



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 03:07 PM UTC

PDB ID : 3P45 / pdb_00003p45
Title : Crystal structure of apo-caspase-6 at physiological pH
Authors : Mueller, I.; Lamers, M.B.A.C.; Ritchie, A.J.; Dominguez, C.; Munoz, I.; Mail-
lard, M.; Kiselyov, A.
Deposited on : 2010-10-06
Resolution : 2.53 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

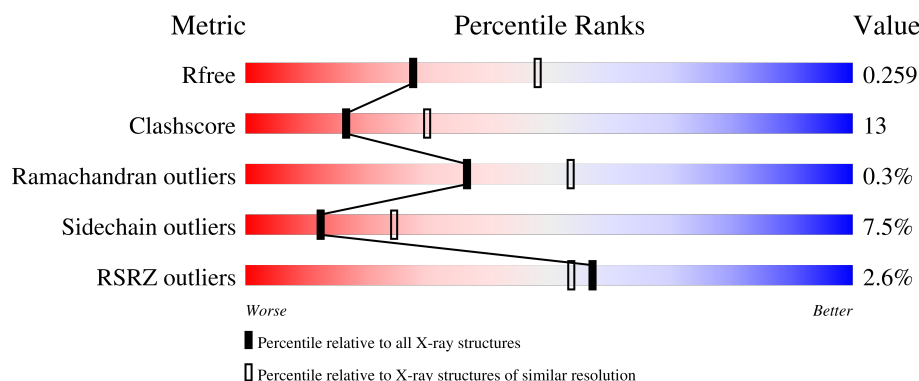
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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))
R_{free}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	179	% 58% 14% • 26%
1	C	179	52% 19% • 26%
1	E	179	2% 51% 20% •• 26%
1	G	179	% 56% 15% • 27%
1	I	179	2% 58% 13% • 26%

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Mol	Chain	Length	Quality of chain
1	K	179	
1	M	179	
1	O	179	
2	B	108	
2	D	108	
2	F	108	
2	H	108	
2	J	108	
2	L	108	
2	N	108	
2	P	108	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12955 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 caspase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1058	678	183	190	7			
1	C	132	Total	C	N	O	S	0	0	0
			1054	676	184	188	6			
1	E	132	Total	C	N	O	S	0	0	0
			1058	679	186	187	6			
1	G	131	Total	C	N	O	S	0	0	0
			1040	666	180	188	6			
1	I	133	Total	C	N	O	S	0	0	0
			1063	681	185	190	7			
1	K	133	Total	C	N	O	S	0	0	0
			1037	665	181	184	7			
1	M	133	Total	C	N	O	S	0	0	0
			1055	677	183	188	7			
1	O	132	Total	C	N	O	S	0	0	0
			1043	670	179	188	6			

- Molecule 2 is a protein called caspase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	72	Total	C	N	O	S	0	0	0
			579	377	94	102	6			
2	D	70	Total	C	N	O	S	0	0	0
			554	361	89	98	6			
2	F	68	Total	C	N	O	S	0	0	0
			535	348	86	95	6			
2	H	68	Total	C	N	O	S	0	0	0
			545	356	89	94	6			
2	J	70	Total	C	N	O	S	0	0	0
			543	353	87	97	6			
2	L	66	Total	C	N	O	S	0	0	0
			521	339	84	92	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	67	Total	C	N	O	S	0	0	0
			531	345	85	95	6			
2	P	68	Total	C	N	O	S	0	0	0
			538	349	87	96	6			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	294	ARG	-	expression tag	UNP P55212
B	295	HIS	-	expression tag	UNP P55212
B	296	HIS	-	expression tag	UNP P55212
B	297	HIS	-	expression tag	UNP P55212
B	298	HIS	-	expression tag	UNP P55212
B	299	HIS	-	expression tag	UNP P55212
B	300	HIS	-	expression tag	UNP P55212
D	294	ARG	-	expression tag	UNP P55212
D	295	HIS	-	expression tag	UNP P55212
D	296	HIS	-	expression tag	UNP P55212
D	297	HIS	-	expression tag	UNP P55212
D	298	HIS	-	expression tag	UNP P55212
D	299	HIS	-	expression tag	UNP P55212
D	300	HIS	-	expression tag	UNP P55212
F	294	ARG	-	expression tag	UNP P55212
F	295	HIS	-	expression tag	UNP P55212
F	296	HIS	-	expression tag	UNP P55212
F	297	HIS	-	expression tag	UNP P55212
F	298	HIS	-	expression tag	UNP P55212
F	299	HIS	-	expression tag	UNP P55212
F	300	HIS	-	expression tag	UNP P55212
H	294	ARG	-	expression tag	UNP P55212
H	295	HIS	-	expression tag	UNP P55212
H	296	HIS	-	expression tag	UNP P55212
H	297	HIS	-	expression tag	UNP P55212
H	298	HIS	-	expression tag	UNP P55212
H	299	HIS	-	expression tag	UNP P55212
H	300	HIS	-	expression tag	UNP P55212
J	294	ARG	-	expression tag	UNP P55212
J	295	HIS	-	expression tag	UNP P55212
J	296	HIS	-	expression tag	UNP P55212
J	297	HIS	-	expression tag	UNP P55212
J	298	HIS	-	expression tag	UNP P55212
J	299	HIS	-	expression tag	UNP P55212

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Chain	Residue	Modelled	Actual	Comment	Reference
J	300	HIS	-	expression tag	UNP P55212
L	294	ARG	-	expression tag	UNP P55212
L	295	HIS	-	expression tag	UNP P55212
L	296	HIS	-	expression tag	UNP P55212
L	297	HIS	-	expression tag	UNP P55212
L	298	HIS	-	expression tag	UNP P55212
L	299	HIS	-	expression tag	UNP P55212
L	300	HIS	-	expression tag	UNP P55212
N	294	ARG	-	expression tag	UNP P55212
N	295	HIS	-	expression tag	UNP P55212
N	296	HIS	-	expression tag	UNP P55212
N	297	HIS	-	expression tag	UNP P55212
N	298	HIS	-	expression tag	UNP P55212
N	299	HIS	-	expression tag	UNP P55212
N	300	HIS	-	expression tag	UNP P55212
P	294	ARG	-	expression tag	UNP P55212
P	295	HIS	-	expression tag	UNP P55212
P	296	HIS	-	expression tag	UNP P55212
P	297	HIS	-	expression tag	UNP P55212
P	298	HIS	-	expression tag	UNP P55212
P	299	HIS	-	expression tag	UNP P55212
P	300	HIS	-	expression tag	UNP P55212

- Molecule 3 is water.

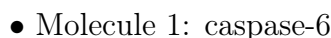
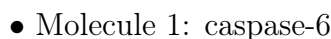
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	7	Total O 7 7	0	0
3	C	8	Total O 8 8	0	0
3	D	8	Total O 8 8	0	0
3	E	30	Total O 30 30	0	0
3	F	11	Total O 11 11	0	0
3	G	8	Total O 8 8	0	0
3	H	7	Total O 7 7	0	0

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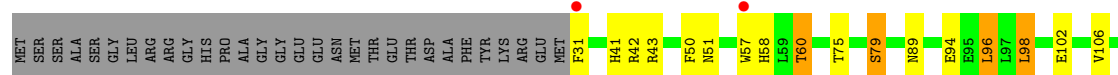
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	21	Total 21	O 21	0	0
3	J	10	Total 10	O 10	0	0
3	K	14	Total 14	O 14	0	0
3	L	6	Total 6	O 6	0	0
3	M	29	Total 29	O 29	0	0
3	N	4	Total 4	O 4	0	0
3	O	8	Total 8	O 8	0	0
3	P	6	Total 6	O 6	0	0

- Molecule 1: caspase-6

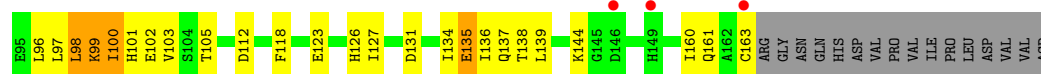
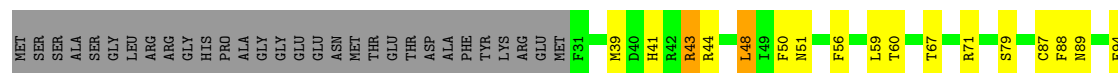




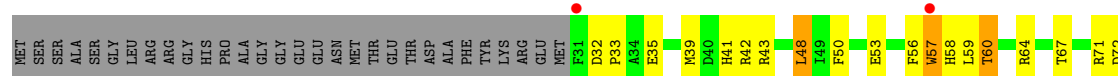
- Molecule 1: caspase-6



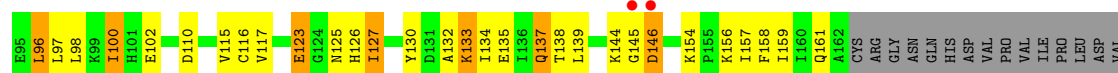
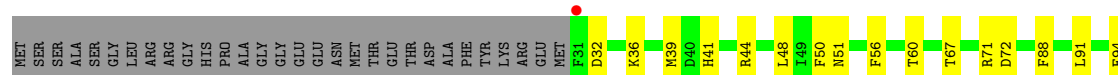
- Molecule 1: caspase-6



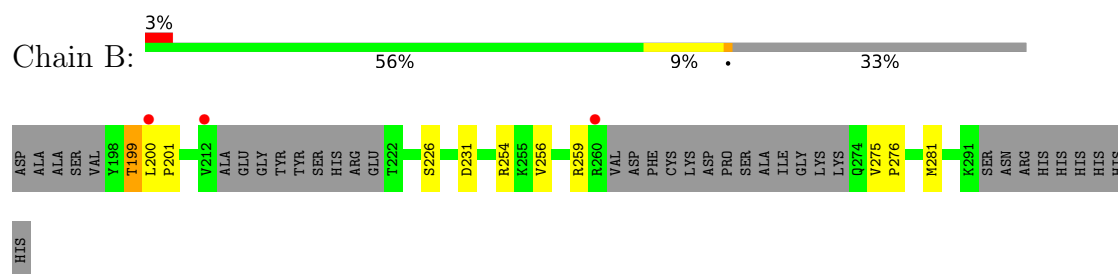
- Molecule 1: caspase-6



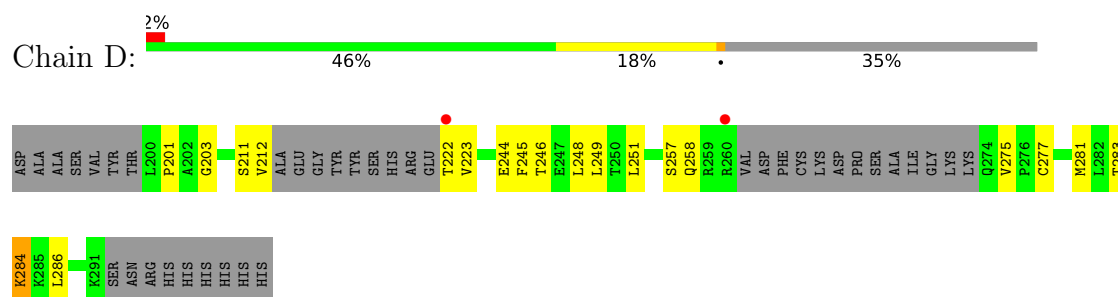
- Molecule 1: caspase-6



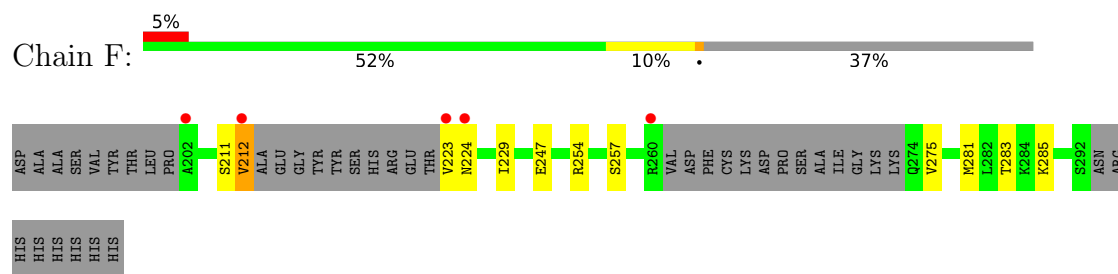
- Molecule 2: caspase-6



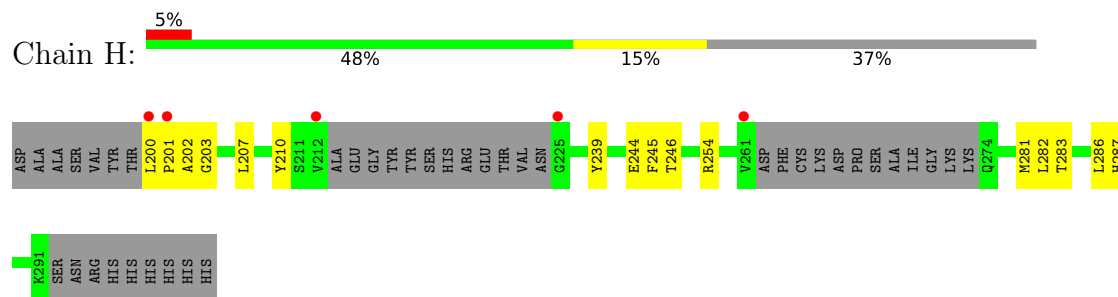
- Molecule 2: caspase-6



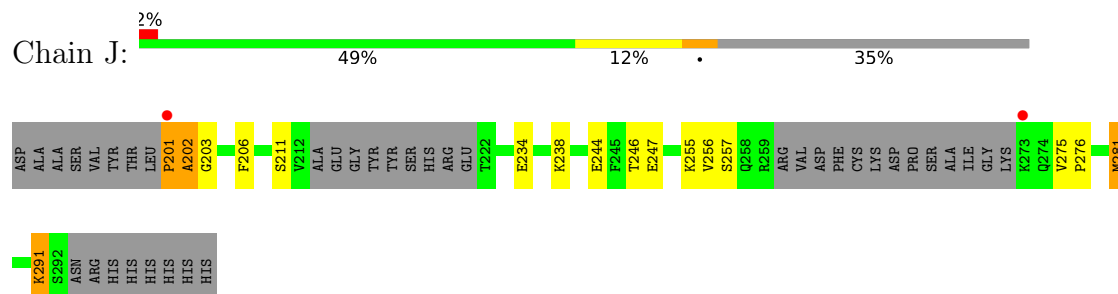
- Molecule 2: caspase-6



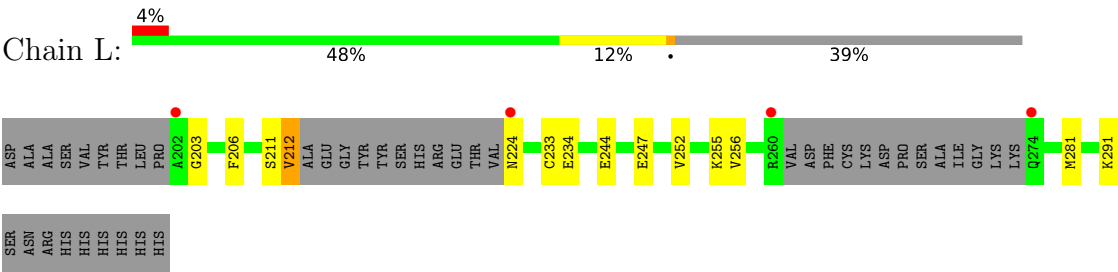
- Molecule 2: caspase-6



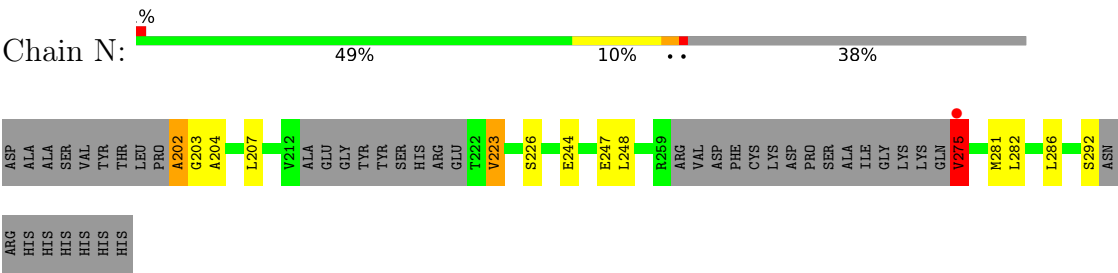
- Molecule 2: caspase-6



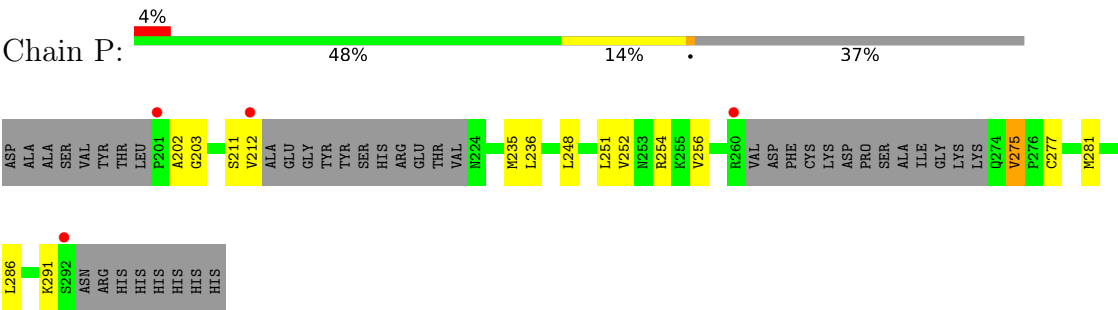
● Molecule 2: caspase-6



● Molecule 2: caspase-6



● Molecule 2: caspase-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.23Å 161.24Å 88.92Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	29.96 – 2.53 29.96 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.96-2.53) 99.8 (29.96-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.54Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.264 0.207 , 0.259	Depositor DCC
R_{free} test set	3815 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12955	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.24	1/1083 (0.1%)	1.17	3/1460 (0.2%)
1	C	1.09	2/1080 (0.2%)	1.03	0/1457
1	E	1.19	2/1083 (0.2%)	1.14	5/1458 (0.3%)
1	G	1.02	0/1065	1.04	4/1437 (0.3%)
1	I	1.16	1/1089 (0.1%)	1.09	2/1468 (0.1%)
1	K	0.94	0/1061	1.05	0/1431
1	M	1.16	0/1080	1.15	0/1456
1	O	0.96	0/1068	1.05	3/1442 (0.2%)
2	B	1.03	0/591	1.08	1/794 (0.1%)
2	D	1.09	0/565	1.04	0/759
2	F	1.16	0/545	1.05	1/730 (0.1%)
2	H	1.01	0/556	0.97	1/745 (0.1%)
2	J	1.17	0/554	1.08	1/743 (0.1%)
2	L	0.97	0/531	1.04	0/711
2	N	1.07	0/541	1.14	2/725 (0.3%)
2	P	1.02	0/549	1.08	1/735 (0.1%)
All	All	1.09	6/13041 (0.0%)	1.08	24/17551 (0.1%)

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	C	0	2
1	I	0	1
1	O	0	1
2	J	0	1
2	N	0	2
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	49	ILE	CA-CB	-7.00	1.45	1.54
1	C	70	ASP	C-O	-5.64	1.17	1.24
1	E	137	GLN	N-CA	5.44	1.53	1.46
1	I	159	ILE	C-O	-5.43	1.18	1.24
1	C	116	CYS	C-O	-5.22	1.17	1.23
1	A	136	ILE	C-O	-5.12	1.18	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	202	ALA	N-CA-C	10.45	123.94	111.82
1	A	110	ASP	CB-CA-C	-7.19	97.06	110.36
2	F	247	GLU	N-CA-C	-6.36	104.27	111.07
2	N	203	GLY	N-CA-C	-6.26	98.33	113.18
1	A	131	ASP	N-CA-CB	-6.07	101.21	110.26
1	O	32	ASP	CA-C-N	6.04	125.52	119.24
1	O	32	ASP	C-N-CA	6.04	125.52	119.24
1	E	73	ASN	N-CA-C	-5.85	104.27	111.40
2	H	245	PHE	N-CA-C	5.55	117.33	111.28
1	E	67	THR	N-CA-C	5.48	117.26	111.28
2	P	236	LEU	N-CA-C	-5.43	105.26	111.07
2	B	199	THR	N-CA-C	5.39	120.13	113.50
1	E	65	ARG	N-CA-C	5.30	117.05	111.28
2	N	275	VAL	CB-CA-C	-5.24	101.44	111.40
1	G	65	ARG	N-CA-C	5.20	117.68	111.71
1	E	134	ILE	CB-CA-C	-5.18	102.77	110.33
1	I	102	GLU	N-CA-C	-5.16	105.55	111.07
1	E	105	THR	N-CA-CB	-5.09	103.27	110.81
1	A	157	ILE	N-CA-C	5.05	115.37	107.99
1	O	102	GLU	N-CA-C	-5.05	105.67	111.07
1	G	61	LEU	CA-C-N	-5.03	115.05	120.03
1	G	61	LEU	C-N-CA	-5.03	115.05	120.03
1	G	131	ASP	N-CA-CB	-5.01	102.76	110.42
1	I	131	ASP	N-CA-CB	-5.00	102.04	110.49

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	130	TYR	Peptide
1	C	31	PHE	Peptide
1	I	130	TYR	Peptide

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Mol	Chain	Res	Type	Group
2	J	201	PRO	Peptide
2	N	202	ALA	Mainchain,Peptide
1	O	130	TYR	Peptide

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	1058	0	1020	26	0
1	C	1054	0	1013	32	0
1	E	1058	0	1033	39	0
1	G	1040	0	1000	20	0
1	I	1063	0	1025	35	0
1	K	1037	0	996	35	0
1	M	1055	0	1018	40	0
1	O	1043	0	997	40	0
2	B	579	0	582	11	0
2	D	554	0	555	18	0
2	F	535	0	531	8	0
2	H	545	0	553	17	0
2	J	543	0	533	16	0
2	L	521	0	515	14	0
2	N	531	0	532	13	0
2	P	538	0	534	16	0
3	A	24	0	0	1	0
3	B	7	0	0	1	0
3	C	8	0	0	0	0
3	D	8	0	0	0	0
3	E	30	0	0	3	0
3	F	11	0	0	0	0
3	G	8	0	0	0	0
3	H	7	0	0	1	0
3	I	21	0	0	0	0
3	J	10	0	0	0	0
3	K	14	0	0	4	0
3	L	6	0	0	0	0
3	M	29	0	0	1	0
3	N	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	8	0	0	0	0
3	P	6	0	0	0	0
All	All	12955	0	12437	324	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 13.

All (324) 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)
2:H:201:PRO:HB2	2:H:281:MET:SD	1.77	1.24
1:O:88:PHE:HB3	1:O:91:LEU:HD21	1.34	1.09
1:I:161:GLN:HA	1:I:161:GLN:HE21	1.12	1.09
2:B:201:PRO:HB2	2:B:281:MET:SD	1.97	1.03
1:I:127:ILE:HD12	1:I:127:ILE:O	1.60	1.01
1:I:60:THR:HG22	1:I:60:THR:O	1.61	0.99
1:I:60:THR:O	1:I:60:THR:CG2	2.11	0.97
1:I:161:GLN:HE21	1:I:161:GLN:CA	1.80	0.94
2:D:201:PRO:HB2	2:D:281:MET:SD	2.10	0.90
1:M:98:LEU:H	1:M:98:LEU:HD12	1.36	0.90
2:B:275:VAL:HB	2:D:281:MET:HE3	1.55	0.87
1:M:59:LEU:O	1:M:60:THR:HG22	1.76	0.86
2:L:203:GLY:HA2	2:L:281:MET:HE1	1.60	0.83
1:E:51:ASN:ND2	1:E:67:THR:CG2	2.42	0.83
1:G:51:ASN:HD21	1:G:67:THR:HG23	1.44	0.82
1:I:127:ILE:HD12	1:I:127:ILE:C	2.00	0.82
1:O:127:ILE:O	1:O:127:ILE:HD12	1.79	0.82
1:I:127:ILE:C	1:I:127:ILE:CD1	2.54	0.81
1:E:59:LEU:O	1:E:60:THR:HG22	1.81	0.80
1:E:51:ASN:ND2	1:E:67:THR:HG22	1.97	0.80
2:N:275:VAL:HB	2:P:281:MET:HE3	1.63	0.80
1:M:98:LEU:HD13	1:M:99:LYS:N	1.97	0.79
1:G:60:THR:HG22	1:G:60:THR:O	1.82	0.78
1:M:95:GLU:O	1:M:98:LEU:CD1	2.32	0.78
1:M:60:THR:HG23	1:M:60:THR:O	1.84	0.76
1:M:98:LEU:HD13	1:M:98:LEU:C	2.10	0.75
1:O:88:PHE:HB3	1:O:91:LEU:CD2	2.16	0.75
1:E:118:PHE:CZ	1:E:139:LEU:HD13	2.22	0.75
1:A:110:ASP:HB2	3:A:194:HOH:O	1.86	0.74
1:K:97:LEU:HD23	1:K:100:ILE:HD11	1.69	0.74
1:A:133:LYS:HZ3	1:E:126:HIS:HE1	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:204:ALA:HB2	2:P:275:VAL:HG21	1.70	0.73
1:A:51:ASN:HB3	1:A:89:ASN:ND2	2.04	0.73
1:G:144:LYS:HD3	2:H:202:ALA:HB1	1.70	0.71
1:C:101:HIS:O	1:C:105:THR:HG22	1.91	0.71
1:M:161:GLN:NE2	2:N:226:SER:OG	2.17	0.70
2:N:202:ALA:HA	2:N:281:MET:SD	2.32	0.70
1:M:98:LEU:CD1	1:M:98:LEU:N	2.55	0.70
1:I:50:PHE:CE1	1:I:96:LEU:HD13	2.27	0.69
2:J:275:VAL:HB	2:L:281:MET:CE	2.23	0.69
1:O:97:LEU:HA	1:O:100:ILE:HG22	1.75	0.69
1:G:51:ASN:HD21	1:G:67:THR:CG2	2.06	0.69
1:A:75:THR:HG23	1:A:85:VAL:HG11	1.75	0.68
2:B:201:PRO:HG2	2:B:281:MET:HG3	1.75	0.68
2:J:275:VAL:HB	2:L:281:MET:HE3	1.74	0.68
1:M:120:SER:HB3	1:M:127:ILE:HD11	1.76	0.68
2:D:211:SER:OG	2:D:212:VAL:HG23	1.93	0.68
1:E:60:THR:O	1:E:60:THR:HG23	1.94	0.67
2:B:254:ARG:NE	3:B:96:HOH:O	2.22	0.67
1:E:51:ASN:HD21	1:E:67:THR:CG2	2.05	0.67
1:C:51:ASN:HD21	1:C:67:THR:HG23	1.58	0.67
1:C:56:PHE:HZ	1:G:98:LEU:HD22	1.59	0.67
2:F:275:VAL:HB	2:H:281:MET:HE3	1.77	0.67
1:A:133:LYS:NZ	1:E:126:HIS:HE1	1.93	0.66
1:A:126:HIS:HE1	1:E:133:LYS:NZ	1.94	0.65
1:M:120:SER:HB3	1:M:127:ILE:CD1	2.26	0.65
2:F:275:VAL:HB	2:H:281:MET:CE	2.27	0.65
2:J:201:PRO:C	2:J:281:MET:HE1	2.21	0.65
1:E:74:LEU:HD11	2:F:229:ILE:HD12	1.79	0.65
1:O:145:GLY:O	1:O:146:ASP:CB	2.44	0.65
1:I:127:ILE:O	1:I:127:ILE:CD1	2.43	0.64
2:B:275:VAL:HB	2:D:281:MET:CE	2.27	0.64
1:K:48:LEU:HD12	1:K:103:VAL:HG21	1.77	0.64
1:K:97:LEU:HA	1:K:100:ILE:HD11	1.78	0.64
1:K:118:PHE:CD2	1:K:127:ILE:HD13	2.33	0.64
1:M:95:GLU:O	1:M:98:LEU:HD11	1.96	0.64
2:L:203:GLY:HA2	2:L:281:MET:CE	2.28	0.64
1:M:98:LEU:HD12	1:M:98:LEU:N	2.03	0.64
1:I:161:GLN:HA	1:I:161:GLN:NE2	1.97	0.64
1:M:48:LEU:HD13	1:M:50:PHE:CE2	2.33	0.63
1:A:51:ASN:HB3	1:A:89:ASN:HD22	1.63	0.63
2:D:248:LEU:C	2:D:248:LEU:HD23	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:207:LEU:HD22	2:H:282:LEU:HD11	1.78	0.63
2:D:248:LEU:HD23	2:D:248:LEU:O	1.99	0.62
1:O:127:ILE:HD12	1:O:127:ILE:C	2.24	0.62
1:K:59:LEU:O	1:K:60:THR:HG22	1.99	0.62
1:G:47:ALA:HB3	1:G:85:VAL:HG22	1.81	0.61
2:J:256:VAL:HG11	2:J:276:PRO:HD3	1.83	0.61
1:O:144:LYS:CE	2:P:202:ALA:HB1	2.31	0.61
1:A:127:ILE:HD12	1:A:127:ILE:O	2.00	0.61
1:G:48:LEU:HD13	1:G:50:PHE:CE2	2.35	0.61
1:C:118:PHE:CZ	1:C:139:LEU:HD13	2.36	0.60
1:G:48:LEU:HD13	1:G:50:PHE:CZ	2.35	0.60
1:C:48:LEU:HD11	1:C:103:VAL:HG11	1.83	0.60
1:O:127:ILE:C	1:O:127:ILE:CD1	2.75	0.60
1:A:118:PHE:CZ	1:A:139:LEU:HD13	2.35	0.60
1:K:39:MET:O	2:L:291:LYS:NZ	2.33	0.60
1:O:39:MET:HE3	1:O:44:ARG:HH11	1.66	0.59
2:J:202:ALA:HB3	2:J:206:PHE:CD1	2.37	0.59
2:J:202:ALA:HB3	2:J:206:PHE:CG	2.37	0.59
1:A:133:LYS:NZ	1:E:135:GLU:OE1	2.34	0.59
1:I:161:GLN:CA	1:I:161:GLN:NE2	2.57	0.58
1:I:118:PHE:CZ	1:I:139:LEU:HD13	2.38	0.58
1:E:102:GLU:CD	3:E:185:HOH:O	2.47	0.57
2:P:235:MET:HE2	2:P:235:MET:HA	1.85	0.57
1:C:100:ILE:O	1:C:103:VAL:HG22	2.04	0.57
1:O:96:LEU:HD12	1:O:134:ILE:CD1	2.34	0.57
2:F:283:THR:O	2:H:254:ARG:HD3	2.04	0.57
1:E:96:LEU:HD13	1:E:96:LEU:C	2.30	0.57
2:F:223:VAL:HG12	2:F:224:ASN:N	2.20	0.56
1:O:134:ILE:HG21	1:O:139:LEU:HD21	1.87	0.56
1:K:126:HIS:HE1	1:O:133:LYS:NZ	2.05	0.55
1:E:51:ASN:ND2	1:E:67:THR:HG21	2.20	0.55
1:C:51:ASN:HD21	1:C:67:THR:CG2	2.19	0.55
1:G:71:ARG:NH2	1:G:72:ASP:OD1	2.40	0.55
1:I:98:LEU:HD22	1:M:56:PHE:HZ	1.71	0.55
1:M:42:ARG:HH11	1:M:43:ARG:HE	1.54	0.54
1:O:41:HIS:HB3	1:O:110:ASP:O	2.07	0.54
1:E:51:ASN:HD21	1:E:67:THR:HG22	1.64	0.54
2:P:252:VAL:O	2:P:256:VAL:HG23	2.08	0.54
1:C:127:ILE:HD12	1:C:127:ILE:O	2.08	0.54
1:I:75:THR:O	1:I:79:SER:HB2	2.07	0.54
1:I:161:GLN:NE2	2:J:211:SER:CB	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:96:LEU:O	1:K:100:ILE:HG13	2.08	0.53
1:O:50:PHE:CE1	1:O:96:LEU:HD22	2.44	0.53
1:C:100:ILE:HA	1:C:103:VAL:HG22	1.90	0.53
1:A:31:PHE:HE2	2:D:258:GLN:NE2	2.07	0.53
1:M:59:LEU:O	1:M:60:THR:CG2	2.55	0.53
1:C:48:LEU:HD21	1:C:103:VAL:HG11	1.91	0.53
1:O:71:ARG:HD2	1:O:72:ASP:OD1	2.07	0.53
1:O:51:ASN:HD21	1:O:67:THR:HG23	1.74	0.53
1:A:94:GLU:HG2	1:E:56:PHE:CE1	2.44	0.52
2:P:203:GLY:C	2:P:281:MET:HE2	2.35	0.52
1:A:133:LYS:NZ	1:E:126:HIS:CE1	2.77	0.52
1:I:41:HIS:O	2:J:291:LYS:HE3	2.10	0.52
1:K:48:LEU:CD1	1:K:103:VAL:HG21	2.40	0.51
2:L:211:SER:OG	2:L:212:VAL:HG12	2.11	0.51
2:D:245:PHE:CE2	2:D:249:LEU:HD11	2.45	0.51
1:E:127:ILE:C	1:E:127:ILE:HD12	2.35	0.51
1:K:48:LEU:HD22	1:K:50:PHE:CE2	2.45	0.51
1:M:41:HIS:HD2	1:M:112:ASP:OD1	1.93	0.51
2:P:248:LEU:O	2:P:248:LEU:HD23	2.11	0.51
1:A:59:LEU:O	1:A:60:THR:HG22	2.11	0.51
1:I:161:GLN:HE22	2:J:211:SER:CB	2.24	0.51
1:E:51:ASN:HD22	1:E:67:THR:CG2	2.21	0.51
1:O:144:LYS:HE2	2:P:202:ALA:HB1	1.92	0.50
2:H:254:ARG:NE	3:H:122:HOH:O	2.44	0.50
1:C:43:ARG:O	1:C:111:ALA:HA	2.12	0.50
1:G:42:ARG:HD2	1:G:43:ARG:HG3	1.94	0.50
1:K:131:ASP:OD1	1:O:94:GLU:HG3	2.12	0.50
2:F:254:ARG:NH1	2:H:283:THR:O	2.37	0.50
1:I:41:HIS:CD2	1:I:112:ASP:HA	2.46	0.50
1:E:96:LEU:C	1:E:96:LEU:CD1	2.84	0.50
1:E:98:LEU:HD12	3:E:186:HOH:O	2.11	0.50
1:K:126:HIS:HE1	1:O:133:LYS:HZ1	1.60	0.50
2:B:201:PRO:HB2	2:B:281:MET:CG	2.41	0.49
1:E:33:PRO:HG3	2:H:239:TYR:CZ	2.47	0.49
1:E:71:ARG:NH2	3:E:194:HOH:O	2.46	0.49
1:E:118:PHE:CE2	1:E:139:LEU:HD13	2.47	0.49
1:C:102:GLU:HA	1:C:105:THR:CG2	2.43	0.49
1:M:95:GLU:HA	1:M:98:LEU:HD11	1.95	0.49
1:O:127:ILE:O	1:O:127:ILE:CD1	2.57	0.49
2:N:207:LEU:HD22	2:N:282:LEU:HD11	1.95	0.48
1:E:101:HIS:O	1:E:105:THR:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:224:ASN:OD1	2:L:224:ASN:O	2.30	0.48
1:C:41:HIS:CD2	1:C:112:ASP:HA	2.48	0.48
1:C:71:ARG:HE	1:C:89:ASN:HD21	1.62	0.48
1:C:122:GLY:HA3	1:C:162:ALA:HB1	1.96	0.48
1:M:42:ARG:HH11	1:M:43:ARG:NE	2.11	0.48
2:H:201:PRO:HG2	2:H:281:MET:HG3	1.95	0.48
2:J:244:GLU:OE1	2:J:246:THR:OG1	2.21	0.48
1:O:50:PHE:CD1	1:O:96:LEU:HD22	2.48	0.48
2:D:201:PRO:CB	2:D:281:MET:SD	2.96	0.48
1:M:64:ARG:O	1:M:67:THR:HG22	2.13	0.48
1:E:91:LEU:HB3	1:E:95:GLU:HG3	1.96	0.48
1:I:43:ARG:HH12	1:I:110:ASP:HB2	1.79	0.48
1:M:121:HIS:O	1:M:127:ILE:HD13	2.14	0.47
1:O:154:LYS:O	1:O:156:LYS:HE2	2.14	0.47
1:A:60:THR:HG23	1:A:60:THR:O	2.15	0.47
1:O:126:HIS:HB3	1:O:133:LYS:HB2	1.96	0.47
2:L:244:GLU:O	2:L:247:GLU:HB2	2.15	0.47
2:J:203:GLY:O	2:J:206:PHE:HD2	1.97	0.47
2:H:201:PRO:CB	2:H:281:MET:SD	2.73	0.47
2:J:244:GLU:O	2:J:247:GLU:HB2	2.14	0.47
2:N:281:MET:HG2	2:P:277:CYS:HB3	1.97	0.47
1:K:94:GLU:O	1:K:98:LEU:HG	2.14	0.47
2:P:248:LEU:HD23	2:P:248:LEU:C	2.39	0.47
1:A:31:PHE:CE2	2:D:258:GLN:NE2	2.83	0.47
1:A:127:ILE:HD12	1:A:127:ILE:C	2.40	0.47
2:N:223:VAL:O	2:N:223:VAL:CG1	2.64	0.46
1:E:50:PHE:CE1	1:E:96:LEU:HD22	2.49	0.46
1:E:64:ARG:NH1	1:E:67:THR:OG1	2.48	0.46
1:K:94:GLU:HG2	1:O:56:PHE:CE1	2.50	0.46
1:O:116:CYS:O	1:O:158:PHE:HA	2.16	0.46
1:A:33:PRO:HB3	2:D:251:LEU:HD11	1.96	0.46
1:O:135:GLU:O	1:O:138:THR:HB	2.15	0.46
1:K:98:LEU:CD1	3:K:188:HOH:O	2.62	0.46
1:K:135:GLU:HG2	1:O:133:LYS:HZ3	1.81	0.46
2:N:275:VAL:HB	2:P:281:MET:CE	2.40	0.46
2:H:286:LEU:HD12	2:H:287:HIS:N	2.30	0.46
1:I:60:THR:O	1:I:60:THR:HG23	2.07	0.46
1:K:98:LEU:HD12	3:K:188:HOH:O	2.16	0.46
2:L:252:VAL:O	2:L:256:VAL:HG23	2.16	0.46
1:M:135:GLU:O	1:M:138:THR:HB	2.15	0.46
1:O:115:VAL:HG22	1:O:157:ILE:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:57:TRP:HE1	1:M:58:HIS:CE1	2.34	0.46
2:B:201:PRO:CG	2:B:281:MET:HG3	2.45	0.46
1:M:71:ARG:HD2	1:M:72:ASP:OD1	2.15	0.46
1:A:77:ARG:HD2	1:A:77:ARG:HA	1.68	0.46
1:G:108:HIS:HB2	1:G:150:SER:OG	2.16	0.46
1:E:151:LEU:O	1:E:156:LYS:NZ	2.49	0.46
1:C:56:PHE:CZ	1:G:98:LEU:HD22	2.46	0.45
1:C:157:ILE:HD11	2:D:286:LEU:HD21	1.97	0.45
1:K:134:ILE:CG2	1:K:139:LEU:HD21	2.46	0.45
1:O:125:ASN:HB3	1:O:137:GLN:HE22	1.81	0.45
1:I:50:PHE:CE1	1:I:96:LEU:CD1	2.99	0.45
2:F:211:SER:OG	2:F:212:VAL:N	2.50	0.45
2:B:201:PRO:CB	2:B:281:MET:SD	2.88	0.45
1:E:55:PHE:N	1:E:55:PHE:CD2	2.84	0.45
1:K:71:ARG:HE	1:K:89:ASN:HD21	1.64	0.45
2:N:248:LEU:C	2:N:248:LEU:HD23	2.41	0.45
1:M:94:GLU:O	1:M:98:LEU:HD12	2.15	0.45
1:O:157:ILE:HD11	2:P:286:LEU:HD21	1.98	0.45
3:K:180:HOH:O	1:O:132:ALA:HB1	2.17	0.45
1:I:94:GLU:OE1	1:M:92:LYS:NZ	2.41	0.45
1:K:87:CYS:N	3:K:187:HOH:O	2.41	0.45
2:N:281:MET:HG2	2:P:277:CYS:CB	2.47	0.45
1:A:96:LEU:CD1	1:A:96:LEU:C	2.90	0.45
1:E:50:PHE:CD1	1:E:96:LEU:HD22	2.52	0.45
1:I:119:LEU:HD23	1:I:161:GLN:HB3	1.98	0.45
1:M:60:THR:O	1:M:60:THR:CG2	2.55	0.45
1:M:95:GLU:C	1:M:98:LEU:CD1	2.90	0.45
1:K:44:ARG:HA	1:K:112:ASP:OD2	2.17	0.44
2:N:244:GLU:O	2:N:247:GLU:HB2	2.17	0.44
1:C:108:HIS:O	1:C:109:ALA:C	2.59	0.44
2:H:203:GLY:O	2:H:281:MET:HE2	2.16	0.44
2:L:233:CYS:O	2:L:234:GLU:C	2.60	0.44
1:C:127:ILE:HD12	1:C:127:ILE:C	2.41	0.44
1:M:98:LEU:H	1:M:98:LEU:CD1	2.11	0.44
1:I:98:LEU:HD22	1:M:56:PHE:CZ	2.52	0.44
1:C:102:GLU:HA	1:C:105:THR:HG22	2.00	0.44
1:C:100:ILE:O	1:C:103:VAL:CG2	2.66	0.43
1:C:127:ILE:HD11	1:C:139:LEU:HD11	2.00	0.43
1:A:78:PHE:O	1:A:83:PHE:HB2	2.18	0.43
1:E:41:HIS:CD2	1:E:112:ASP:HA	2.53	0.43
1:G:77:ARG:HA	1:G:77:ARG:HD3	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:39:MET:SD	1:K:112:ASP:HB3	2.58	0.43
1:I:51:ASN:HD22	1:I:119:LEU:HD12	1.84	0.43
1:K:101:HIS:O	1:K:105:THR:HG23	2.18	0.43
2:D:244:GLU:OE1	2:D:246:THR:OG1	2.29	0.43
1:M:48:LEU:HD13	1:M:50:PHE:HE2	1.79	0.43
1:G:98:LEU:HD13	1:G:98:LEU:HA	1.70	0.43
1:K:48:LEU:CD2	1:K:50:PHE:CE2	3.00	0.43
1:M:33:PRO:HA	2:P:251:LEU:HD21	2.00	0.43
1:I:31:PHE:CZ	2:L:255:LYS:HD2	2.53	0.43
1:M:41:HIS:CD2	1:M:112:ASP:OD1	2.71	0.43
1:O:117:VAL:HG22	1:O:159:ILE:HB	2.01	0.43
1:G:51:ASN:ND2	1:G:67:THR:OG1	2.52	0.43
2:J:234:GLU:OE2	2:J:238:LYS:HE2	2.18	0.43
1:C:95:GLU:O	1:C:96:LEU:C	2.61	0.43
2:D:283:THR:C	2:D:284:LYS:HG3	2.44	0.43
1:A:96:LEU:C	1:A:96:LEU:HD13	2.44	0.43
1:E:124:GLY:O	1:E:125:ASN:HB2	2.19	0.43
2:H:244:GLU:OE1	2:H:246:THR:OG1	2.25	0.43
1:I:50:PHE:CD1	1:I:96:LEU:HD13	2.52	0.43
2:L:211:SER:OG	2:L:212:VAL:N	2.52	0.43
1:C:96:LEU:C	1:C:96:LEU:CD1	2.92	0.42
1:I:51:ASN:HB3	1:I:89:ASN:ND2	2.34	0.42
1:K:134:ILE:HG21	1:K:139:LEU:HD21	2.01	0.42
1:O:137:GLN:H	1:O:137:GLN:NE2	2.17	0.42
1:C:50:PHE:CD1	1:C:96:LEU:HD22	2.54	0.42
1:E:50:PHE:CD1	1:E:96:LEU:CD2	3.01	0.42
1:M:32:ASP:HA	1:M:33:PRO:HD2	1.94	0.42
1:A:59:LEU:C	1:A:60:THR:HG22	2.44	0.42
1:I:50:PHE:CZ	1:I:96:LEU:CD1	3.01	0.42
1:O:96:LEU:O	1:O:100:ILE:HG22	2.20	0.42
1:O:97:LEU:HA	1:O:100:ILE:CG2	2.48	0.42
2:B:200:LEU:HD12	2:D:277:CYS:SG	2.59	0.42
1:C:41:HIS:HD2	1:C:112:ASP:OD1	2.02	0.42
2:D:248:LEU:C	2:D:248:LEU:CD2	2.92	0.42
1:G:60:THR:O	1:G:60:THR:CG2	2.53	0.42
1:O:123:GLU:O	1:O:126:HIS:HD2	2.02	0.42
2:B:256:VAL:HG11	2:B:276:PRO:HD3	2.01	0.42
2:H:200:LEU:N	2:H:210:TYR:HH	2.18	0.42
1:M:96:LEU:C	1:M:96:LEU:HD23	2.45	0.42
1:M:71:ARG:HE	1:M:89:ASN:HD21	1.66	0.42
1:E:124:GLY:O	1:E:125:ASN:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:256:VAL:CG1	2:J:276:PRO:HD3	2.50	0.41
1:O:97:LEU:CA	1:O:100:ILE:HG22	2.48	0.41
1:C:151:LEU:O	1:C:156:LYS:NZ	2.53	0.41
1:I:57:TRP:CD1	1:I:58:HIS:CE1	3.08	0.41
1:I:118:PHE:CE2	1:I:139:LEU:HD13	2.55	0.41
1:K:59:LEU:O	1:K:60:THR:CG2	2.65	0.41
1:K:96:LEU:C	1:K:96:LEU:HD23	2.45	0.41
1:M:100:ILE:HG21	1:M:139:LEU:HD22	2.02	0.41
1:M:108:HIS:O	1:M:154:LYS:NZ	2.53	0.41
1:A:133:LYS:HZ3	1:E:126:HIS:CE1	2.26	0.41
2:D:203:GLY:C	2:D:281:MET:HE2	2.45	0.41
1:G:34:ALA:O	1:G:35:GLU:C	2.63	0.41
1:G:48:LEU:HD23	1:G:48:LEU:HA	1.86	0.41
2:H:203:GLY:C	2:H:281:MET:HE2	2.45	0.41
1:O:115:VAL:HA	1:O:157:ILE:O	2.20	0.41
1:C:56:PHE:O	1:C:59:LEU:HB2	2.21	0.41
1:K:88:PHE:CE1	1:K:99:LYS:HE3	2.56	0.41
1:K:41:HIS:CD2	1:K:112:ASP:HA	2.56	0.41
1:K:51:ASN:ND2	1:K:67:THR:OG1	2.53	0.41
1:M:39:MET:HE2	2:N:286:LEU:HD11	2.03	0.41
1:A:94:GLU:HG2	1:E:56:PHE:CZ	2.56	0.41
1:C:65:ARG:HH21	2:D:223:VAL:HG13	1.85	0.41
1:C:97:LEU:O	1:C:100:ILE:HG22	2.21	0.41
1:I:161:GLN:NE2	2:J:211:SER:HB3	2.35	0.41
2:N:204:ALA:CB	2:P:275:VAL:HG21	2.45	0.41
1:O:123:GLU:O	1:O:123:GLU:HG3	2.20	0.41
1:I:120:SER:O	1:I:162:ALA:HA	2.21	0.41
1:I:138:THR:HG21	3:M:207:HOH:O	2.21	0.41
1:O:51:ASN:HD21	1:O:67:THR:CG2	2.33	0.41
2:P:211:SER:OG	2:P:212:VAL:N	2.53	0.41
1:C:96:LEU:C	1:C:96:LEU:HD13	2.46	0.41
1:E:51:ASN:HD21	1:E:67:THR:CB	2.34	0.41
1:I:57:TRP:HD1	1:I:58:HIS:CE1	2.38	0.41
1:K:97:LEU:CD2	1:K:100:ILE:HD11	2.45	0.41
2:B:231:ASP:OD2	2:B:259:ARG:HD2	2.20	0.40
2:J:281:MET:HE3	2:J:281:MET:HB2	1.90	0.40
1:K:112:ASP:OD2	2:L:291:LYS:NZ	2.48	0.40
2:F:275:VAL:CB	2:H:281:MET:HE3	2.49	0.40
1:K:56:PHE:HD2	1:K:59:LEU:HD23	1.86	0.40
1:K:136:ILE:O	1:K:137:GLN:C	2.63	0.40
1:A:41:HIS:HD2	1:A:112:ASP:OD1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:PHE:CZ	1:G:98:LEU:CD2	3.04	0.40
1:G:37:TYR:O	1:G:39:MET:HG2	2.21	0.40
1:K:43:ARG:HE	1:K:43:ARG:HB2	1.66	0.40
1:M:41:HIS:CE1	1:M:154:LYS:HE2	2.57	0.40
1:E:59:LEU:O	1:E:60:THR:CG2	2.60	0.40
2:L:203:GLY:O	2:L:206:PHE:HD2	2.04	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	131/179 (73%)	126 (96%)	4 (3%)	1 (1%)	16	29
1	C	130/179 (73%)	123 (95%)	6 (5%)	1 (1%)	16	29
1	E	130/179 (73%)	120 (92%)	9 (7%)	1 (1%)	16	29
1	G	129/179 (72%)	120 (93%)	9 (7%)	0	100	100
1	I	131/179 (73%)	127 (97%)	4 (3%)	0	100	100
1	K	131/179 (73%)	127 (97%)	4 (3%)	0	100	100
1	M	131/179 (73%)	127 (97%)	4 (3%)	0	100	100
1	O	130/179 (73%)	122 (94%)	6 (5%)	2 (2%)	8	15
2	B	66/108 (61%)	62 (94%)	4 (6%)	0	100	100
2	D	64/108 (59%)	62 (97%)	2 (3%)	0	100	100
2	F	62/108 (57%)	57 (92%)	5 (8%)	0	100	100
2	H	62/108 (57%)	59 (95%)	3 (5%)	0	100	100
2	J	64/108 (59%)	61 (95%)	3 (5%)	0	100	100
2	L	60/108 (56%)	57 (95%)	3 (5%)	0	100	100
2	N	61/108 (56%)	57 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	62/108 (57%)	60 (97%)	2 (3%)	0	100	100
All	All	1544/2296 (67%)	1467 (95%)	72 (5%)	5 (0%)	36	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	123	GLU
1	E	146	ASP
1	O	146	ASP
1	A	144	LYS
1	C	149	HIS

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	111/154 (72%)	102 (92%)	9 (8%)	11	22
1	C	110/154 (71%)	102 (93%)	8 (7%)	13	25
1	E	111/154 (72%)	103 (93%)	8 (7%)	13	26
1	G	109/154 (71%)	99 (91%)	10 (9%)	8	17
1	I	112/154 (73%)	104 (93%)	8 (7%)	13	27
1	K	107/154 (70%)	93 (87%)	14 (13%)	4	7
1	M	110/154 (71%)	96 (87%)	14 (13%)	4	8
1	O	108/154 (70%)	98 (91%)	10 (9%)	8	17
2	B	65/95 (68%)	63 (97%)	2 (3%)	35	60
2	D	62/95 (65%)	58 (94%)	4 (6%)	15	30
2	F	59/95 (62%)	55 (93%)	4 (7%)	14	28
2	H	61/95 (64%)	61 (100%)	0	100	100
2	J	59/95 (62%)	55 (93%)	4 (7%)	14	28
2	L	57/95 (60%)	56 (98%)	1 (2%)	51	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	60/95 (63%)	57 (95%)	3 (5%)	22	42
2	P	60/95 (63%)	57 (95%)	3 (5%)	22	42
All	All	1361/1992 (68%)	1259 (92%)	102 (8%)	12	24

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	48	LEU
1	A	59	LEU
1	A	77	ARG
1	A	96	LEU
1	A	103	VAL
1	A	123	GLU
1	A	138	THR
1	A	144	LYS
2	B	199	THR
2	B	226	SER
1	C	48	LEU
1	C	57	TRP
1	C	59	LEU
1	C	96	LEU
1	C	98	LEU
1	C	101	HIS
1	C	107	SER
1	C	127	ILE
2	D	222	THR
2	D	257	SER
2	D	275	VAL
2	D	284	LYS
1	E	36	LYS
1	E	59	LEU
1	E	79	SER
1	E	96	LEU
1	E	98	LEU
1	E	103	VAL
1	E	105	THR
1	E	106	VAL
2	F	212	VAL
2	F	257	SER
2	F	281	MET

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Mol	Chain	Res	Type
2	F	285	LYS
1	G	42	ARG
1	G	48	LEU
1	G	57	TRP
1	G	59	LEU
1	G	92	LYS
1	G	98	LEU
1	G	106	VAL
1	G	125	ASN
1	G	135	GLU
1	G	146	ASP
1	I	42	ARG
1	I	60	THR
1	I	79	SER
1	I	96	LEU
1	I	98	LEU
1	I	106	VAL
1	I	127	ILE
1	I	161	GLN
2	J	255	LYS
2	J	257	SER
2	J	281	MET
2	J	291	LYS
1	K	43	ARG
1	K	48	LEU
1	K	79	SER
1	K	98	LEU
1	K	99	LYS
1	K	100	ILE
1	K	102	GLU
1	K	123	GLU
1	K	135	GLU
1	K	138	THR
1	K	144	LYS
1	K	160	ILE
1	K	161	GLN
1	K	163	CYS
2	L	212	VAL
1	M	35	GLU
1	M	48	LEU
1	M	53	GLU
1	M	57	TRP

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Mol	Chain	Res	Type
1	M	60	THR
1	M	97	LEU
1	M	98	LEU
1	M	99	LYS
1	M	100	ILE
1	M	103	VAL
1	M	106	VAL
1	M	127	ILE
1	M	144	LYS
1	M	161	GLN
2	N	223	VAL
2	N	275	VAL
2	N	292	SER
1	O	36	LYS
1	O	48	LEU
1	O	60	THR
1	O	96	LEU
1	O	98	LEU
1	O	100	ILE
1	O	127	ILE
1	O	133	LYS
1	O	137	GLN
1	O	161	GLN
2	P	254	ARG
2	P	275	VAL
2	P	291	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	51	ASN
1	A	89	ASN
1	A	101	HIS
1	A	125	ASN
1	A	126	HIS
2	B	230	GLN
2	B	274	GLN
1	C	41	HIS
1	C	51	ASN
1	C	89	ASN
1	C	121	HIS

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Mol	Chain	Res	Type
1	C	126	HIS
2	D	287	HIS
1	E	41	HIS
1	E	51	ASN
1	E	58	HIS
1	E	89	ASN
1	E	126	HIS
2	F	230	GLN
1	G	51	ASN
1	G	58	HIS
1	G	101	HIS
1	G	125	ASN
2	H	230	GLN
1	I	41	HIS
1	I	51	ASN
1	I	52	HIS
1	I	58	HIS
1	I	89	ASN
1	I	161	GLN
2	J	230	GLN
2	J	274	GLN
1	K	51	ASN
1	K	52	HIS
1	K	89	ASN
1	K	126	HIS
2	L	224	ASN
1	M	41	HIS
1	M	51	ASN
1	M	89	ASN
1	M	161	GLN
1	O	41	HIS
1	O	51	ASN
1	O	89	ASN
1	O	125	ASN
1	O	126	HIS
1	O	137	GLN
2	P	287	HIS

5.3.3 RNA ⓘ

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](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	133/179 (74%)	-0.34	1 (0%) 82 80	13, 22, 41, 55	0
1	C	132/179 (73%)	-0.11	0 100 100	17, 34, 58, 66	0
1	E	132/179 (73%)	-0.38	3 (2%) 61 57	12, 23, 40, 56	0
1	G	131/179 (73%)	-0.11	1 (0%) 82 80	20, 35, 52, 67	0
1	I	133/179 (74%)	-0.41	3 (2%) 61 57	11, 20, 41, 61	0
1	K	133/179 (74%)	0.11	3 (2%) 61 57	23, 38, 53, 62	0
1	M	133/179 (74%)	-0.36	2 (1%) 72 69	12, 23, 44, 60	0
1	O	132/179 (73%)	0.09	3 (2%) 61 57	23, 37, 68, 77	0
2	B	72/108 (66%)	-0.03	3 (4%) 40 37	17, 27, 48, 67	0
2	D	70/108 (64%)	0.03	2 (2%) 53 50	19, 33, 53, 62	0
2	F	68/108 (62%)	0.05	5 (7%) 20 18	13, 28, 56, 72	0
2	H	68/108 (62%)	0.13	5 (7%) 20 18	18, 34, 53, 74	0
2	J	70/108 (64%)	-0.07	2 (2%) 53 50	14, 27, 44, 52	0
2	L	66/108 (61%)	0.06	4 (6%) 27 24	21, 36, 52, 64	0
2	N	67/108 (62%)	-0.06	1 (1%) 72 69	16, 31, 51, 55	0
2	P	68/108 (62%)	-0.01	4 (5%) 28 25	23, 35, 53, 78	0
All	All	1608/2296 (70%)	-0.12	42 (2%) 57 53	11, 30, 54, 78	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	223	VAL	5.1
2	H	225	GLY	4.4
2	H	261	VAL	4.1
1	O	31	PHE	3.6
1	E	57	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	31	PHE	3.3
2	D	260	ARG	3.3
2	L	224	ASN	3.2
1	G	57	TRP	3.2
2	P	260	ARG	3.1
2	F	260	ARG	3.1
2	F	224	ASN	3.1
1	I	31	PHE	3.0
1	I	57	TRP	3.0
2	H	212	VAL	2.9
1	A	31	PHE	2.9
2	L	260	ARG	2.9
1	K	163	CYS	2.7
2	B	200	LEU	2.6
1	I	163	CYS	2.6
2	J	201	PRO	2.5
1	E	124	GLY	2.5
2	H	200	LEU	2.4
2	P	212	VAL	2.4
1	M	57	TRP	2.4
1	O	146	ASP	2.4
2	B	212	VAL	2.4
2	L	274	GLN	2.3
2	F	212	VAL	2.3
1	K	149	HIS	2.3
2	P	292	SER	2.3
1	O	145	GLY	2.2
2	L	202	ALA	2.2
2	N	275	VAL	2.2
2	J	273	LYS	2.2
2	D	222	THR	2.2
2	B	260	ARG	2.2
2	H	201	PRO	2.2
2	F	202	ALA	2.1
2	P	201	PRO	2.1
1	M	31	PHE	2.1
1	K	146	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.