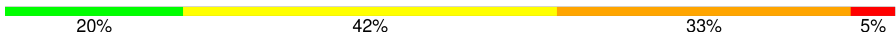

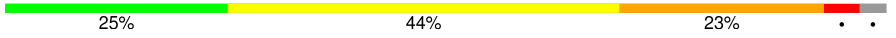



Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	95	
1	B	95	
1	C	95	
2	D	8	
2	E	8	
2	F	8	

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.

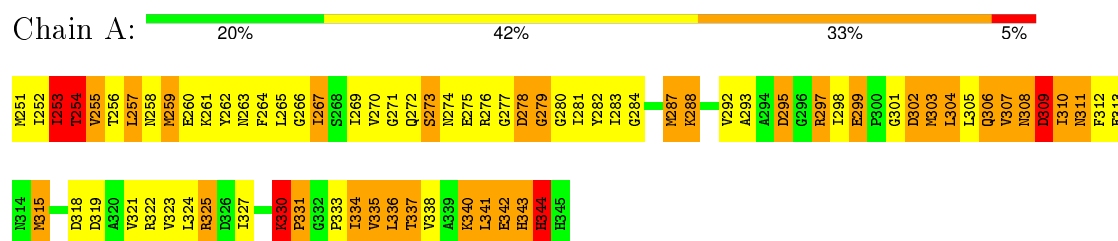
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	3	Total	O	0	0
			3	3		
3	C	4	Total	O	0	0
			4	4		
3	E	1	Total	O	0	0
			1	1		
3	F	1	Total	O	0	0
			1	1		

3 Residue-property plots

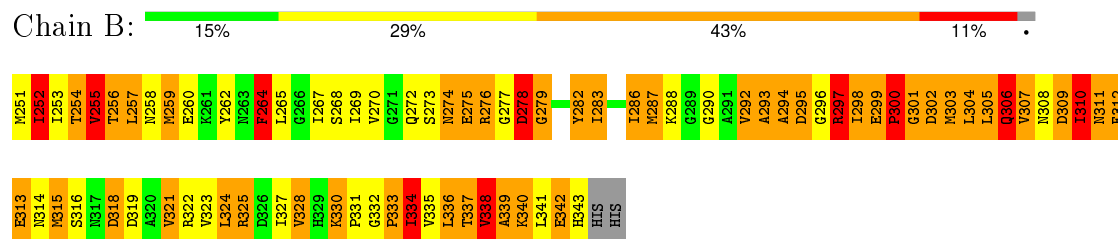
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

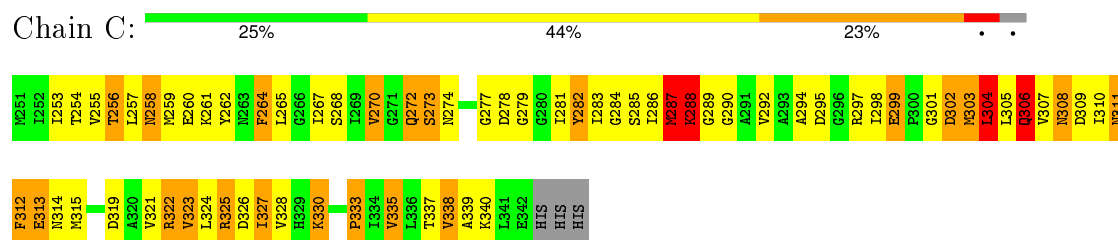
- Molecule 1: Segment polarity protein dishevelled homolog DVL-2



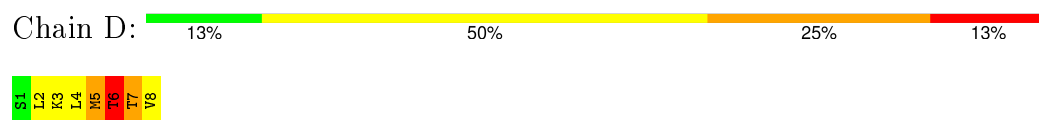
- Molecule 1: Segment polarity protein dishevelled homolog DVL-2



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



- Molecule 2: Dapper 1




- Molecule 2: Dapper 1

Chain E: 



• Molecule 2: Dapper 1

Chain F: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.73 Å 84.73 Å 123.15 Å 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	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	3.02	72/730 (9.9%)	2.33	38/977 (3.9%)
1	B	2.90	65/707 (9.2%)	2.63	50/947 (5.3%)
1	C	2.68	47/696 (6.8%)	2.18	31/932 (3.3%)
2	D	3.50	8/60 (13.3%)	2.27	3/78 (3.8%)
2	E	3.52	6/60 (10.0%)	2.95	8/78 (10.3%)
2	F	3.94	10/60 (16.7%)	2.65	4/78 (5.1%)
All	All	2.94	208/2313 (9.0%)	2.41	134/3090 (4.3%)

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 (208) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	338	VAL	CB-CG2	-17.09	1.17	1.52
1	A	303	MSE	SE-CE	-13.79	1.14	1.95
2	F	6	THR	CB-CG2	-12.63	1.10	1.52
1	A	284	GLY	C-O	-12.06	1.04	1.23
1	B	315	MSE	SE-CE	-12.04	1.24	1.95
2	F	6	THR	CA-CB	11.97	1.84	1.53
1	A	262	TYR	CG-CD1	-11.74	1.23	1.39
2	E	3	LYS	CD-CE	11.31	1.79	1.51
1	C	286	ILE	C-O	-11.19	1.02	1.23
1	C	264	PHE	CB-CG	-10.80	1.32	1.51
2	D	5	MET	SD-CE	-10.56	1.18	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	288	LYS	CB-CG	-10.55	1.24	1.52
1	A	255	VAL	CB-CG2	-10.39	1.31	1.52
1	B	312	PHE	CB-CG	-10.39	1.33	1.51
1	A	311	ASN	C-O	-10.31	1.03	1.23
1	C	325	ARG	CG-CD	9.98	1.76	1.51
2	D	8	VAL	CB-CG1	-9.83	1.32	1.52
2	E	5	MET	SD-CE	-9.69	1.23	1.77
1	B	270	VAL	CB-CG1	-9.61	1.32	1.52
1	B	311	ASN	CB-CG	9.59	1.73	1.51
2	F	5	MET	N-CA	9.44	1.65	1.46
1	C	314	ASN	CB-CG	9.27	1.72	1.51
1	A	293	ALA	CA-CB	9.07	1.71	1.52
1	C	330	LYS	CD-CE	9.05	1.73	1.51
1	B	321	VAL	C-O	9.05	1.40	1.23
1	B	336	LEU	CA-C	-8.96	1.29	1.52
1	C	333	PRO	CB-CG	8.84	1.94	1.50
1	A	262	TYR	CD2-CE2	-8.84	1.26	1.39
1	B	272	GLN	CG-CD	8.77	1.71	1.51
2	E	6	THR	CA-CB	8.76	1.76	1.53
1	C	283	ILE	CA-CB	-8.69	1.34	1.54
1	B	335	VAL	CB-CG2	8.63	1.71	1.52
1	B	270	VAL	N-CA	-8.52	1.29	1.46
1	B	303	MSE	CA-C	8.37	1.74	1.52
1	A	331	PRO	CA-C	-8.32	1.36	1.52
1	A	283	ILE	CA-C	8.19	1.74	1.52
1	C	288	LYS	C-N	-8.18	1.18	1.33
2	D	7	THR	CA-CB	8.17	1.74	1.53
1	C	292	VAL	CB-CG1	-8.14	1.35	1.52
2	D	6	THR	CB-CG2	-8.10	1.25	1.52
2	D	5	MET	N-CA	7.93	1.62	1.46
1	A	306	GLN	CB-CG	-7.85	1.31	1.52
2	F	4	LEU	CG-CD1	7.84	1.80	1.51
1	C	311	ASN	C-O	-7.83	1.08	1.23
1	C	285	SER	CB-OG	7.75	1.52	1.42
1	C	282	TYR	CE2-CZ	7.74	1.48	1.38
1	A	253	ILE	CB-CG2	7.70	1.76	1.52
1	B	299	GLU	CD-OE1	7.69	1.34	1.25
1	A	262	TYR	CD1-CE1	-7.56	1.28	1.39
1	C	270	VAL	CA-CB	7.54	1.70	1.54
1	B	316	SER	CB-OG	7.50	1.52	1.42
1	A	292	VAL	CB-CG1	7.46	1.68	1.52
1	A	280	GLY	C-O	7.42	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337	THR	N-CA	-7.39	1.31	1.46
1	B	282	TYR	CE1-CZ	7.39	1.48	1.38
1	B	306	GLN	C-O	7.33	1.37	1.23
1	B	342	GLU	CG-CD	7.33	1.62	1.51
1	A	313	GLU	CG-CD	7.29	1.62	1.51
1	C	338	VAL	CB-CG2	-7.26	1.37	1.52
1	B	307	VAL	CB-CG2	-7.25	1.37	1.52
1	A	281	ILE	N-CA	-7.23	1.31	1.46
1	B	319	ASP	CA-C	-7.23	1.34	1.52
1	C	299	GLU	CD-OE1	7.23	1.33	1.25
1	A	264	PHE	CE2-CZ	7.21	1.51	1.37
2	E	8	VAL	CB-CG1	-7.20	1.37	1.52
1	C	313	GLU	CG-CD	7.16	1.62	1.51
1	B	312	PHE	CG-CD2	-7.13	1.28	1.38
1	B	302	ASP	CB-CG	7.07	1.66	1.51
1	C	313	GLU	CB-CG	7.06	1.65	1.52
1	B	328	VAL	CB-CG1	7.04	1.67	1.52
1	A	262	TYR	CE1-CZ	-7.00	1.29	1.38
1	A	310	ILE	CB-CG2	6.99	1.74	1.52
1	C	301	GLY	CA-C	6.93	1.62	1.51
1	A	337	THR	CA-CB	6.92	1.71	1.53
1	C	255	VAL	CB-CG2	-6.90	1.38	1.52
1	A	307	VAL	N-CA	-6.89	1.32	1.46
1	C	328	VAL	C-O	-6.88	1.10	1.23
1	B	269	ILE	C-O	-6.86	1.10	1.23
1	B	324	LEU	CG-CD1	6.82	1.77	1.51
1	A	302	ASP	CG-OD1	6.81	1.41	1.25
1	A	255	VAL	CA-CB	6.80	1.69	1.54
2	F	1	SER	CB-OG	-6.79	1.33	1.42
1	B	306	GLN	CB-CG	6.77	1.70	1.52
1	B	334	ILE	CA-C	-6.75	1.35	1.52
2	F	4	LEU	N-CA	-6.72	1.32	1.46
1	A	278	ASP	CB-CG	6.71	1.65	1.51
1	A	322	ARG	NE-CZ	-6.70	1.24	1.33
1	A	330	LYS	CD-CE	6.68	1.68	1.51
1	B	292	VAL	CA-CB	-6.66	1.40	1.54
1	C	289	GLY	N-CA	6.65	1.56	1.46
1	C	264	PHE	CE1-CZ	6.64	1.50	1.37
1	B	318	ASP	CB-CG	-6.64	1.37	1.51
1	C	306	GLN	N-CA	-6.61	1.33	1.46
1	A	311	ASN	CA-CB	6.60	1.70	1.53
1	C	322	ARG	CG-CD	6.58	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	GLY	N-CA	-6.56	1.36	1.46
1	B	335	VAL	N-CA	-6.54	1.33	1.46
1	A	312	PHE	CD1-CE1	6.52	1.52	1.39
1	A	306	GLN	C-O	-6.51	1.10	1.23
1	A	313	GLU	CD-OE1	6.46	1.32	1.25
1	B	286	ILE	C-O	-6.45	1.11	1.23
1	B	318	ASP	CA-CB	-6.43	1.39	1.53
1	B	338	VAL	CA-C	-6.42	1.36	1.52
1	A	325	ARG	CB-CG	6.41	1.69	1.52
1	A	295	ASP	CB-CG	-6.40	1.38	1.51
1	C	323	VAL	CA-C	-6.37	1.36	1.52
1	B	254	THR	N-CA	-6.35	1.33	1.46
1	B	267	ILE	CB-CG2	6.32	1.72	1.52
1	A	297	ARG	CG-CD	6.29	1.67	1.51
1	A	327	ILE	CA-CB	-6.29	1.40	1.54
1	A	262	TYR	C-O	-6.29	1.11	1.23
1	C	312	PHE	CG-CD1	6.27	1.48	1.38
1	A	292	VAL	CA-C	-6.26	1.36	1.52
1	A	336	LEU	N-CA	-6.26	1.33	1.46
1	A	299	GLU	CG-CD	6.22	1.61	1.51
1	B	254	THR	C-O	-6.21	1.11	1.23
1	A	264	PHE	CE1-CZ	6.20	1.49	1.37
1	C	322	ARG	N-CA	6.20	1.58	1.46
1	A	272	GLN	CA-CB	-6.20	1.40	1.53
2	D	8	VAL	CB-CG2	6.18	1.65	1.52
1	C	321	VAL	C-O	6.18	1.35	1.23
1	B	313	GLU	CD-OE2	6.12	1.32	1.25
1	B	309	ASP	C-O	-6.10	1.11	1.23
2	E	4	LEU	CG-CD1	6.09	1.74	1.51
1	A	315	MSE	CB-CG	-6.09	1.34	1.52
1	B	333	PRO	C-O	6.07	1.35	1.23
1	C	264	PHE	CE2-CZ	6.05	1.48	1.37
1	C	288	LYS	CA-CB	-6.04	1.40	1.53
1	B	322	ARG	N-CA	6.01	1.58	1.46
1	A	335	VAL	CA-CB	-6.00	1.42	1.54
1	A	262	TYR	CG-CD2	-5.97	1.31	1.39
1	A	338	VAL	C-O	-5.93	1.12	1.23
1	B	335	VAL	CB-CG1	-5.92	1.40	1.52
1	A	297	ARG	NE-CZ	-5.91	1.25	1.33
1	A	298	ILE	N-CA	-5.90	1.34	1.46
2	D	4	LEU	N-CA	-5.88	1.34	1.46
1	B	272	GLN	CA-C	-5.87	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	LEU	CG-CD2	5.86	1.73	1.51
1	B	297	ARG	CZ-NH1	-5.84	1.25	1.33
1	A	334	ILE	CA-CB	-5.84	1.41	1.54
1	A	315	MSE	CG-SE	5.83	2.15	1.95
1	A	340	LYS	CE-NZ	5.82	1.63	1.49
1	B	264	PHE	CE1-CZ	5.80	1.48	1.37
1	C	322	ARG	C-O	5.78	1.34	1.23
1	B	305	LEU	CG-CD2	-5.77	1.30	1.51
1	A	261	LYS	N-CA	-5.75	1.34	1.46
1	B	270	VAL	CA-CB	5.71	1.66	1.54
1	C	313	GLU	CD-OE1	5.70	1.31	1.25
1	A	319	ASP	CA-CB	5.70	1.66	1.53
1	A	267	ILE	C-O	-5.70	1.12	1.23
1	B	339	ALA	CA-C	5.68	1.67	1.52
1	B	264	PHE	CG-CD2	5.68	1.47	1.38
1	A	307	VAL	CB-CG2	5.67	1.64	1.52
1	A	319	ASP	CB-CG	5.67	1.63	1.51
1	C	305	LEU	CA-C	5.65	1.67	1.52
1	A	279	GLY	C-O	-5.64	1.14	1.23
1	C	335	VAL	CB-CG1	-5.62	1.41	1.52
1	A	327	ILE	C-O	-5.61	1.12	1.23
1	B	325	ARG	CB-CG	-5.60	1.37	1.52
1	A	265	LEU	C-O	-5.59	1.12	1.23
1	A	254	THR	CB-OG1	-5.59	1.32	1.43
1	C	273	SER	N-CA	-5.59	1.35	1.46
1	C	324	LEU	CG-CD2	5.55	1.72	1.51
1	B	259	MSE	SE-CE	-5.55	1.62	1.95
1	B	301	GLY	CA-C	5.54	1.60	1.51
1	A	315	MSE	SE-CE	-5.54	1.62	1.95
1	B	252	ILE	N-CA	-5.50	1.35	1.46
1	B	303	MSE	CA-CB	-5.49	1.41	1.53
1	C	297	ARG	NE-CZ	5.48	1.40	1.33
1	A	311	ASN	CG-OD1	-5.47	1.11	1.24
1	C	294	ALA	C-O	-5.47	1.12	1.23
2	F	8	VAL	CB-CG1	-5.47	1.41	1.52
1	A	254	THR	CA-CB	-5.46	1.39	1.53
2	F	7	THR	CA-CB	-5.46	1.39	1.53
1	C	319	ASP	C-O	-5.41	1.13	1.23
1	B	282	TYR	CB-CG	-5.40	1.43	1.51
1	B	283	ILE	CA-C	5.40	1.67	1.52
1	C	330	LYS	CG-CD	5.40	1.70	1.52
1	B	255	VAL	CB-CG1	-5.37	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	VAL	CB-CG2	-5.34	1.41	1.52
1	B	279	GLY	CA-C	-5.33	1.43	1.51
1	B	293	ALA	CA-CB	-5.29	1.41	1.52
1	A	269	ILE	C-O	-5.27	1.13	1.23
1	A	282	TYR	CA-CB	5.25	1.65	1.53
1	A	270	VAL	C-O	-5.24	1.13	1.23
2	F	2	LEU	CA-CB	-5.23	1.41	1.53
1	B	325	ARG	NE-CZ	-5.19	1.26	1.33
1	B	259	MSE	CG-SE	5.19	2.13	1.95
1	C	304	LEU	C-O	5.18	1.33	1.23
1	C	264	PHE	N-CA	-5.18	1.35	1.46
1	A	282	TYR	CG-CD1	-5.12	1.32	1.39
2	F	2	LEU	CA-C	-5.12	1.39	1.52
1	A	280	GLY	N-CA	5.11	1.53	1.46
2	E	5	MET	C-O	-5.11	1.13	1.23
1	B	297	ARG	CG-CD	-5.09	1.39	1.51
1	B	327	ILE	CA-C	-5.08	1.39	1.52
1	A	309	ASP	CB-CG	5.07	1.62	1.51
1	A	262	TYR	CZ-OH	5.06	1.46	1.37
1	C	322	ARG	CA-CB	-5.06	1.42	1.53
1	A	252	ILE	N-CA	-5.05	1.36	1.46
1	C	267	ILE	C-O	-5.04	1.13	1.23
1	B	286	ILE	CA-C	-5.04	1.39	1.52
1	B	334	ILE	CB-CG2	-5.02	1.37	1.52
1	C	272	GLN	CD-NE2	5.02	1.45	1.32
1	C	335	VAL	CB-CG2	-5.02	1.42	1.52
1	B	288	LYS	CA-CB	-5.02	1.43	1.53
1	B	259	MSE	CA-C	-5.00	1.40	1.52
1	A	266	GLY	N-CA	5.00	1.53	1.46

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	PHE	CB-CG-CD1	14.96	131.27	120.80
1	B	312	PHE	CB-CG-CD2	-14.77	110.46	120.80
1	C	288	LYS	C-N-CA	-13.85	93.22	122.30
1	B	318	ASP	CB-CG-OD1	-13.68	105.99	118.30
1	B	324	LEU	CB-CG-CD2	-13.46	88.11	111.00
1	B	319	ASP	CB-CG-OD2	13.33	130.30	118.30
1	C	288	LYS	N-CA-CB	13.05	134.09	110.60
1	B	297	ARG	NE-CZ-NH1	-12.63	113.99	120.30
1	A	304	LEU	CB-CG-CD1	12.18	131.70	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	302	ASP	CB-CG-OD2	12.13	129.22	118.30
1	B	302	ASP	CB-CG-OD1	-11.30	108.13	118.30
1	A	295	ASP	CB-CG-OD2	10.60	127.84	118.30
1	B	334	ILE	CG1-CB-CG2	-10.33	88.68	111.40
1	A	304	LEU	CB-CG-CD2	-10.21	93.64	111.00
1	A	297	ARG	NE-CZ-NH2	10.16	125.38	120.30
1	A	315	MSE	CG-SE-CE	-9.80	77.35	98.90
1	B	334	ILE	CB-CA-C	-9.80	92.01	111.60
1	C	278	ASP	CB-CG-OD2	9.59	126.93	118.30
2	E	6	THR	OG1-CB-CG2	-9.45	88.26	110.00
1	A	295	ASP	CB-CG-OD1	-9.36	109.88	118.30
1	A	297	ARG	NE-CZ-NH1	-9.24	115.68	120.30
1	B	302	ASP	CB-CG-OD2	9.13	126.52	118.30
1	B	325	ARG	NE-CZ-NH1	-8.76	115.92	120.30
2	F	5	MET	CG-SD-CE	-8.76	86.18	100.20
1	B	295	ASP	CB-CG-OD2	8.49	125.94	118.30
1	B	254	THR	N-CA-CB	-8.47	94.20	110.30
2	F	8	VAL	CA-C-O	-8.44	102.38	120.10
1	A	308	ASN	C-N-CA	-8.42	100.64	121.70
1	A	278	ASP	CB-CG-OD1	8.40	125.86	118.30
2	D	7	THR	OG1-CB-CG2	-8.40	90.69	110.00
1	C	288	LYS	O-C-N	-8.29	109.11	123.20
1	B	324	LEU	CB-CG-CD1	8.27	125.06	111.00
1	A	342	GLU	CB-CA-C	-8.04	94.31	110.40
1	C	304	LEU	CA-CB-CG	7.95	133.57	115.30
1	B	309	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	B	310	ILE	CB-CA-C	-7.90	95.80	111.60
1	C	287	MSE	C-N-CA	-7.72	102.39	121.70
2	E	4	LEU	CB-CG-CD2	-7.68	97.94	111.00
1	C	295	ASP	CB-CG-OD2	7.68	125.21	118.30
1	B	257	LEU	CA-CB-CG	-7.60	97.83	115.30
1	B	304	LEU	CA-CB-CG	7.46	132.46	115.30
1	B	297	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	B	318	ASP	CB-CG-OD2	7.18	124.76	118.30
1	A	341	LEU	CB-CG-CD2	-7.08	98.97	111.00
2	F	7	THR	CA-CB-OG1	-7.07	94.15	109.00
1	A	302	ASP	CB-CG-OD1	7.05	124.65	118.30
1	B	298	ILE	CG1-CB-CG2	-7.04	95.91	111.40
1	B	323	VAL	CA-CB-CG2	-7.01	100.38	110.90
1	B	305	LEU	CB-CG-CD2	-6.92	99.23	111.00
1	A	341	LEU	CB-CG-CD1	-6.89	99.29	111.00
1	B	290	GLY	N-CA-C	-6.73	96.28	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	GLU	OE1-CD-OE2	6.72	131.37	123.30
1	B	343	HIS	CA-C-O	6.71	134.19	120.10
1	C	268	SER	CA-CB-OG	-6.67	93.18	111.20
1	A	337	THR	OG1-CB-CG2	-6.60	94.82	110.00
2	E	2	LEU	CB-CG-CD2	-6.44	100.05	111.00
1	B	334	ILE	N-CA-C	-6.41	93.71	111.00
2	E	1	SER	N-CA-CB	-6.38	100.93	110.50
1	B	254	THR	O-C-N	-6.38	112.50	122.70
1	A	273	SER	CA-C-N	-6.36	103.21	117.20
1	A	343	HIS	N-CA-C	6.32	128.05	111.00
1	A	292	VAL	CA-CB-CG1	6.29	120.33	110.90
2	E	5	MET	CA-C-N	6.20	130.84	117.20
1	C	290	GLY	CA-C-O	6.20	131.75	120.60
1	A	333	PRO	N-CD-CG	-6.18	93.92	103.20
1	B	319	ASP	N-CA-CB	-6.15	99.54	110.60
1	B	338	VAL	CG1-CB-CG2	-6.14	101.07	110.90
1	C	297	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	259	MSE	CG-SE-CE	-6.09	85.50	98.90
1	B	314	ASN	N-CA-CB	-6.08	99.65	110.60
1	A	335	VAL	CB-CA-C	-6.08	99.85	111.40
1	A	309	ASP	N-CA-C	6.05	127.35	111.00
1	C	295	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	C	256	THR	OG1-CB-CG2	-6.05	96.09	110.00
1	C	338	VAL	CB-CA-C	-6.04	99.92	111.40
1	A	257	LEU	CA-CB-CG	-6.03	101.44	115.30
1	B	251	MSE	CA-CB-CG	-6.02	103.06	113.30
1	A	288	LYS	N-CA-CB	-6.01	99.77	110.60
1	B	338	VAL	CB-CA-C	-6.00	100.00	111.40
1	B	336	LEU	O-C-N	5.97	132.26	122.70
1	C	337	THR	O-C-N	-5.97	113.15	122.70
1	B	336	LEU	N-CA-C	-5.97	94.89	111.00
1	B	294	ALA	C-N-CA	-5.94	106.85	121.70
1	A	264	PHE	CB-CG-CD2	-5.92	116.66	120.80
1	C	287	MSE	CA-CB-CG	-5.90	103.27	113.30
2	F	6	THR	CB-CA-C	-5.90	95.68	111.60
1	A	251	MSE	CG-SE-CE	-5.86	86.02	98.90
1	C	303	MSE	C-N-CA	-5.85	107.07	121.70
2	E	5	MET	CB-CG-SD	5.81	129.83	112.40
1	A	259	MSE	CG-SE-CE	-5.78	86.18	98.90
1	C	278	ASP	OD1-CG-OD2	-5.75	112.37	123.30
2	D	7	THR	CA-CB-OG1	-5.72	96.98	109.00
2	E	8	VAL	CA-CB-CG1	-5.71	102.34	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	268	SER	C-N-CA	-5.68	107.49	121.70
1	A	270	VAL	CG1-CB-CG2	5.67	119.98	110.90
1	B	300	PRO	C-N-CA	5.66	134.19	122.30
1	C	288	LYS	CA-C-O	5.66	131.99	120.10
1	C	290	GLY	CA-C-N	-5.62	104.83	117.20
1	C	302	ASP	CB-CG-OD1	-5.62	113.25	118.30
1	A	298	ILE	CA-CB-CG1	-5.60	100.36	111.00
1	A	343	HIS	N-CA-CB	-5.57	100.57	110.60
1	B	274	ASN	N-CA-C	-5.52	96.09	111.00
1	C	284	GLY	CA-C-O	-5.51	110.69	120.60
1	C	337	THR	CA-C-O	5.50	131.64	120.10
1	A	256	THR	N-CA-C	5.49	125.83	111.00
1	A	309	ASP	CB-CG-OD2	5.46	123.22	118.30
1	C	281	ILE	CG1-CB-CG2	5.44	123.36	111.40
1	A	297	ARG	CB-CA-C	5.43	121.27	110.40
1	A	253	ILE	CA-CB-CG2	5.42	121.74	110.90
1	B	313	GLU	C-N-CA	-5.41	108.18	121.70
1	B	309	ASP	C-N-CA	-5.41	108.18	121.70
1	B	340	LYS	CA-C-O	5.40	131.43	120.10
1	B	254	THR	C-N-CA	-5.39	108.23	121.70
1	B	311	ASN	N-CA-CB	5.38	120.28	110.60
1	B	334	ILE	CA-CB-CG1	5.35	121.17	111.00
1	A	321	VAL	CA-CB-CG2	-5.35	102.88	110.90
1	C	310	ILE	CB-CG1-CD1	-5.34	98.95	113.90
1	C	292	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	B	267	ILE	CB-CA-C	-5.28	101.05	111.60
1	B	288	LYS	N-CA-CB	-5.25	101.16	110.60
1	A	343	HIS	CB-CA-C	-5.24	99.92	110.40
1	C	265	LEU	CB-CG-CD1	-5.20	102.16	111.00
1	B	270	VAL	CB-CA-C	-5.19	101.53	111.40
1	C	322	ARG	C-N-CA	-5.19	108.73	121.70
1	B	312	PHE	CZ-CE2-CD2	-5.16	113.91	120.10
1	A	325	ARG	C-N-CA	-5.15	108.82	121.70
2	E	7	THR	N-CA-CB	-5.15	100.51	110.30
2	D	6	THR	CB-CA-C	-5.14	97.73	111.60
1	A	288	LYS	O-C-N	-5.13	114.48	123.20
1	C	265	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	B	298	ILE	CB-CA-C	-5.09	101.42	111.60
1	B	272	GLN	CB-CA-C	-5.06	100.28	110.40
1	A	305	LEU	CB-CG-CD2	5.02	119.53	111.00
1	A	306	GLN	N-CA-CB	-5.02	101.56	110.60

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	97	0
1	B	703	0	713	89	0
1	C	693	0	705	76	0
2	D	61	0	74	18	0
2	E	61	0	74	12	0
2	F	61	0	74	19	0
3	A	16	0	0	17	0
3	B	3	0	0	2	0
3	C	4	0	0	1	0
3	E	1	0	0	0	0
3	F	1	0	0	1	0
All	All	2328	0	2367	296	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 63.

All (296) 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:324:LEU:CD1	1:B:324:LEU:CG	1.77	1.60
2:E:6:THR:CA	2:E:6:THR:CB	1.76	1.59
2:D:7:THR:CB	2:D:7:THR:CA	1.74	1.58
1:C:325:ARG:CG	1:C:325:ARG:CD	1.76	1.58
2:E:3:LYS:CD	2:E:3:LYS:CE	1.79	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:LEU:CD1	2:F:4:LEU:CG	1.80	1.57
1:A:253:ILE:CG1	1:A:253:ILE:CD1	1.82	1.56
1:A:253:ILE:CB	1:A:253:ILE:CG2	1.76	1.56
1:B:303:MSE:CA	1:B:303:MSE:C	1.74	1.56
2:F:6:THR:CA	2:F:6:THR:CB	1.84	1.53
1:C:287:MSE:SE	1:C:287:MSE:CE	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:CE	2:D:5:MET:SD	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:HE1	2:D:5:MET:SD	1.76	1.16
1:B:315:MSE:SE	1:B:315:MSE:HE2	1.81	1.13
2:D:5:MET:HE3	2:D:5:MET:SD	1.76	1.13
1:B:315:MSE:SE	1:B:315:MSE:HE1	1.81	1.12
1:A:303:MSE:CG	1:A:303:MSE:CE	2.29	1.10
2:D:5:MET:HE2	2:D:5:MET:SD	1.76	1.08
1:B:315:MSE:SE	1:B:315:MSE:HE3	1.81	1.06
1:A:308:ASN:O	1:A:309:ASP:HB2	1.26	1.06
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:HE1	1:A:303:MSE:SE	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
1:A:315:MSE:HB3	1:A:315:MSE:CE	2.01	0.91
1:A:341:LEU:HD12	3:A:12:HOH:O	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:MSE:CB	1:A:315:MSE:HE2	2.03	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:HD13	1:A:253:ILE:CG2	2.05	0.86
1:A:253:ILE:CG1	1:A:253:ILE:CG2	2.53	0.86
2:F:7:THR:OG1	2:F:7:THR:O	1.87	0.86
1:A:253:ILE:HG21	1:A:253:ILE:CD1	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:F:5:MET:CA	2:F:5:MET:HE3	2.06	0.83
2:D:7:THR:CG2	2:D:7:THR:CA	2.54	0.83
1:C:270:VAL:CG1	2:F:2:LEU:HD22	2.09	0.83
1:A:253:ILE:CB	1:A:253:ILE:CD1	2.57	0.82
1:C:272:GLN:HB2	3:F:16:HOH:O	1.79	0.82
2:F:6:THR:CB	2:F:6:THR:C	2.48	0.81
2:F:5:MET:CA	2:F:5:MET:CE	2.59	0.81
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
1:A:315:MSE:HB3	1:A:315:MSE:HE3	1.64	0.78
2:F:5:MET:HA	2:F:5:MET:CE	2.15	0.77
1:C:270:VAL:HG11	2:F:2:LEU:HD22	1.67	0.77
1:A:342:GLU:N	3:A:12:HOH:O	2.17	0.77
2:D:7:THR:OG1	2:D:7:THR:CA	2.34	0.76
1:B:274:ASN:HB3	1:B:279:GLY:H	0.65	0.76
1:B:324:LEU:CD1	1:B:324:LEU:HG	2.10	0.75
2:E:6:THR:C	2:E:6:THR:CB	2.53	0.75
1:B:307:VAL:HG22	1:B:336:LEU:HD23	1.68	0.75
1:B:287:MSE:HE2	1:B:287:MSE:N	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:303:MSE:CB	1:B:303:MSE:C	2.55	0.73
1:B:274:ASN:N	1:B:274:ASN:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:THR:N	2:D:7:THR:CB	2.53	0.72
1:C:307:VAL:CG2	1:C:312:PHE:CZ	2.72	0.72
1:B:254:THR:C	1:B:255:VAL:HG12	2.11	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:HA	1:A:260:GLU:OE2	1.92	0.69
1:A:276:ARG:HG3	1:A:276:ARG:NH1	2.08	0.69
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
2:E:7:THR:C	2:E:8:VAL:HG13	2.13	0.67
1:C:338:VAL:CG2	1:C:339:ALA:N	2.57	0.66
1:A:341:LEU:HD21	2:E:4:LEU:HB2	1.75	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
2:E:6:THR:CG2	2:E:6:THR:CA	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:O	1:B:292:VAL:HG12	1.98	0.64
2:E:3:LYS:HB2	2:E:3:LYS:CE	2.28	0.64
2:F:5:MET:HE3	2:F:5:MET:HA	1.76	0.64
2:D:5:MET:HE3	2:D:5:MET:CG	2.16	0.63
1:C:258:ASN:ND2	1:C:260:GLU:H	1.96	0.62
2:F:5:MET:HE2	2:F:5:MET:HA	1.80	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:311:ASN:CG	3:A:23:HOH:O	2.30	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:C:307:VAL:CG2	1:C:312:PHE:HZ	2.13	0.61
1:B:287:MSE:HE2	1:B:287:MSE:H	1.64	0.61
1:C:272:GLN:CD	1:C:282:TYR:OH	2.39	0.61
1:C:272:GLN:HG2	1:C:282:TYR:HE1	1.64	0.61
1:C:259:MSE:HE2	1:C:259:MSE:N	2.14	0.61
1:B:293:ALA:O	1:B:296:GLY:N	2.33	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:C:312:PHE:HD2	1:C:315:MSE:CE	2.14	0.61
1:B:303:MSE:CA	1:B:304:LEU:N	2.58	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ILE:HG21	1:A:253:ILE:HD13	1.73	0.60
1:B:274:ASN:HB2	1:B:278:ASP:HA	1.83	0.60
1:A:310:ILE:CG2	1:A:310:ILE:CG1	2.72	0.60
1:B:338:VAL:O	1:B:338:VAL:CG1	2.50	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:B:258:ASN:C	1:B:260:GLU:H	2.03	0.59
2:F:5:MET:HE2	2:F:5:MET:CA	2.32	0.59
1:B:338:VAL:HG22	1:B:339:ALA:N	2.16	0.58
1:A:253:ILE:HG23	1:A:253:ILE:HD13	1.85	0.58
1:B:282:TYR:CE2	1:B:303:MSE:HB2	2.38	0.58
1:A:274:ASN:CG	1:A:275:GLU:H	2.06	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:HD3	1:C:288:LYS:N	2.17	0.57
1:B:315:MSE:HB3	1:B:315:MSE:HE2	1.85	0.57
1:B:302:ASP:OD1	1:B:340:LYS:HD3	2.05	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:298:ILE:HG13	3:C:11:HOH:O	2.04	0.56
1:B:256:THR:C	1:B:257:LEU:HD23	2.25	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
2:E:7:THR:C	2:E:8:VAL:CG1	2.72	0.56
1:A:274:ASN:CG	1:A:275:GLU:N	2.59	0.55
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:343:HIS:O	1:A:344:HIS:C	2.45	0.55
1:C:325:ARG:HD2	2:F:6:THR:HG21	1.89	0.55
1:A:341:LEU:CA	3:A:12:HOH:O	1.95	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:HB	1:A:253:ILE:CG2	2.19	0.54
2:D:7:THR:N	2:D:7:THR:CG2	2.70	0.54
1:A:308:ASN:HD21	1:A:335:VAL:H	1.52	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ILE:HB	1:A:310:ILE:CG2	2.17	0.54
1:A:315:MSE:CG	1:A:315:MSE:HE3	2.34	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:C:308:ASN:HD21	1:C:335:VAL:H	1.55	0.53
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:HD3	3:A:22:HOH:O	2.07	0.52
1:A:330:LYS:HB3	1:A:331:PRO:CD	2.39	0.52
1:C:258:ASN:HD21	1:C:260:GLU:HB2	1.73	0.52
1:C:258:ASN:C	1:C:259:MSE:HE2	2.30	0.52
1:A:299:GLU:OE2	1:C:287:MSE:HB3	2.10	0.52
1:C:272:GLN:CD	1:C:282:TYR:HH	2.13	0.51
2:F:4:LEU:CD1	2:F:4:LEU:CB	2.78	0.51
1:A:259:MSE:HG3	1:A:334:ILE:CD1	2.40	0.51
1:B:283:ILE:CD1	1:B:304:LEU:HD21	2.40	0.51
1:C:272:GLN:HG3	1:C:279:GLY:HA3	1.91	0.51
1:B:286:ILE:HD12	1:B:300:PRO:HD3	1.93	0.51
1:C:302:ASP:HB3	1:C:338:VAL:HG21	1.93	0.51
1:C:325:ARG:NE	1:C:325:ARG:CG	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:C:322:ARG:O	1:C:323:VAL:C	2.49	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:HG2	1:A:303:MSE:CE	2.36	0.50
1:B:252:ILE:HG22	1:B:253:ILE:N	2.27	0.50
1:C:287:MSE:O	1:C:288:LYS:C	2.40	0.50
1:B:325:ARG:NH2	3:B:10:HOH:O	2.45	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
2:F:5:MET:N	2:F:5:MET:HE3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ILE:HD11	1:B:304:LEU:HD21	1.94	0.48
1:B:258:ASN:C	1:B:260:GLU:N	2.67	0.48
1:C:308:ASN:O	1:C:309:ASP:CB	2.57	0.48
1:B:303:MSE:CG	1:B:303:MSE:C	2.82	0.48
1:C:253:ILE:HG21	1:C:253:ILE:HD13	1.45	0.48
1:A:259:MSE:HG3	1:A:334:ILE:HD12	1.94	0.48
1:A:276:ARG:HG3	1:A:276:ARG:HH11	1.75	0.48
1:B:338:VAL:HG13	1:B:338:VAL:O	2.12	0.47
1:B:315:MSE:HE2	1:B:315:MSE:CB	2.45	0.47
1:C:299:GLU:N	1:C:299:GLU:OE1	2.47	0.47
1:B:330:LYS:C	1:B:331:PRO:O	2.52	0.47
1:B:305:LEU:O	1:B:312:PHE:HB2	2.14	0.47
1:C:306:GLN:HB2	1:C:311:ASN:HA	1.97	0.47
1:A:340:LYS:HE3	1:A:340:LYS:HB3	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:274:ASN:N	1:C:277:GLY:O	2.47	0.46
1:C:256:THR:O	1:C:256:THR:CG2	2.64	0.46
1:B:257:LEU:O	1:B:259:MSE:HG2	2.16	0.46
1:A:260:GLU:OE2	1:A:260:GLU:CA	2.58	0.46
1:C:311:ASN:OD1	1:C:313:GLU:HG3	2.16	0.46
1:A:307:VAL:HG22	1:A:336:LEU:HD23	1.97	0.46
1:A:315:MSE:HB2	1:A:315:MSE:HE2	1.92	0.46
1:B:334:ILE:HG21	1:B:334:ILE:HD13	1.21	0.45
1:B:306:GLN:HB2	1:B:311:ASN:HA	1.98	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:311:ASN:HD22	1:B:313:GLU:H	1.62	0.45
1:B:274:ASN:HB2	1:B:278:ASP:CA	2.44	0.45
1:B:252:ILE:O	1:B:253:ILE:HB	2.17	0.45
1:A:288:LYS:HA	1:A:288:LYS:HD2	1.71	0.45
1:B:277:GLY:O	1:B:278:ASP:C	2.54	0.45
1:A:340:LYS:HE2	1:C:287:MSE:HE2	1.98	0.45
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:B:255:VAL:HG22	1:B:257:LEU:HD21	1.95	0.44
1:A:307:VAL:HG22	1:A:336:LEU:CD2	2.47	0.44
1:A:274:ASN:H	1:A:277:GLY:CA	2.21	0.44
1:A:297:ARG:HG3	2:F:7:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:278:ASP:O	1:A:279:GLY:C	2.54	0.43
1:C:272:GLN:NE2	1:C:282:TYR:OH	2.51	0.43
1:A:276:ARG:CG	1:A:276:ARG:HH11	2.31	0.43
1:B:303:MSE:HG2	1:B:303:MSE:C	2.38	0.43
1:C:323:VAL:O	1:C:327:ILE:CG1	2.66	0.43
1:A:307:VAL:HG21	1:A:324:LEU:HD13	1.99	0.43
2:D:7:THR:HG23	2:D:7:THR:N	2.33	0.43
1:A:271:GLY:O	2:D:2:LEU:HA	2.19	0.43
1:B:274:ASN:O	1:B:275:GLU:O	2.36	0.43
1:B:254:THR:O	1:B:255:VAL:CB	2.57	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:C:299:GLU:OE1	1:C:302:ASP:OD2	2.36	0.42
1:B:276:ARG:CA	1:B:276:ARG:HE	2.12	0.42
1:C:299:GLU:N	1:C:302:ASP:OD2	2.34	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: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:293:ALA:C	1:B:295:ASP:N	2.71	0.42
2:E:4:LEU:HG	2:E:5:MET:N	2.34	0.42
1:B:299:GLU:N	1:B:302:ASP:OD2	2.29	0.42
1:B:262:TYR:OH	1:B:294:ALA:CB	2.68	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: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:B:332:GLY:C	1:B:333:PRO:O	2.56	0.41
2:E:6:THR:OG1	2:E:6:THR:CA	2.56	0.41
1:A:287:MSE:HG2	1:A:287:MSE:H	1.67	0.41
1:B:254:THR:C	1:B:255:VAL:CG1	2.73	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:A:257:LEU:HA	1:A:257:LEU:HD23	1.89	0.41
1:C:299:GLU:CD	1:C:340:LYS:HE2	2.41	0.41
2:F:6:THR:CB	2:F:7:THR:N	2.84	0.41
1:C:307:VAL:CG2	1:C:312:PHE:CE1	2.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:HIS:CG	1:A:344:HIS:H	2.10	0.40
2:D:6:THR:HB	2:D:7:THR:H	1.73	0.40
1:C:257:LEU:CB	1:C:259:MSE:HE1	2.51	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	93/95 (98%)	87 (94%)	4 (4%)	2 (2%)	8	4
1	B	91/95 (96%)	75 (82%)	12 (13%)	4 (4%)	3	1
1	C	90/95 (95%)	82 (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	292/309 (94%)	261 (89%)	25 (9%)	6 (2%)	9	5

All (6) 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
1	B	334	ILE

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%)	70 (89%)	9 (11%)	7	6
1	B	77/74 (104%)	65 (84%)	12 (16%)	3	2
1	C	76/74 (103%)	67 (88%)	9 (12%)	6	5
2	D	8/8 (100%)	8 (100%)	0	100	100
2	E	8/8 (100%)	6 (75%)	2 (25%)	1	0
2	F	8/8 (100%)	5 (62%)	3 (38%)	0	0
All	All	256/246 (104%)	221 (86%)	35 (14%)	4	3

All (35) 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	330	LYS
1	A	344	HIS
1	B	255	VAL
1	B	256	THR
1	B	264	PHE
1	B	273	SER
1	B	276	ARG
1	B	278	ASP
1	B	287	MSE
1	B	297	ARG
1	B	306	GLN
1	B	330	LYS
1	B	337	THR
1	B	338	VAL
1	C	258	ASN

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Mol	Chain	Res	Type
1	C	264	PHE
1	C	273	SER
1	C	287	MSE
1	C	288	LYS
1	C	304	LEU
1	C	306	GLN
1	C	308	ASN
1	C	327	ILE
2	E	3	LYS
2	E	5	MET
2	F	1	SER
2	F	5	MET
2	F	6	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	A	306	GLN
1	A	308	ASN
1	B	272	GLN
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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.