



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:46 PM UTC

PDB ID : 2TUN / pdb_00002tun
Title : CONFORMATIONAL CHANGES IN THE (ALA-84-VAL) MUTANT OF
TUMOR NECROSIS FACTOR
Authors : Saludjian, P.; Prange, T.
Deposited on : 1993-10-06
Resolution : 3.10 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) : **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

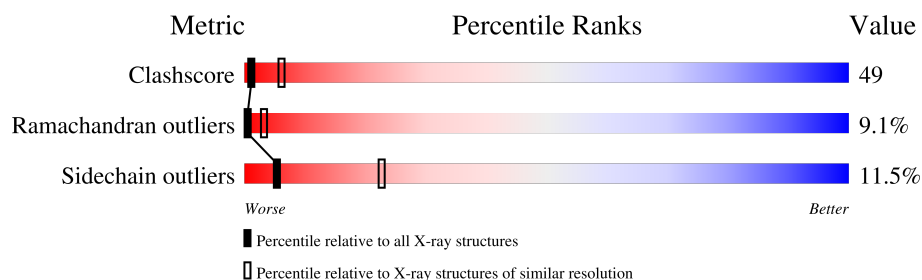
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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	157	
1	B	157	
1	C	157	
1	D	157	
1	E	157	
1	F	157	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7086 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 TUMOR NECROSIS FACTOR-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1181	756	203	220	2			
1	B	151	Total	C	N	O	S	0	0	0
			1181	756	203	220	2			
1	C	151	Total	C	N	O	S	0	0	0
			1181	756	203	220	2			
1	D	151	Total	C	N	O	S	0	0	0
			1181	756	203	220	2			
1	E	151	Total	C	N	O	S	0	0	0
			1181	756	203	220	2			
1	F	151	Total	C	N	O	S	0	0	0
			1181	756	203	220	2			

There are 12 discrepancies between the modelled and reference sequences:

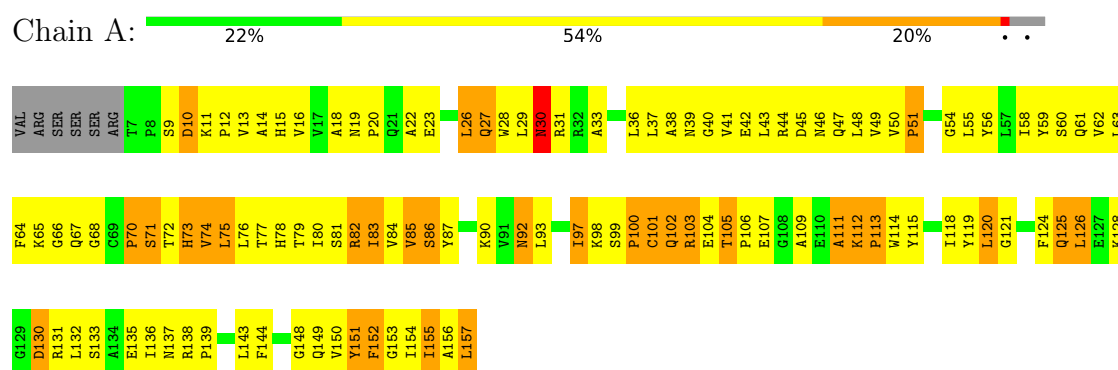
Chain	Residue	Modelled	Actual	Comment	Reference
A	84	VAL	ALA	engineered mutation	UNP P01375
A	143	LEU	ASP	conflict	UNP P01375
B	84	VAL	ALA	engineered mutation	UNP P01375
B	143	LEU	ASP	conflict	UNP P01375
C	84	VAL	ALA	engineered mutation	UNP P01375
C	143	LEU	ASP	conflict	UNP P01375
D	84	VAL	ALA	engineered mutation	UNP P01375
D	143	LEU	ASP	conflict	UNP P01375
E	84	VAL	ALA	engineered mutation	UNP P01375
E	143	LEU	ASP	conflict	UNP P01375
F	84	VAL	ALA	engineered mutation	UNP P01375
F	143	LEU	ASP	conflict	UNP P01375

3 Residue-property plots [i](#)

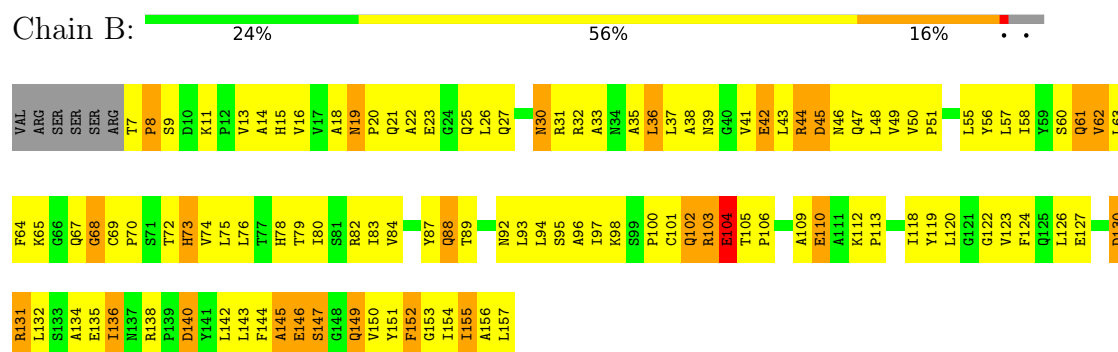
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: TUMOR NECROSIS FACTOR-ALPHA



• Molecule 1: TUMOR NECROSIS FACTOR-ALPHA

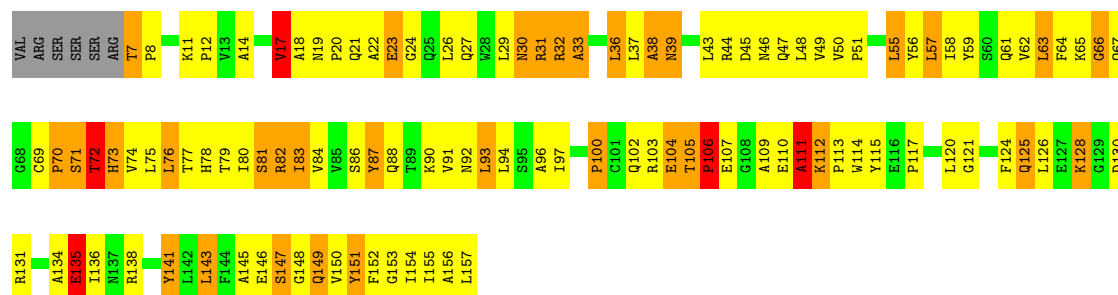


• Molecule 1: TUMOR NECROSIS FACTOR-ALPHA



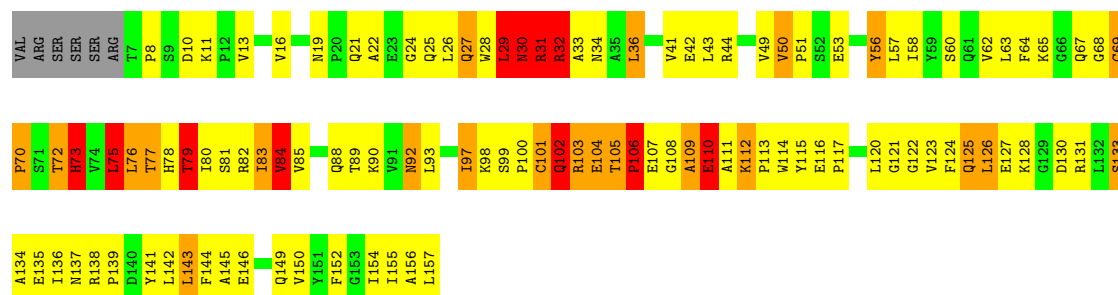
- Molecule 1: TUMOR NECROSIS FACTOR-ALPHA

Chain D: 24% 48% 21% . .

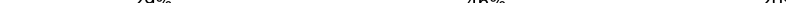


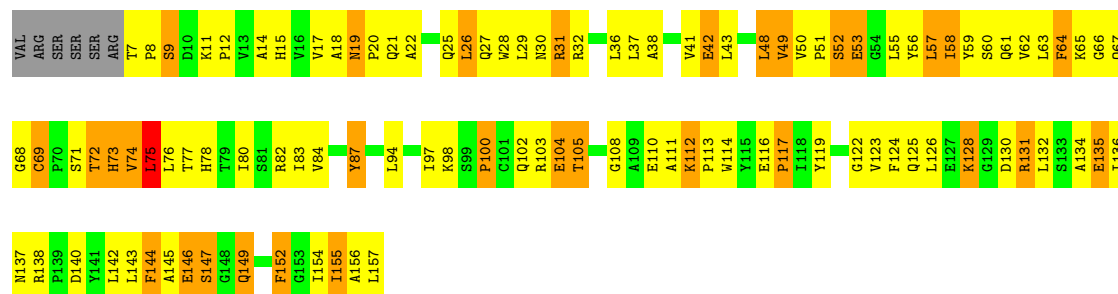
● Molecule 1: TUMOR NECROSIS FACTOR-ALPHA

Chain E:  26% 49% 14% 7% .



● Molecule 1: TUMOR NECROSIS FACTOR-ALPHA

Chain F:  29% 46% 20% . .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.00 Å 166.00 Å 93.70 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (9.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7086	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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	0.92	0/1208	1.93	37/1645 (2.2%)
1	B	0.95	1/1208 (0.1%)	2.03	39/1645 (2.4%)
1	C	1.05	2/1208 (0.2%)	2.73	56/1645 (3.4%)
1	D	0.98	5/1208 (0.4%)	2.09	46/1645 (2.8%)
1	E	0.96	1/1208 (0.1%)	1.96	35/1645 (2.1%)
1	F	0.89	0/1208	1.83	21/1645 (1.3%)
All	All	0.96	9/7248 (0.1%)	2.12	234/9870 (2.4%)

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	1
1	D	0	2
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	8	PRO	N-CD	11.23	1.63	1.47
1	D	7	THR	C-O	8.18	1.40	1.23
1	B	8	PRO	N-CD	7.55	1.58	1.47
1	D	73	HIS	CA-CB	6.22	1.62	1.53
1	D	105	THR	N-CA	5.78	1.50	1.46
1	E	69	CYS	CA-C	5.72	1.60	1.52
1	C	8	PRO	N-CA	-5.54	1.40	1.47
1	D	72	THR	CA-CB	5.36	1.62	1.53
1	D	149	GLN	N-CA	5.13	1.50	1.46

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	THR	CA-C-N	46.69	178.20	119.84
1	C	7	THR	C-N-CA	46.69	178.20	119.84
1	D	7	THR	CA-C-O	-21.64	84.01	120.80
1	C	7	THR	O-C-N	18.06	151.90	123.00
1	C	8	PRO	CA-N-CD	-18.05	86.73	112.00
1	C	8	PRO	N-CA-CB	17.48	121.61	103.25
1	B	8	PRO	CA-N-CD	-16.18	88.85	111.50
1	B	7	THR	CA-C-N	15.46	164.10	127.00
1	B	7	THR	C-N-CA	15.46	164.10	127.00
1	D	7	THR	O-C-N	-15.12	98.81	123.00
1	E	50	VAL	N-CA-C	12.02	118.97	108.63
1	B	152	PHE	CA-CB-CG	11.26	125.06	113.80
1	E	69	CYS	CA-CB-SG	-11.07	88.93	114.40
1	E	69	CYS	N-CA-CB	10.93	127.72	110.12
1	C	7	THR	CA-C-O	-9.92	103.94	120.80
1	D	73	HIS	N-CA-C	9.53	126.39	107.62
1	E	101	CYS	CB-CA-C	-9.45	94.97	111.22
1	E	101	CYS	N-CA-C	9.28	125.90	107.62
1	B	7	THR	O-C-N	9.21	137.73	123.00
1	F	50	VAL	N-CA-C	9.16	115.90	107.56
1	F	147	SER	N-CA-C	-9.01	100.41	111.40
1	D	73	HIS	CA-CB-CG	-8.76	105.05	113.80
1	F	19	ASN	CB-CA-C	8.68	119.19	110.33
1	C	53	GLU	CA-CB-CG	8.68	131.46	114.10
1	D	151	TYR	N-CA-C	8.68	122.26	109.07
1	B	149	GLN	N-CA-C	-8.62	103.27	113.88
1	D	105	THR	CB-CA-C	8.59	118.48	111.00
1	D	152	PHE	CA-CB-CG	8.40	122.20	113.80
1	F	146	GLU	N-CA-C	8.34	123.76	108.58
1	E	102	GLN	N-CA-C	-8.25	100.16	112.04
1	B	101	CYS	CA-C-N	8.25	137.29	121.54
1	B	101	CYS	C-N-CA	8.25	137.29	121.54
1	C	104	GLU	CA-CB-CG	8.19	130.47	114.10
1	C	54	GLY	N-CA-C	8.18	127.57	112.77
1	C	7	THR	C-N-CD	-8.12	91.69	125.00
1	A	124	PHE	CA-C-N	8.12	131.16	120.28
1	A	124	PHE	C-N-CA	8.12	131.16	120.28
1	C	112	LYS	N-CA-C	-8.08	91.96	109.81
1	C	87	TYR	CA-C-O	-8.05	111.87	121.05
1	A	144	PHE	CA-CB-CG	8.00	121.80	113.80
1	D	135	GLU	CB-CG-CD	7.99	126.18	112.60
1	B	8	PRO	N-CA-CB	7.99	111.39	102.60
1	E	69	CYS	CB-CA-C	-7.91	102.26	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	CYS	CB-CA-C	7.89	122.29	110.14
1	E	146	GLU	N-CA-C	7.88	118.65	108.24
1	E	31	ARG	CA-C-N	7.87	136.57	121.54
1	E	31	ARG	C-N-CA	7.87	136.57	121.54
1	C	53	GLU	CB-CG-CD	7.78	125.83	112.60
1	D	71	SER	CA-C-N	7.50	135.87	121.54
1	D	71	SER	C-N-CA	7.50	135.87	121.54
1	C	105	THR	CA-C-N	7.48	129.19	119.84
1	C	105	THR	C-N-CA	7.48	129.19	119.84
1	A	64	PHE	CA-CB-CG	7.41	121.21	113.80
1	A	152	PHE	N-CA-CB	7.36	123.18	110.81
1	A	103	ARG	CA-CB-CG	7.30	128.70	114.10
1	D	38	ALA	CA-C-N	7.26	135.41	121.54
1	D	38	ALA	C-N-CA	7.26	135.41	121.54
1	B	104	GLU	CB-CG-CD	7.22	124.88	112.60
1	F	19	ASN	CA-CB-CG	7.15	119.75	112.60
1	B	146	GLU	CB-CG-CD	7.07	124.61	112.60
1	C	145	ALA	N-CA-C	-7.04	101.79	110.65
1	B	144	PHE	CA-CB-CG	7.03	120.83	113.80
1	C	111	ALA	N-CA-C	7.02	125.75	110.80
1	A	152	PHE	N-CA-C	-7.01	96.28	108.69
1	C	32	ARG	CD-NE-CZ	7.00	134.20	124.40
1	D	110	GLU	CA-C-N	6.98	134.87	121.54
1	D	110	GLU	C-N-CA	6.98	134.87	121.54
1	B	7	THR	C-N-CD	-6.95	105.32	120.60
1	C	102	GLN	N-CA-C	-6.91	97.97	108.96
1	E	30	ASN	N-CA-C	-6.88	100.62	110.59
1	C	113	PRO	CA-N-CD	-6.86	102.39	112.00
1	F	69	CYS	O-C-N	6.84	128.09	121.66
1	D	17	VAL	CA-C-N	6.84	130.83	121.05
1	D	17	VAL	C-N-CA	6.84	130.83	121.05
1	B	7	THR	CA-C-O	-6.83	109.18	120.80
1	C	116	GLU	CB-CG-CD	6.79	124.14	112.60
1	A	54	GLY	N-CA-C	6.78	119.79	111.45
1	C	146	GLU	CA-C-O	6.75	130.16	120.51
1	B	100	PRO	N-CA-C	6.75	123.38	114.27
1	E	135	GLU	N-CA-C	6.72	120.46	109.24
1	C	8	PRO	N-CD-CG	6.69	113.23	103.20
1	C	146	GLU	CA-C-N	6.68	134.31	121.54
1	C	146	GLU	C-N-CA	6.68	134.31	121.54
1	F	113	PRO	N-CA-C	6.67	120.97	110.50
1	F	64	PHE	CA-CB-CG	6.66	120.46	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ARG	CB-CG-CD	6.62	126.52	111.30
1	A	103	ARG	N-CA-CB	6.60	121.64	110.49
1	D	105	THR	CA-C-N	6.58	128.07	119.84
1	D	105	THR	C-N-CA	6.58	128.07	119.84
1	A	71	SER	N-CA-C	6.52	120.25	110.14
1	B	110	GLU	CB-CG-CD	6.51	123.67	112.60
1	B	36	LEU	N-CA-C	6.50	120.05	109.59
1	C	44	ARG	O-C-N	6.48	125.62	120.83
1	A	71	SER	CA-C-N	6.35	133.67	121.54
1	A	71	SER	C-N-CA	6.35	133.67	121.54
1	C	50	VAL	N-CA-C	6.35	114.17	107.76
1	D	79	THR	N-CA-C	6.34	119.14	107.73
1	E	69	CYS	O-C-N	6.34	127.55	120.83
1	D	45	ASP	CA-CB-CG	6.30	118.90	112.60
1	B	131	ARG	CA-CB-CG	6.25	126.59	114.10
1	E	83	ILE	CB-CA-C	6.23	118.50	110.96
1	D	81	SER	N-CA-C	6.22	117.63	108.86
1	A	85	VAL	N-CA-C	-6.21	100.81	109.45
1	A	133	SER	N-CA-C	6.20	118.91	107.99
1	A	152	PHE	CA-CB-CG	-6.19	107.61	113.80
1	D	141	TYR	CA-CB-CG	6.19	125.05	113.90
1	E	124	PHE	CA-CB-CG	6.18	119.98	113.80
1	D	55	LEU	CB-CA-C	6.17	119.72	109.53
1	B	146	GLU	CA-C-N	6.17	133.32	121.54
1	B	146	GLU	C-N-CA	6.17	133.32	121.54
1	D	87	TYR	CA-CB-CG	6.13	124.94	113.90
1	D	135	GLU	CA-CB-CG	6.12	126.34	114.10
1	C	89	THR	CA-C-N	6.12	133.22	121.54
1	C	89	THR	C-N-CA	6.12	133.22	121.54
1	C	114	TRP	CA-CB-CG	6.11	125.21	113.60
1	A	30	ASN	CA-C-N	6.10	133.19	121.54
1	A	30	ASN	C-N-CA	6.10	133.19	121.54
1	E	110	GLU	CA-CB-CG	6.10	126.30	114.10
1	A	102	GLN	N-CA-CB	6.09	120.78	110.49
1	B	147	SER	N-CA-CB	6.03	120.69	110.49
1	A	90	LYS	N-CA-C	6.02	118.59	108.23
1	B	100	PRO	CA-C-N	-6.01	113.50	122.39
1	B	100	PRO	C-N-CA	-6.01	113.50	122.39
1	A	75	LEU	N-CA-CB	-5.98	102.29	111.74
1	F	152	PHE	CA-CB-CG	5.96	119.76	113.80
1	D	125	GLN	N-CA-CB	5.95	119.98	110.16
1	C	39	ASN	CA-CB-CG	5.95	118.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	GLN	N-CA-C	5.94	117.75	111.28
1	E	133	SER	N-CA-C	5.88	118.10	108.52
1	C	88	GLN	CA-C-N	5.87	132.75	121.54
1	C	88	GLN	C-N-CA	5.87	132.75	121.54
1	C	106	PRO	N-CA-C	5.87	124.56	112.47
1	C	99	SER	CA-C-N	5.86	127.16	119.84
1	C	99	SER	C-N-CA	5.86	127.16	119.84
1	E	36	LEU	N-CA-C	5.83	119.21	109.95
1	A	115	TYR	CA-CB-CG	5.82	124.38	113.90
1	D	93	LEU	N-CA-C	-5.82	105.84	113.12
1	A	120	LEU	N-CA-CB	-5.82	101.57	111.69
1	C	111	ALA	N-CA-CB	-5.78	100.72	110.49
1	F	104	GLU	N-CA-C	-5.78	105.24	112.93
1	C	125	GLN	CB-CG-CD	5.75	122.38	112.60
1	C	8	PRO	CB-CA-C	-5.74	102.08	111.56
1	F	22	ALA	CA-C-N	5.67	128.15	120.38
1	F	22	ALA	C-N-CA	5.67	128.15	120.38
1	E	30	ASN	CA-C-O	-5.65	115.28	121.89
1	C	131	ARG	CG-CD-NE	5.63	124.38	112.00
1	E	144	PHE	CA-CB-CG	5.62	119.42	113.80
1	B	130	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	38	ALA	CA-C-N	5.59	132.21	121.54
1	B	38	ALA	C-N-CA	5.59	132.21	121.54
1	D	147	SER	CA-C-N	5.58	132.35	121.41
1	D	147	SER	C-N-CA	5.58	132.35	121.41
1	B	134	ALA	CA-C-N	5.57	128.62	120.71
1	B	134	ALA	C-N-CA	5.57	128.62	120.71
1	E	34	ASN	CA-CB-CG	5.57	118.17	112.60
1	D	145	ALA	N-CA-C	-5.55	107.06	113.88
1	C	46	ASN	CA-CB-CG	5.54	118.14	112.60
1	E	146	GLU	CB-CA-C	-5.53	100.72	112.78
1	D	106	PRO	CA-N-CD	-5.51	104.28	112.00
1	D	63	LEU	CB-CA-C	5.50	119.77	109.71
1	E	105	THR	CB-CA-C	5.50	115.10	111.20
1	D	102	GLN	CA-C-N	5.50	132.03	121.54
1	D	102	GLN	C-N-CA	5.50	132.03	121.54
1	E	79	THR	CA-C-N	5.50	131.11	122.70
1	E	79	THR	C-N-CA	5.50	131.11	122.70
1	E	106	PRO	N-CA-C	5.49	123.77	112.47
1	A	101	CYS	N-CA-C	5.49	117.05	109.15
1	E	56	TYR	CA-CB-CG	5.47	123.75	113.90
1	F	50	VAL	O-C-N	5.44	125.41	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	GLU	CA-CB-CG	5.43	124.96	114.10
1	B	127	GLU	CB-CG-CD	5.43	121.83	112.60
1	C	10	ASP	CA-CB-CG	-5.42	107.18	112.60
1	A	137	ASN	CA-CB-CG	5.41	118.01	112.60
1	C	38	ALA	CA-C-N	5.40	131.86	121.54
1	C	38	ALA	C-N-CA	5.40	131.86	121.54
1	D	111	ALA	N-CA-C	5.39	122.29	110.80
1	A	73	HIS	CA-C-N	5.39	131.67	121.97
1	A	73	HIS	C-N-CA	5.39	131.67	121.97
1	D	56	TYR	CA-CB-CG	5.38	123.59	113.90
1	E	84	VAL	N-CA-CB	-5.36	102.39	111.23
1	B	145	ALA	CA-C-N	5.36	131.77	121.54
1	B	145	ALA	C-N-CA	5.36	131.77	121.54
1	D	31	ARG	CD-NE-CZ	5.36	131.90	124.40
1	A	71	SER	CA-C-O	5.35	128.03	121.56
1	C	102	GLN	CB-CA-C	5.34	119.14	110.22
1	A	111	ALA	CA-C-N	5.32	130.20	123.34
1	A	111	ALA	C-N-CA	5.32	130.20	123.34
1	C	12	PRO	CB-CA-C	5.32	120.33	111.56
1	D	57	LEU	N-CA-C	-5.31	100.07	108.73
1	C	127	GLU	CA-CB-CG	5.30	124.70	114.10
1	C	12	PRO	N-CA-C	-5.30	101.56	112.47
1	A	79	THR	N-CA-C	5.28	118.01	109.40
1	B	62	VAL	N-CA-CB	-5.25	107.40	112.65
1	B	102	GLN	N-CA-CB	5.25	119.36	110.49
1	F	38	ALA	N-CA-C	5.24	115.05	108.45
1	F	135	GLU	N-CA-C	5.24	117.37	109.41
1	F	87	TYR	CA-CB-CG	5.22	123.30	113.90
1	C	113	PRO	N-CA-CB	-5.22	97.77	103.25
1	D	36	LEU	N-CA-C	5.21	117.44	107.75
1	C	32	ARG	CA-CB-CG	5.20	124.50	114.10
1	A	102	GLN	N-CA-C	-5.19	99.74	110.80
1	A	130	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	106	PRO	N-CA-C	5.17	119.47	112.48
1	F	49	VAL	CA-C-N	5.17	126.12	122.60
1	F	49	VAL	C-N-CA	5.17	126.12	122.60
1	D	82	ARG	N-CA-CB	5.17	119.19	110.77
1	E	29	LEU	N-CA-C	5.16	116.93	108.52
1	C	114	TRP	N-CA-C	-5.15	100.90	108.99
1	D	32	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	E	112	LYS	O-C-N	5.12	125.71	121.35
1	F	117	PRO	CB-CA-C	5.12	118.07	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	68	GLY	CA-C-N	5.11	134.26	121.80
1	B	68	GLY	C-N-CA	5.11	134.26	121.80
1	E	50	VAL	CB-CA-C	-5.08	106.21	110.94
1	C	127	GLU	CB-CG-CD	5.08	121.24	112.60
1	D	102	GLN	N-CA-CB	5.08	117.96	110.49
1	E	84	VAL	N-CA-C	5.08	119.91	109.34
1	A	90	LYS	CA-C-N	5.06	128.70	122.37
1	A	90	LYS	C-N-CA	5.06	128.70	122.37
1	D	23	GLU	CA-C-N	5.06	127.75	120.11
1	D	23	GLU	C-N-CA	5.06	127.75	120.11
1	C	102	GLN	CA-C-N	5.05	131.19	121.54
1	C	102	GLN	C-N-CA	5.05	131.19	121.54
1	E	75	LEU	CA-C-N	5.04	128.26	121.05
1	E	75	LEU	C-N-CA	5.04	128.26	121.05
1	E	144	PHE	N-CA-C	-5.04	106.38	112.88
1	C	15	HIS	N-CA-CB	5.03	118.98	110.79
1	F	104	GLU	CB-CG-CD	5.03	121.14	112.60
1	D	149	GLN	CA-CB-CG	5.02	124.15	114.10
1	B	102	GLN	N-CA-C	-5.02	100.10	110.80
1	C	146	GLU	N-CA-C	5.02	121.49	110.80
1	F	42	GLU	CA-CB-CG	5.01	124.13	114.10
1	D	30	ASN	CA-CB-CG	5.00	117.61	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	7	THR	Peptide
1	D	7	THR	Mainchain,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	1181	0	1183	139	2
1	B	1181	0	1183	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1181	0	1183	136	0
1	D	1181	0	1183	121	2
1	E	1181	0	1183	126	0
1	F	1181	0	1183	118	0
All	All	7086	0	7098	700	2

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 49.

All (700) 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:C:98:LYS:HD3	1:C:118:ILE:HG12	1.31	1.06
1:A:19:ASN:HB2	1:A:29:LEU:HD23	1.37	1.04
1:C:14:ALA:HB2	1:C:41:VAL:HG21	1.38	1.03
1:F:42:GLU:HB3	1:F:49:VAL:HB	1.39	1.00
1:D:19:ASN:HB2	1:D:29:LEU:HD13	1.44	1.00
1:F:68:GLY:HA3	1:F:111:ALA:HB1	1.41	0.99
1:D:80:ILE:HB	1:D:94:LEU:HB2	1.44	0.99
1:F:65:LYS:HD3	1:F:143:LEU:HD13	1.46	0.98
1:C:112:LYS:O	1:C:113:PRO:O	1.83	0.97
1:B:49:VAL:HG22	1:B:131:ARG:HG3	1.43	0.96
1:B:69:CYS:HB2	1:B:104:GLU:HB3	1.49	0.94
1:F:58:ILE:HG23	1:F:154:ILE:HG22	1.50	0.93
1:F:80:ILE:HG23	1:F:132:LEU:HD21	1.52	0.92
1:C:112:LYS:H	1:C:112:LYS:HD3	1.35	0.90
1:B:98:LYS:HG3	1:B:118:ILE:HG12	1.51	0.90
1:E:56:TYR:HB2	1:E:126:LEU:HD11	1.52	0.89
1:B:69:CYS:CB	1:B:104:GLU:HB3	2.01	0.89
1:C:47:GLN:HB3	1:C:133:SER:HB3	1.51	0.89
1:E:84:VAL:HG22	1:E:85:VAL:HG12	1.56	0.87
1:A:13:VAL:HG22	1:A:38:ALA:HB2	1.57	0.86
1:C:83:ILE:HB	1:C:131:ARG:HG3	1.56	0.86
1:F:83:ILE:HB	1:F:131:ARG:HG2	1.58	0.86
1:C:106:PRO:HB3	1:C:110:GLU:HB2	1.57	0.85
1:A:83:ILE:HG23	1:A:131:ARG:HB2	1.58	0.85
1:B:48:LEU:HD21	1:B:154:ILE:HG12	1.57	0.85
1:F:146:GLU:HA	1:F:149:GLN:HB2	1.56	0.85
1:F:58:ILE:HD13	1:F:132:LEU:HD11	1.60	0.84
1:A:12:PRO:HB3	1:A:51:PRO:HG2	1.59	0.84
1:A:82:ARG:HD2	1:A:84:VAL:HG12	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ALA:HB3	1:B:120:LEU:HD21	1.58	0.83
1:E:75:LEU:HG	1:E:99:SER:HB3	1.60	0.83
1:D:76:LEU:HD22	1:D:76:LEU:H	1.41	0.83
1:A:13:VAL:HG12	1:A:155:ILE:HD13	1.60	0.83
1:B:79:THR:HB	1:B:92:ASN:HD21	1.43	0.83
1:D:72:THR:HG23	1:D:73:HIS:H	1.41	0.82
1:F:17:VAL:HG12	1:F:18:ALA:H	1.43	0.82
1:C:80:ILE:HB	1:C:94:LEU:HD21	1.62	0.81
1:A:74:VAL:HG21	1:A:100:PRO:HD2	1.62	0.81
1:E:103:ARG:HD2	1:E:104:GLU:N	1.94	0.81
1:C:16:VAL:HG21	1:C:48:LEU:HD21	1.62	0.81
1:C:62:VAL:HA	1:C:150:VAL:HG12	1.62	0.81
1:A:73:HIS:HB2	1:B:112:LYS:HD2	1.62	0.80
1:E:60:SER:HB3	1:E:80:ILE:HD11	1.62	0.80
1:C:60:SER:HB3	1:C:80:ILE:HD11	1.62	0.80
1:F:29:LEU:HD12	1:F:32:ARG:HG3	1.64	0.80
1:A:138:ARG:HH21	1:D:138:ARG:NH2	1.77	0.80
1:D:26:LEU:HD13	1:D:136:ILE:HG13	1.61	0.80
1:A:74:VAL:HG11	1:A:100:PRO:HG2	1.63	0.79
1:C:65:LYS:HD3	1:C:143:LEU:HG	1.64	0.79
1:A:85:VAL:O	1:A:86:SER:HB3	1.81	0.79
1:C:146:GLU:HB3	1:C:149:GLN:HB2	1.64	0.79
1:A:74:VAL:HG13	1:A:101:CYS:HB2	1.63	0.79
1:D:76:LEU:HD21	1:D:100:PRO:HG3	1.64	0.79
1:D:82:ARG:HG2	1:D:93:LEU:HD21	1.64	0.79
1:A:16:VAL:HG22	1:A:152:PHE:HB3	1.64	0.78
1:D:83:ILE:HG23	1:D:131:ARG:HB2	1.66	0.77
1:C:43:LEU:HD13	1:C:48:LEU:HD22	1.67	0.77
1:B:80:ILE:HB	1:B:94:LEU:HB2	1.65	0.77
1:A:92:ASN:HD22	1:A:93:LEU:N	1.83	0.77
1:E:30:ASN:H	1:E:30:ASN:HD22	1.30	0.77
1:A:14:ALA:HB3	1:A:154:ILE:HG12	1.67	0.76
1:A:148:GLY:HA3	1:C:94:LEU:HA	1.66	0.76
1:E:30:ASN:O	1:E:31:ARG:HB2	1.83	0.76
1:E:104:GLU:HB3	1:E:106:PRO:HD3	1.65	0.76
1:E:11:LYS:HG2	1:E:156:ALA:HB3	1.67	0.76
1:B:60:SER:HB3	1:B:80:ILE:HD11	1.68	0.76
1:E:49:VAL:HG22	1:E:131:ARG:HG2	1.66	0.75
1:B:65:LYS:NZ	1:B:143:LEU:HG	2.02	0.75
1:E:76:LEU:HD21	1:E:100:PRO:HG3	1.69	0.75
1:F:14:ALA:HB3	1:F:154:ILE:HG12	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:PRO:HD2	1:A:156:ALA:HB3	1.69	0.74
1:C:25:GLN:HG3	1:C:26:LEU:H	1.51	0.73
1:C:84:VAL:HB	1:C:87:TYR:O	1.86	0.73
1:F:71:SER:O	1:F:72:THR:HB	1.85	0.73
1:F:104:GLU:O	1:F:105:THR:C	2.31	0.73
1:C:84:VAL:HG11	1:C:87:TYR:HD2	1.52	0.73
1:C:63:LEU:HG	1:C:117:PRO:HB3	1.70	0.73
1:E:125:GLN:HG3	1:F:36:LEU:HD11	1.70	0.73
1:E:143:LEU:HD22	1:E:145:ALA:H	1.54	0.73
1:E:72:THR:O	1:E:73:HIS:HB2	1.87	0.73
1:F:30:ASN:O	1:F:31:ARG:HB2	1.88	0.73
1:A:13:VAL:HG11	1:C:55:LEU:HD13	1.71	0.72
1:E:77:THR:HB	1:E:97:ILE:HG23	1.70	0.72
1:C:16:VAL:CG1	1:C:28:TRP:HB3	2.19	0.72
1:A:92:ASN:HB3	1:B:147:SER:CB	2.19	0.72
1:B:143:LEU:HD22	1:B:149:GLN:OE1	1.90	0.72
1:F:76:LEU:HD23	1:F:100:PRO:HG3	1.72	0.72
1:A:82:ARG:CD	1:A:84:VAL:HG12	2.20	0.72
1:A:78:HIS:HB3	1:A:118:ILE:HG21	1.72	0.71
1:E:50:VAL:HB	1:E:130:ASP:H	1.54	0.71
1:C:57:LEU:HB3	1:C:155:ILE:HG23	1.71	0.71
1:D:61:GLN:HG2	1:D:62:VAL:N	2.06	0.71
1:F:25:GLN:HG3	1:F:26:LEU:H	1.55	0.71
1:A:92:ASN:HB3	1:B:147:SER:HB2	1.73	0.71
1:E:126:LEU:HD13	1:E:126:LEU:H	1.55	0.71
1:B:11:LYS:HD2	1:B:156:ALA:O	1.91	0.71
1:D:18:ALA:HA	1:D:27:GLN:O	1.91	0.71
1:B:31:ARG:HH21	1:B:37:LEU:HD23	1.54	0.70
1:D:36:LEU:HD23	1:D:36:LEU:H	1.56	0.70
1:E:13:VAL:O	1:E:41:VAL:HG21	1.91	0.70
1:D:134:ALA:O	1:D:135:GLU:O	2.10	0.69
1:E:125:GLN:CG	1:F:36:LEU:HD11	2.22	0.69
1:B:69:CYS:SG	1:B:104:GLU:HG3	2.32	0.69
1:D:143:LEU:HD12	1:D:146:GLU:OE1	1.92	0.69
1:B:84:VAL:HG12	1:B:130:ASP:OD2	1.93	0.69
1:E:103:ARG:HD2	1:E:104:GLU:H	1.57	0.69
1:A:56:TYR:HB2	1:A:126:LEU:HD12	1.74	0.68
1:A:102:GLN:NE2	1:B:69:CYS:SG	2.66	0.68
1:D:80:ILE:HD12	1:D:94:LEU:HD22	1.74	0.68
1:D:94:LEU:HD23	1:D:120:LEU:HB3	1.76	0.68
1:A:84:VAL:HG23	1:A:85:VAL:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ILE:HG21	1:C:131:ARG:HH11	1.57	0.68
1:D:50:VAL:CG2	1:D:130:ASP:HB2	2.25	0.67
1:D:94:LEU:HB3	1:D:120:LEU:HD23	1.76	0.67
1:D:17:VAL:HB	1:D:32:ARG:HH11	1.58	0.67
1:C:76:LEU:HD22	1:C:100:PRO:HD3	1.77	0.67
1:D:81:SER:HB2	1:D:92:ASN:HA	1.76	0.66
1:C:14:ALA:HB2	1:C:41:VAL:CG2	2.23	0.66
1:B:69:CYS:HB2	1:B:104:GLU:CB	2.24	0.66
1:D:83:ILE:HA	1:D:90:LYS:HA	1.78	0.66
1:D:57:LEU:HB3	1:D:155:ILE:HG23	1.77	0.66
1:E:82:ARG:HB2	1:E:93:LEU:HD12	1.76	0.66
1:B:69:CYS:CB	1:B:104:GLU:CB	2.73	0.66
1:C:30:ASN:O	1:C:31:ARG:HB2	1.95	0.66
1:D:138:ARG:HD2	1:D:141:TYR:CE2	2.30	0.66
1:B:96:ALA:CB	1:B:120:LEU:HD21	2.27	0.65
1:F:77:THR:HG22	1:F:97:ILE:HG23	1.79	0.65
1:E:83:ILE:HG23	1:E:131:ARG:HB2	1.79	0.65
1:A:14:ALA:HB2	1:A:41:VAL:HG11	1.79	0.64
1:D:69:CYS:O	1:D:106:PRO:HD2	1.95	0.64
1:B:146:GLU:OE1	1:B:150:VAL:HG12	1.97	0.64
1:D:155:ILE:HD11	1:F:157:LEU:HD13	1.78	0.64
1:A:74:VAL:CG1	1:A:101:CYS:HB2	2.27	0.64
1:A:27:GLN:NE2	1:A:46:ASN:OD1	2.31	0.64
1:C:84:VAL:HG11	1:C:87:TYR:CD2	2.31	0.64
1:A:41:VAL:HG22	1:A:154:ILE:HD11	1.78	0.63
1:D:97:ILE:O	1:E:115:TYR:HB3	1.97	0.63
1:B:126:LEU:HD21	1:B:132:LEU:HD11	1.80	0.63
1:C:25:GLN:HG3	1:C:26:LEU:N	2.14	0.63
1:D:50:VAL:HG11	1:D:126:LEU:HD13	1.80	0.63
1:F:84:VAL:HG13	1:F:87:TYR:H	1.64	0.63
1:E:84:VAL:HG22	1:E:85:VAL:N	2.14	0.63
1:C:106:PRO:HB3	1:C:110:GLU:CB	2.27	0.63
1:D:128:LYS:HB2	1:D:128:LYS:NZ	2.14	0.63
1:F:82:ARG:HE	1:F:84:VAL:HB	1.64	0.63
1:A:14:ALA:O	1:A:153:GLY:HA2	1.99	0.62
1:D:64:PHE:HA	1:D:141:TYR:O	1.99	0.62
1:B:26:LEU:HD22	1:B:136:ILE:HG21	1.80	0.62
1:E:53:GLU:HG2	1:E:128:LYS:H	1.64	0.62
1:F:60:SER:HB2	1:F:152:PHE:HD1	1.64	0.62
1:C:83:ILE:HG21	1:C:131:ARG:NH1	2.12	0.62
1:B:19:ASN:HD22	1:B:21:GLN:H	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:LYS:HZ3	1:F:112:LYS:HB3	1.64	0.62
1:A:26:LEU:HD23	1:A:136:ILE:HD11	1.81	0.62
1:A:44:ARG:HH22	1:D:44:ARG:NH1	1.97	0.62
1:A:49:VAL:HA	1:A:130:ASP:O	1.99	0.62
1:A:74:VAL:CG2	1:A:100:PRO:HD2	2.30	0.62
1:A:149:GLN:HG3	1:A:150:VAL:HG12	1.81	0.62
1:C:16:VAL:HG11	1:C:28:TRP:HB3	1.79	0.62
1:D:12:PRO:HA	1:D:39:ASN:HB2	1.81	0.62
1:E:136:ILE:HD13	1:E:142:LEU:HD21	1.80	0.62
1:B:78:HIS:ND1	1:B:120:LEU:HD23	2.15	0.62
1:C:143:LEU:CD2	1:C:145:ALA:H	2.12	0.62
1:A:112:LYS:HB3	1:C:102:GLN:OE1	2.00	0.62
1:B:65:LYS:HZ1	1:B:143:LEU:HG	1.64	0.62
1:C:15:HIS:O	1:C:35:ALA:HB1	1.99	0.62
1:C:48:LEU:O	1:C:131:ARG:HA	2.00	0.62
1:D:81:SER:CB	1:D:92:ASN:HA	2.30	0.62
1:D:17:VAL:HB	1:D:32:ARG:NH1	2.14	0.62
1:E:32:ARG:HE	1:E:32:ARG:C	2.08	0.62
1:B:19:ASN:HB2	1:B:27:GLN:O	2.00	0.61
1:E:57:LEU:HD12	1:E:122:GLY:O	2.00	0.61
1:F:26:LEU:HD21	1:F:135:GLU:HA	1.82	0.61
1:A:65:LYS:CD	1:A:143:LEU:HD13	2.30	0.61
1:A:65:LYS:HD2	1:A:143:LEU:HD13	1.80	0.61
1:B:26:LEU:HD11	1:B:150:VAL:HG21	1.82	0.61
1:C:19:ASN:HD22	1:C:29:LEU:HD12	1.66	0.61
1:A:14:ALA:HA	1:A:36:LEU:O	2.00	0.61
1:B:30:ASN:H	1:B:30:ASN:HD22	1.47	0.61
1:A:82:ARG:HB2	1:A:93:LEU:HD11	1.82	0.61
1:B:16:VAL:HG11	1:B:43:LEU:HD22	1.82	0.61
1:B:69:CYS:HB2	1:B:104:GLU:OE1	2.01	0.61
1:B:55:LEU:HD13	1:C:13:VAL:HG11	1.83	0.60
1:E:102:GLN:O	1:F:112:LYS:HD3	2.00	0.60
1:F:42:GLU:O	1:F:48:LEU:HD13	2.02	0.60
1:C:38:ALA:O	1:C:41:VAL:HG12	2.00	0.60
1:E:84:VAL:HG13	1:E:85:VAL:H	1.66	0.60
1:E:29:LEU:HD12	1:E:30:ASN:O	2.01	0.60
1:D:30:ASN:H	1:D:31:ARG:HH21	1.48	0.60
1:E:75:LEU:HG	1:E:99:SER:CB	2.30	0.60
1:A:151:TYR:OH	1:C:94:LEU:HB2	2.01	0.60
1:A:68:GLY:HA2	1:A:112:LYS:H	1.65	0.60
1:F:132:LEU:HD22	1:F:152:PHE:CZ	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:HD12	1:A:55:LEU:H	1.67	0.60
1:A:50:VAL:HG21	1:A:126:LEU:HB3	1.83	0.59
1:E:25:GLN:OE1	1:E:27:GLN:NE2	2.35	0.59
1:F:7:THR:HB	1:F:8:PRO:HD3	1.84	0.59
1:A:73:HIS:NE2	1:B:113:PRO:O	2.35	0.59
1:C:143:LEU:HD22	1:C:145:ALA:H	1.66	0.59
1:B:83:ILE:CG1	1:B:131:ARG:HB2	2.32	0.59
1:E:32:ARG:HE	1:E:33:ALA:N	2.00	0.59
1:E:60:SER:CB	1:E:80:ILE:HD11	2.32	0.59
1:A:18:ALA:CB	1:A:150:VAL:HG11	2.32	0.59
1:A:92:ASN:HD22	1:A:93:LEU:H	1.50	0.59
1:B:18:ALA:HB3	1:B:150:VAL:CG1	2.32	0.59
1:A:47:GLN:NE2	1:A:131:ARG:HG3	2.16	0.59
1:D:14:ALA:HA	1:D:36:LEU:O	2.03	0.59
1:F:7:THR:N	1:F:8:PRO:HD2	2.17	0.59
1:A:77:THR:HG22	1:A:97:ILE:HG23	1.83	0.59
1:B:102:GLN:O	1:B:103:ARG:HB2	2.02	0.59
1:C:80:ILE:HB	1:C:94:LEU:CD2	2.31	0.59
1:A:44:ARG:HH22	1:D:44:ARG:CZ	2.14	0.59
1:E:58:ILE:O	1:E:121:GLY:HA2	2.02	0.59
1:A:12:PRO:CB	1:A:51:PRO:HG2	2.31	0.59
1:D:155:ILE:HD11	1:F:157:LEU:HD22	1.84	0.59
1:B:67:GLN:HG3	1:B:113:PRO:HG3	1.85	0.58
1:D:77:THR:HA	1:D:96:ALA:O	2.03	0.58
1:A:71:SER:OG	1:D:71:SER:HB2	2.02	0.58
1:C:19:ASN:OD1	1:C:21:GLN:HB2	2.03	0.58
1:C:29:LEU:HD22	1:C:30:ASN:O	2.03	0.58
1:F:82:ARG:HD2	1:F:126:LEU:CD2	2.33	0.58
1:B:123:VAL:HG12	1:C:59:TYR:OH	2.02	0.58
1:C:16:VAL:HG12	1:C:28:TRP:HB3	1.83	0.58
1:B:69:CYS:HB3	1:B:104:GLU:HB3	1.85	0.58
1:D:109:ALA:HB2	1:F:103:ARG:HH21	1.69	0.58
1:D:58:ILE:O	1:D:121:GLY:HA2	2.04	0.58
1:F:14:ALA:HB2	1:F:41:VAL:HG21	1.85	0.58
1:B:87:TYR:HD2	1:B:89:THR:OG1	1.87	0.58
1:C:26:LEU:HD22	1:C:136:ILE:CD1	2.33	0.58
1:C:26:LEU:HD22	1:C:136:ILE:HD11	1.84	0.58
1:F:65:LYS:CD	1:F:143:LEU:HD13	2.27	0.58
1:A:75:LEU:HD12	1:A:97:ILE:HG21	1.85	0.58
1:B:79:THR:HB	1:B:92:ASN:ND2	2.16	0.58
1:C:55:LEU:HA	1:C:124:PHE:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:LEU:HD22	1:E:136:ILE:HG12	1.86	0.58
1:F:8:PRO:O	1:F:9:SER:O	2.21	0.58
1:C:25:GLN:O	1:C:26:LEU:HB3	2.04	0.58
1:F:71:SER:HA	1:F:105:THR:HG21	1.85	0.58
1:E:76:LEU:HD23	1:E:76:LEU:H	1.68	0.57
1:B:41:VAL:HG21	1:B:154:ILE:HD11	1.85	0.57
1:D:61:GLN:HG2	1:D:62:VAL:H	1.69	0.57
1:E:19:ASN:OD1	1:E:27:GLN:HB3	2.03	0.57
1:F:63:LEU:HB3	1:F:149:GLN:HG3	1.86	0.57
1:B:18:ALA:HB3	1:B:150:VAL:HG13	1.86	0.57
1:C:57:LEU:HB3	1:C:155:ILE:CG2	2.35	0.57
1:A:18:ALA:O	1:A:20:PRO:HD3	2.05	0.57
1:A:100:PRO:HG2	1:A:101:CYS:H	1.70	0.57
1:C:13:VAL:HG13	1:C:36:LEU:HG	1.86	0.57
1:C:74:VAL:HG21	1:C:100:PRO:HG2	1.87	0.57
1:E:57:LEU:O	1:E:154:ILE:HA	2.05	0.57
1:D:80:ILE:CG2	1:D:94:LEU:HD13	2.35	0.57
1:E:102:GLN:HE22	1:F:114:TRP:HB3	1.69	0.57
1:A:82:ARG:CZ	1:A:126:LEU:HA	2.35	0.57
1:E:98:LYS:HE3	1:F:117:PRO:HD2	1.86	0.57
1:F:15:HIS:HB3	1:F:36:LEU:HB2	1.87	0.56
1:B:57:LEU:O	1:B:154:ILE:HA	2.05	0.56
1:B:61:GLN:HB3	1:B:151:TYR:CE1	2.41	0.56
1:C:155:ILE:HD12	1:C:156:ALA:H	1.70	0.56
1:B:104:GLU:O	1:B:105:THR:C	2.48	0.56
1:A:60:SER:HB3	1:A:80:ILE:HD11	1.88	0.56
1:B:61:GLN:HA	1:B:118:ILE:O	2.04	0.56
1:D:27:GLN:HG2	1:D:46:ASN:HD21	1.70	0.56
1:F:73:HIS:CD2	1:F:75:LEU:HD11	2.40	0.56
1:E:89:THR:O	1:E:90:LYS:HB2	2.06	0.56
1:F:57:LEU:CB	1:F:123:VAL:HG22	2.35	0.56
1:C:79:THR:HG23	1:C:95:SER:HB2	1.89	0.55
1:E:78:HIS:ND1	1:E:120:LEU:HD12	2.22	0.55
1:C:112:LYS:HD3	1:C:112:LYS:N	2.15	0.55
1:A:23:GLU:HB3	1:D:135:GLU:HG2	1.87	0.55
1:F:74:VAL:HG22	1:F:76:LEU:HD22	1.88	0.55
1:A:56:TYR:CB	1:A:126:LEU:HD12	2.35	0.55
1:E:84:VAL:HG22	1:E:85:VAL:H	1.71	0.55
1:A:62:VAL:CG2	1:A:118:ILE:HB	2.37	0.55
1:C:146:GLU:CB	1:C:149:GLN:HB2	2.33	0.55
1:D:22:ALA:HB2	1:D:27:GLN:HE21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:THR:HG22	1:D:97:ILE:HG13	1.89	0.55
1:D:104:GLU:HB3	1:D:106:PRO:HD3	1.89	0.55
1:A:55:LEU:O	1:A:156:ALA:HA	2.05	0.55
1:F:61:GLN:HB2	1:F:119:TYR:CD2	2.42	0.55
1:E:92:ASN:HB3	1:F:147:SER:HB2	1.87	0.55
1:A:13:VAL:H	1:A:38:ALA:CB	2.20	0.54
1:A:74:VAL:HG21	1:A:100:PRO:CD	2.35	0.54
1:B:87:TYR:HD2	1:B:89:THR:HG1	1.53	0.54
1:A:55:LEU:HD11	1:B:9:SER:H	1.72	0.54
1:A:44:ARG:HH12	1:D:44:ARG:HH22	1.54	0.54
1:A:63:LEU:HG	1:A:149:GLN:O	2.08	0.54
1:C:65:LYS:HE2	1:C:143:LEU:HA	1.89	0.54
1:B:72:THR:HG22	1:B:73:HIS:H	1.73	0.54
1:B:98:LYS:HB2	1:B:118:ILE:HD11	1.89	0.54
1:D:36:LEU:O	1:D:36:LEU:HG	2.08	0.54
1:E:79:THR:OG1	1:E:80:ILE:N	2.41	0.54
1:E:154:ILE:C	1:E:154:ILE:HD12	2.32	0.54
1:A:85:VAL:O	1:A:86:SER:CB	2.50	0.54
1:B:78:HIS:CE1	1:B:120:LEU:HB2	2.42	0.54
1:C:49:VAL:HG12	1:C:131:ARG:HB3	1.90	0.54
1:E:112:LYS:HD2	1:E:112:LYS:N	2.23	0.54
1:F:17:VAL:HG12	1:F:18:ALA:N	2.20	0.54
1:F:20:PRO:HD2	1:F:21:GLN:OE1	2.07	0.54
1:B:11:LYS:HE3	1:B:155:ILE:HD11	1.89	0.54
1:B:14:ALA:HB3	1:B:154:ILE:HG13	1.90	0.54
1:B:103:ARG:O	1:B:104:GLU:HB2	2.08	0.54
1:D:87:TYR:HE1	1:D:91:VAL:HG21	1.73	0.54
1:D:26:LEU:HD23	1:D:26:LEU:H	1.73	0.53
1:F:64:PHE:HE1	1:F:136:ILE:HD12	1.72	0.53
1:F:94:LEU:HG	1:F:124:PHE:CE2	2.43	0.53
1:D:155:ILE:CD1	1:F:157:LEU:HD13	2.37	0.53
1:C:76:LEU:HB2	1:C:98:LYS:O	2.09	0.53
1:E:19:ASN:CG	1:E:27:GLN:HB3	2.33	0.53
1:A:92:ASN:ND2	1:A:93:LEU:H	2.07	0.53
1:A:30:ASN:HB2	1:A:37:LEU:HD21	1.89	0.53
1:A:82:ARG:HD3	1:A:126:LEU:CD2	2.39	0.53
1:E:67:GLN:HA	1:E:113:PRO:HA	1.91	0.52
1:F:57:LEU:HB2	1:F:123:VAL:HG22	1.90	0.52
1:F:25:GLN:CG	1:F:26:LEU:H	2.23	0.52
1:E:30:ASN:ND2	1:E:43:LEU:HD21	2.24	0.52
1:A:15:HIS:CE1	1:A:151:TYR:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:HIS:HA	1:B:152:PHE:O	2.09	0.52
1:C:59:TYR:HA	1:C:120:LEU:O	2.10	0.52
1:C:83:ILE:HB	1:C:131:ARG:CG	2.35	0.52
1:D:50:VAL:HG23	1:D:130:ASP:HB2	1.91	0.52
1:B:57:LEU:HB3	1:B:155:ILE:HG23	1.90	0.52
1:C:19:ASN:HB2	1:C:29:LEU:HB2	1.92	0.52
1:E:50:VAL:HG23	1:E:130:ASP:O	2.09	0.52
1:A:13:VAL:H	1:A:38:ALA:HB3	1.75	0.52
1:A:67:GLN:O	1:A:67:GLN:HG2	2.10	0.52
1:A:82:ARG:HD3	1:A:126:LEU:HD23	1.91	0.52
1:D:11:LYS:HB3	1:D:156:ALA:HB3	1.92	0.52
1:C:65:LYS:CE	1:C:143:LEU:HA	2.40	0.51
1:D:128:LYS:HB2	1:D:128:LYS:HZ2	1.75	0.51
1:B:146:GLU:OE1	1:B:149:GLN:HB2	2.10	0.51
1:C:127:GLU:O	1:C:130:ASP:HB2	2.10	0.51
1:D:93:LEU:HB2	1:D:94:LEU:HD12	1.91	0.51
1:B:55:LEU:CD1	1:C:13:VAL:HG11	2.41	0.51
1:D:19:ASN:HB2	1:D:29:LEU:CD1	2.30	0.51
1:D:67:GLN:HA	1:D:113:PRO:HA	1.91	0.51
1:D:115:TYR:CE1	1:D:143:LEU:HD21	2.46	0.51
1:F:65:LYS:HB3	1:F:143:LEU:HB2	1.93	0.51
1:F:112:LYS:HZ3	1:F:112:LYS:CB	2.23	0.51
1:B:82:ARG:HH11	1:B:126:LEU:HG	1.75	0.51
1:C:61:GLN:NE2	1:C:118:ILE:O	2.43	0.51
1:D:75:LEU:O	1:D:77:THR:HG23	2.11	0.51
1:F:71:SER:HA	1:F:105:THR:CG2	2.40	0.51
1:A:119:TYR:CE2	1:B:119:TYR:HE2	2.29	0.51
1:B:72:THR:HG22	1:B:73:HIS:N	2.25	0.51
1:D:74:VAL:HG22	1:D:100:PRO:HG2	1.91	0.51
1:D:136:ILE:HD12	1:D:136:ILE:O	2.10	0.51
1:E:109:ALA:O	1:E:110:GLU:HB2	2.11	0.51
1:F:84:VAL:HG13	1:F:87:TYR:N	2.26	0.51
1:A:61:GLN:HB2	1:A:119:TYR:HD1	1.75	0.51
1:E:102:GLN:NE2	1:F:114:TRP:HB3	2.26	0.51
1:C:61:GLN:HE21	1:C:61:GLN:HA	1.76	0.51
1:E:16:VAL:CG2	1:E:28:TRP:HB3	2.41	0.51
1:F:37:LEU:HD21	1:F:43:LEU:CB	2.41	0.51
1:A:11:LYS:O	1:A:13:VAL:HG13	2.11	0.51
1:B:122:GLY:HA2	1:C:59:TYR:CE1	2.45	0.51
1:F:100:PRO:HB3	1:F:116:GLU:HG3	1.92	0.51
1:B:15:HIS:N	1:B:36:LEU:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LEU:HD22	1:B:136:ILE:CG2	2.41	0.50
1:F:82:ARG:HG2	1:F:83:ILE:N	2.26	0.50
1:F:132:LEU:HD22	1:F:152:PHE:HZ	1.74	0.50
1:E:105:THR:N	1:E:106:PRO:CD	2.74	0.50
1:A:104:GLU:O	1:A:105:THR:C	2.54	0.50
1:C:52:SER:N	1:C:128:LYS:HD2	2.27	0.50
1:A:125:GLN:O	1:A:126:LEU:O	2.28	0.50
1:B:83:ILE:HG13	1:B:131:ARG:HB2	1.94	0.50
1:B:138:ARG:C	1:B:140:ASP:H	2.18	0.50
1:C:12:PRO:HD2	1:C:156:ALA:CB	2.41	0.50
1:D:14:ALA:O	1:D:153:GLY:HA2	2.11	0.50
1:A:70:PRO:HD2	1:A:101:CYS:SG	2.52	0.50
1:C:58:ILE:HG22	1:C:122:GLY:O	2.12	0.50
1:E:49:VAL:HA	1:E:130:ASP:O	2.12	0.50
1:E:98:LYS:HZ1	1:F:98:LYS:HZ3	1.59	0.50
1:F:60:SER:HB3	1:F:80:ILE:HD11	1.94	0.50
1:B:58:ILE:HD13	1:B:154:ILE:HG22	1.92	0.50
1:C:57:LEU:HB2	1:C:123:VAL:HG22	1.94	0.50
1:C:111:ALA:O	1:C:113:PRO:CD	2.59	0.50
1:D:81:SER:HA	1:D:93:LEU:H	1.77	0.50
1:C:13:VAL:HG23	1:C:155:ILE:HB	1.93	0.49
1:E:22:ALA:HB1	1:E:25:GLN:CD	2.37	0.49
1:E:84:VAL:HG23	1:E:130:ASP:OD1	2.12	0.49
1:C:56:TYR:HA	1:C:155:ILE:O	2.13	0.49
1:F:77:THR:OG1	1:F:137:ASN:HB3	2.12	0.49
1:B:32:ARG:HB2	1:B:35:ALA:HB3	1.94	0.49
1:B:126:LEU:CD2	1:B:132:LEU:HD11	2.42	0.49
1:F:29:LEU:HD12	1:F:32:ARG:CG	2.40	0.49
1:A:135:GLU:HB3	1:D:23:GLU:HB3	1.95	0.49
1:B:13:VAL:HG23	1:B:155:ILE:HB	1.94	0.49
1:A:19:ASN:CB	1:A:29:LEU:HD23	2.27	0.49
1:A:82:ARG:NE	1:A:126:LEU:HD23	2.28	0.49
1:C:70:PRO:HG3	1:C:141:TYR:OH	2.12	0.49
1:D:49:VAL:HG22	1:D:131:ARG:CD	2.42	0.49
1:E:79:THR:O	1:E:134:ALA:HA	2.12	0.49
1:F:17:VAL:HG11	1:F:32:ARG:NH2	2.27	0.49
1:C:50:VAL:HG21	1:C:126:LEU:HD13	1.93	0.49
1:B:79:THR:CB	1:B:92:ASN:HD21	2.22	0.49
1:D:65:LYS:O	1:D:66:GLY:O	2.30	0.49
1:D:80:ILE:HD12	1:D:120:LEU:HB2	1.93	0.49
1:E:67:GLN:HA	1:E:113:PRO:CA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:ALA:HB1	1:F:48:LEU:HD21	1.94	0.49
1:A:65:LYS:HG2	1:A:66:GLY:N	2.26	0.49
1:A:106:PRO:O	1:A:107:GLU:HB2	2.12	0.49
1:B:95:SER:H	1:C:148:GLY:HA3	1.78	0.49
1:C:74:VAL:O	1:C:75:LEU:HB2	2.13	0.49
1:C:155:ILE:HD12	1:C:156:ALA:N	2.27	0.49
1:F:19:ASN:HB2	1:F:27:GLN:O	2.13	0.49
1:F:52:SER:H	1:F:128:LYS:HZ1	1.60	0.49
1:E:123:VAL:HG12	1:F:59:TYR:OH	2.13	0.48
1:E:43:LEU:HD12	1:E:43:LEU:O	2.13	0.48
1:F:60:SER:CB	1:F:80:ILE:HD11	2.43	0.48
1:B:68:GLY:O	1:B:70:PRO:HD3	2.13	0.48
1:C:56:TYR:O	1:C:123:VAL:HA	2.13	0.48
1:D:73:HIS:CD2	1:D:75:LEU:HD11	2.48	0.48
1:E:57:LEU:HB3	1:E:155:ILE:HG22	1.95	0.48
1:E:125:GLN:HG2	1:F:36:LEU:HD11	1.95	0.48
1:A:55:LEU:HD12	1:A:55:LEU:N	2.28	0.48
1:B:42:GLU:OE1	1:B:49:VAL:HB	2.14	0.48
1:D:58:ILE:HG12	1:D:154:ILE:HG22	1.95	0.48
1:E:63:LEU:HD13	1:E:149:GLN:CD	2.39	0.48
1:E:143:LEU:HB3	1:E:149:GLN:OE1	2.13	0.48
1:F:17:VAL:CG1	1:F:18:ALA:H	2.20	0.48
1:C:57:LEU:O	1:C:154:ILE:HA	2.14	0.48
1:C:65:LYS:HB2	1:C:143:LEU:HB2	1.95	0.48
1:F:30:ASN:ND2	1:F:37:LEU:HD23	2.29	0.48
1:C:61:GLN:HE22	1:C:119:TYR:HB2	1.79	0.48
1:A:58:ILE:HA	1:A:153:GLY:O	2.13	0.48
1:A:112:LYS:HE3	1:A:112:LYS:HA	1.95	0.48
1:B:36:LEU:N	1:B:36:LEU:HD12	2.28	0.48
1:B:97:ILE:H	1:C:63:LEU:HD11	1.79	0.48
1:A:98:LYS:NZ	1:C:98:LYS:NZ	2.61	0.48
1:D:62:VAL:HG13	1:D:78:HIS:CE1	2.49	0.48
1:E:53:GLU:HG2	1:E:128:LYS:N	2.27	0.48
1:A:30:ASN:O	1:A:31:ARG:HD2	2.13	0.48
1:A:125:GLN:O	1:A:126:LEU:C	2.57	0.48
1:C:62:VAL:HA	1:C:150:VAL:CG1	2.38	0.48
1:C:65:LYS:N	1:C:141:TYR:O	2.47	0.48
1:D:112:LYS:HZ3	1:D:112:LYS:HB2	1.79	0.48
1:D:124:PHE:HA	1:E:36:LEU:HD11	1.96	0.48
1:F:77:THR:CG2	1:F:97:ILE:HG23	2.43	0.48
1:F:82:ARG:HH21	1:F:84:VAL:HG21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:NH1	1:A:126:LEU:HA	2.28	0.47
1:B:84:VAL:HG12	1:B:130:ASP:CG	2.38	0.47
1:E:125:GLN:HB2	1:F:36:LEU:HD21	1.96	0.47
1:E:157:LEU:HB3	1:F:11:LYS:HE3	1.95	0.47
1:F:7:THR:N	1:F:8:PRO:CD	2.77	0.47
1:A:16:VAL:CG2	1:A:152:PHE:HB3	2.38	0.47
1:C:82:ARG:HB2	1:C:93:LEU:CD1	2.43	0.47
1:E:109:ALA:O	1:E:110:GLU:CB	2.61	0.47
1:E:154:ILE:HD12	1:E:154:ILE:O	2.14	0.47
1:B:146:GLU:HG3	1:B:147:SER:N	2.29	0.47
1:C:83:ILE:CG2	1:C:131:ARG:HH11	2.27	0.47
1:D:14:ALA:HB1	1:D:37:LEU:HD12	1.96	0.47
1:F:65:LYS:HB2	1:F:143:LEU:HD22	1.96	0.47
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.66	0.47
1:A:62:VAL:HG23	1:A:118:ILE:HB	1.97	0.47
1:D:26:LEU:HD13	1:D:136:ILE:CG1	2.39	0.47
1:E:80:ILE:HG22	1:E:93:LEU:HD13	1.96	0.47
1:F:42:GLU:HB3	1:F:49:VAL:CB	2.28	0.47
1:A:13:VAL:O	1:A:41:VAL:HG21	2.13	0.47
1:A:139:PRO:HG2	1:D:24:GLY:O	2.14	0.47
1:A:98:LYS:HB2	1:A:118:ILE:HD11	1.97	0.47
1:C:71:SER:O	1:C:72:THR:HB	2.14	0.47
1:E:13:VAL:HB	1:E:155:ILE:CD1	2.45	0.47
1:E:57:LEU:HB3	1:E:155:ILE:CG2	2.45	0.47
1:F:63:LEU:HD13	1:F:117:PRO:HB3	1.96	0.47
1:F:94:LEU:HG	1:F:124:PHE:HE2	1.79	0.47
1:B:13:VAL:HG23	1:B:154:ILE:O	2.15	0.47
1:D:82:ARG:HG3	1:D:82:ARG:O	2.14	0.47
1:F:18:ALA:HB3	1:F:146:GLU:OE1	2.15	0.47
1:C:30:ASN:HB3	1:C:31:ARG:NH2	2.30	0.47
1:D:105:THR:N	1:D:106:PRO:CD	2.78	0.47
1:D:117:PRO:HD2	1:F:98:LYS:HE3	1.97	0.47
1:F:12:PRO:HD2	1:F:156:ALA:HB3	1.97	0.47
1:A:92:ASN:ND2	1:A:93:LEU:N	2.57	0.46
1:B:93:LEU:HB3	1:B:124:PHE:CZ	2.50	0.46
1:E:64:PHE:CG	1:E:76:LEU:HD13	2.50	0.46
1:E:104:GLU:O	1:E:105:THR:C	2.58	0.46
1:E:143:LEU:CD2	1:E:145:ALA:HB3	2.46	0.46
1:A:45:ASP:O	1:A:46:ASN:HB2	2.15	0.46
1:B:64:PHE:CE1	1:B:136:ILE:HD11	2.50	0.46
1:D:26:LEU:HD22	1:D:136:ILE:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:GLY:O	1:E:139:PRO:HB2	2.15	0.46
1:A:63:LEU:HD13	1:A:143:LEU:HD23	1.97	0.46
1:A:48:LEU:HB2	1:A:132:LEU:HB2	1.96	0.46
1:A:62:VAL:HG22	1:A:118:ILE:O	2.16	0.46
1:B:143:LEU:HD22	1:B:149:GLN:CD	2.40	0.46
1:D:138:ARG:HD2	1:D:141:TYR:HE2	1.77	0.46
1:E:108:GLY:O	1:E:109:ALA:HB2	2.16	0.46
1:B:20:PRO:HB2	1:B:21:GLN:HE21	1.81	0.46
1:B:69:CYS:HB2	1:B:104:GLU:CG	2.45	0.46
1:D:14:ALA:CB	1:D:37:LEU:HD12	2.45	0.46
1:D:18:ALA:HB3	1:D:150:VAL:HG13	1.98	0.46
1:D:43:LEU:HA	1:D:47:GLN:O	2.16	0.46
1:E:50:VAL:HG21	1:E:130:ASP:HB2	1.98	0.46
1:A:18:ALA:HB2	1:A:150:VAL:HG11	1.96	0.46
1:A:56:TYR:CE1	1:A:156:ALA:HB2	2.51	0.46
1:C:126:LEU:CD2	1:C:132:LEU:HD11	2.46	0.46
1:F:110:GLU:HG2	1:F:111:ALA:N	2.31	0.46
1:A:111:ALA:C	1:A:113:PRO:HD3	2.41	0.46
1:A:157:LEU:HD23	1:B:157:LEU:HD21	1.98	0.46
1:B:82:ARG:HB2	1:B:93:LEU:HD11	1.97	0.46
1:C:8:PRO:O	1:C:9:SER:HB2	2.16	0.46
1:C:37:LEU:HD12	1:C:41:VAL:HG22	1.98	0.46
1:C:63:LEU:HD23	1:C:64:PHE:N	2.31	0.46
1:C:104:GLU:O	1:C:105:THR:C	2.58	0.46
1:F:82:ARG:HD2	1:F:126:LEU:HD22	1.97	0.46
1:E:77:THR:HG23	1:E:137:ASN:CG	2.41	0.46
1:E:92:ASN:HB3	1:F:147:SER:CB	2.46	0.46
1:C:13:VAL:O	1:C:41:VAL:HG11	2.15	0.45
1:E:62:VAL:HG22	1:E:150:VAL:HG13	1.99	0.45
1:C:14:ALA:HB3	1:C:154:ILE:CG1	2.46	0.45
1:C:57:LEU:HD23	1:C:57:LEU:C	2.41	0.45
1:D:66:GLY:HA3	1:D:114:TRP:CZ2	2.51	0.45
1:E:84:VAL:HG23	1:E:130:ASP:CG	2.42	0.45
1:A:11:LYS:HA	1:A:12:PRO:HD3	1.85	0.45
1:D:26:LEU:CD1	1:D:136:ILE:HG13	2.40	0.45
1:A:44:ARG:CZ	1:A:44:ARG:HA	2.47	0.45
1:C:13:VAL:HB	1:C:155:ILE:HD13	1.98	0.45
1:C:77:THR:HG23	1:C:97:ILE:HD11	1.98	0.45
1:C:126:LEU:HD21	1:C:132:LEU:HD11	1.99	0.45
1:D:97:ILE:H	1:E:63:LEU:HD11	1.81	0.45
1:F:65:LYS:HG2	1:F:66:GLY:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:PHE:HE1	1:B:136:ILE:HD11	1.82	0.45
1:D:82:ARG:HG2	1:D:93:LEU:CD2	2.42	0.45
1:D:106:PRO:HB3	1:D:111:ALA:H	1.81	0.45
1:E:67:GLN:NE2	1:E:113:PRO:HD3	2.32	0.45
1:B:62:VAL:HG23	1:B:62:VAL:O	2.17	0.45
1:C:57:LEU:CB	1:C:123:VAL:HG22	2.47	0.45
1:A:61:GLN:O	1:A:150:VAL:HG23	2.17	0.44
1:B:19:ASN:ND2	1:B:21:GLN:H	2.13	0.44
1:B:94:LEU:HB3	1:B:120:LEU:HB3	1.98	0.44
1:C:155:ILE:O	1:C:157:LEU:HD12	2.17	0.44
1:D:80:ILE:CD1	1:D:120:LEU:HB2	2.47	0.44
1:D:81:SER:OG	1:D:82:ARG:N	2.50	0.44
1:E:72:THR:O	1:E:73:HIS:CB	2.61	0.44
1:A:59:TYR:CZ	1:A:153:GLY:HA3	2.52	0.44
1:B:49:VAL:CG2	1:B:131:ARG:HG3	2.32	0.44
1:C:53:GLU:HB2	1:C:126:LEU:O	2.17	0.44
1:F:29:LEU:CD1	1:F:32:ARG:HG3	2.42	0.44
1:E:126:LEU:C	1:E:126:LEU:HD22	2.42	0.44
1:A:99:SER:HA	1:A:100:PRO:HD2	1.86	0.44
1:D:18:ALA:O	1:D:20:PRO:HD3	2.16	0.44
1:F:37:LEU:HD21	1:F:43:LEU:HB2	2.00	0.44
1:A:65:LYS:CG	1:A:66:GLY:N	2.80	0.44
1:A:80:ILE:CD1	1:A:120:LEU:HD23	2.47	0.44
1:E:85:VAL:O	1:E:88:GLN:NE2	2.51	0.44
1:F:83:ILE:HB	1:F:131:ARG:CG	2.38	0.44
1:D:84:VAL:HG13	1:D:87:TYR:O	2.17	0.44
1:E:115:TYR:HE2	1:E:143:LEU:CD1	2.30	0.44
1:A:82:ARG:CD	1:A:126:LEU:HD23	2.48	0.44
1:B:41:VAL:HG23	1:B:49:VAL:O	2.18	0.44
1:E:112:LYS:HB3	1:E:113:PRO:HD2	1.99	0.44
1:A:66:GLY:N	1:A:114:TRP:O	2.49	0.44
1:D:63:LEU:HD11	1:F:97:ILE:H	1.82	0.44
1:D:73:HIS:CE1	1:E:113:PRO:O	2.71	0.44
1:F:37:LEU:HD21	1:F:43:LEU:HB3	1.99	0.44
1:A:55:LEU:H	1:A:55:LEU:CD1	2.30	0.43
1:A:81:SER:HB3	1:A:92:ASN:HA	2.00	0.43
1:B:65:LYS:HE2	1:B:65:LYS:HB3	1.84	0.43
1:C:83:ILE:CB	1:C:131:ARG:HG3	2.39	0.43
1:E:126:LEU:HD22	1:E:126:LEU:O	2.17	0.43
1:E:138:ARG:HA	1:E:139:PRO:HD2	1.87	0.43
1:F:68:GLY:CA	1:F:111:ALA:HB1	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ASN:ND2	1:C:20:PRO:HD2	2.33	0.43
1:D:61:GLN:NE2	1:D:63:LEU:HB2	2.33	0.43
1:E:60:SER:HB2	1:E:152:PHE:CD1	2.53	0.43
1:A:40:GLY:HA3	1:A:51:PRO:HB3	2.00	0.43
1:A:58:ILE:O	1:A:121:GLY:HA2	2.18	0.43
1:C:74:VAL:CG2	1:C:100:PRO:HG2	2.48	0.43
1:E:68:GLY:O	1:E:70:PRO:HD3	2.18	0.43
1:E:136:ILE:O	1:E:136:ILE:HG13	2.18	0.43
1:F:52:SER:O	1:F:53:GLU:CB	2.66	0.43
1:A:75:LEU:CD1	1:A:97:ILE:HG21	2.47	0.43
1:B:50:VAL:HG13	1:B:56:TYR:OH	2.17	0.43
1:C:50:VAL:HA	1:C:51:PRO:HD3	1.75	0.43
1:D:26:LEU:HD21	1:D:135:GLU:HA	1.99	0.43
1:D:76:LEU:H	1:D:76:LEU:CD2	2.20	0.43
1:A:98:LYS:HZ3	1:C:98:LYS:NZ	2.16	0.43
1:C:111:ALA:O	1:C:113:PRO:HD3	2.19	0.43
1:D:32:ARG:O	1:D:33:ALA:C	2.61	0.43
1:D:59:TYR:CE1	1:F:122:GLY:HA2	2.53	0.43
1:E:16:VAL:HG21	1:E:28:TRP:HB3	1.99	0.43
1:E:143:LEU:HD21	1:E:145:ALA:HB3	1.99	0.43
1:A:48:LEU:HG	1:A:152:PHE:CE2	2.53	0.43
1:A:98:LYS:CB	1:A:118:ILE:HD11	2.49	0.43
1:B:98:LYS:HB2	1:B:118:ILE:CD1	2.48	0.43
1:D:11:LYS:HA	1:D:12:PRO:HD3	1.85	0.43
1:D:74:VAL:CG2	1:D:100:PRO:HG2	2.49	0.43
1:E:30:ASN:O	1:E:31:ARG:CB	2.57	0.43
1:A:12:PRO:O	1:A:155:ILE:HA	2.19	0.43
1:A:22:ALA:O	1:A:23:GLU:C	2.62	0.43
1:A:65:LYS:HD3	1:A:143:LEU:HD13	2.01	0.43
1:F:19:ASN:ND2	1:F:29:LEU:HD23	2.34	0.43
1:B:14:ALA:O	1:B:153:GLY:HA2	2.19	0.43
1:B:61:GLN:HG3	1:B:119:TYR:HB2	2.00	0.43
1:D:14:ALA:HB1	1:D:37:LEU:CD1	2.49	0.43
1:D:49:VAL:HG22	1:D:131:ARG:HD3	2.00	0.43
1:F:138:ARG:HB3	1:F:140:ASP:OD1	2.18	0.43
1:B:47:GLN:OE1	1:B:83:ILE:HD11	2.18	0.43
1:D:29:LEU:HB3	1:D:31:ARG:HH21	1.84	0.43
1:F:28:TRP:HE1	1:F:134:ALA:HB3	1.84	0.43
1:F:62:VAL:HG12	1:F:78:HIS:ND1	2.34	0.43
1:B:41:VAL:HG11	1:B:154:ILE:HD11	2.01	0.42
1:C:17:VAL:HG12	1:C:32:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:TYR:HA	1:D:120:LEU:O	2.19	0.42
1:D:69:CYS:HA	1:D:70:PRO:HD3	1.91	0.42
1:B:45:ASP:O	1:B:46:ASN:HB3	2.19	0.42
1:E:65:LYS:HG3	1:E:115:TYR:CZ	2.54	0.42
1:E:115:TYR:HE2	1:E:143:LEU:HD12	1.84	0.42
1:C:56:TYR:HB2	1:C:126:LEU:HD12	2.02	0.42
1:D:157:LEU:HD22	1:E:155:ILE:HG12	2.00	0.42
1:E:42:GLU:OE1	1:E:44:ARG:HD3	2.19	0.42
1:E:63:LEU:HD13	1:E:149:GLN:HG2	2.01	0.42
1:A:18:ALA:HB3	1:A:150:VAL:HG11	2.01	0.42
1:B:143:LEU:HD23	1:B:145:ALA:H	1.84	0.42
1:C:58:ILE:O	1:C:59:TYR:HB3	2.19	0.42
1:E:98:LYS:NZ	1:F:98:LYS:NZ	2.68	0.42
1:A:10:ASP:O	1:A:12:PRO:HD3	2.19	0.42
1:B:31:ARG:NH2	1:B:37:LEU:HD23	2.28	0.42
1:D:61:GLN:HB3	1:D:151:TYR:CZ	2.55	0.42
1:D:112:LYS:HB2	1:D:112:LYS:NZ	2.34	0.42
1:E:116:GLU:HA	1:E:117:PRO:HD3	1.72	0.42
1:F:56:TYR:CB	1:F:126:LEU:HD12	2.49	0.42
1:B:50:VAL:HA	1:B:51:PRO:HD3	1.87	0.42
1:C:79:THR:HG22	1:C:80:ILE:N	2.35	0.42
1:B:18:ALA:HB3	1:B:150:VAL:HG11	2.02	0.42
1:B:84:VAL:O	1:B:88:GLN:HA	2.20	0.42
1:C:72:THR:OG1	1:C:73:HIS:N	2.52	0.42
1:E:84:VAL:HG13	1:E:85:VAL:N	2.33	0.42
1:F:55:LEU:HD22	1:F:55:LEU:N	2.34	0.42
1:A:16:VAL:HG21	1:A:28:TRP:HB3	2.02	0.42
1:C:112:LYS:O	1:C:113:PRO:C	2.60	0.42
1:D:72:THR:CG2	1:D:73:HIS:H	2.11	0.42
1:B:44:ARG:HB3	1:B:45:ASP:H	1.60	0.42
1:B:157:LEU:OXT	1:C:11:LYS:HD3	2.20	0.42
1:C:13:VAL:CG2	1:C:155:ILE:HD13	2.50	0.42
1:D:97:ILE:HD13	1:E:149:GLN:NE2	2.34	0.42
1:F:155:ILE:HD13	1:F:155:ILE:HA	1.83	0.42
1:B:72:THR:CG2	1:B:73:HIS:H	2.33	0.42
1:F:7:THR:HB	1:F:8:PRO:CD	2.49	0.42
1:C:77:THR:HB	1:C:137:ASN:HB3	2.02	0.41
1:E:64:PHE:CD2	1:E:141:TYR:O	2.73	0.41
1:A:42:GLU:HB3	1:A:49:VAL:HB	2.01	0.41
1:A:48:LEU:HG	1:A:152:PHE:HE2	1.84	0.41
1:A:149:GLN:HG3	1:A:150:VAL:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:VAL:HA	1:B:154:ILE:O	2.20	0.41
1:B:30:ASN:HB3	1:B:37:LEU:HD22	2.02	0.41
1:C:79:THR:HG23	1:C:94:LEU:O	2.20	0.41
1:C:105:THR:O	1:C:107:GLU:N	2.39	0.41
1:D:49:VAL:HA	1:D:130:ASP:O	2.20	0.41
1:D:94:LEU:CD2	1:D:120:LEU:HB3	2.48	0.41
1:A:18:ALA:H	1:A:150:VAL:CG1	2.33	0.41
1:A:48:LEU:O	1:A:132:LEU:HD13	2.21	0.41
1:A:98:LYS:NZ	1:C:98:LYS:HZ1	2.18	0.41
1:C:63:LEU:O	1:C:142:LEU:HA	2.20	0.41
1:E:92:ASN:HD22	1:E:92:ASN:HA	1.67	0.41
1:E:123:VAL:HG11	1:F:155:ILE:CG1	2.50	0.41
1:A:74:VAL:HG11	1:A:100:PRO:CG	2.44	0.41
1:C:100:PRO:HG3	1:C:114:TRP:CH2	2.55	0.41
1:D:77:THR:O	1:D:136:ILE:HA	2.20	0.41
1:E:81:SER:HA	1:E:93:LEU:H	1.83	0.41
1:F:12:PRO:HB2	1:F:56:TYR:CE2	2.56	0.41
1:F:83:ILE:O	1:F:130:ASP:HA	2.20	0.41
1:B:26:LEU:HD11	1:B:150:VAL:CG2	2.49	0.41
1:B:41:VAL:HB	1:B:51:PRO:HD3	2.02	0.41
1:C:37:LEU:HA	1:C:41:VAL:HG13	2.02	0.41
1:C:76:LEU:O	1:C:97:ILE:HG23	2.21	0.41
1:A:65:LYS:HB3	1:A:143:LEU:HB2	2.02	0.41
1:D:30:ASN:OD1	1:D:31:ARG:NH2	2.54	0.41
1:C:14:ALA:HB3	1:C:154:ILE:HG12	2.01	0.41
1:E:63:LEU:HD13	1:E:149:GLN:CG	2.50	0.41
1:F:136:ILE:HD13	1:F:142:LEU:HD21	2.03	0.41
1:B:76:LEU:HB2	1:B:98:LYS:O	2.21	0.41
1:F:143:LEU:HD12	1:F:144:PHE:N	2.36	0.41
1:A:30:ASN:C	1:A:31:ARG:HD2	2.45	0.41
1:B:30:ASN:CB	1:B:37:LEU:HD22	2.51	0.41
1:B:50:VAL:HG13	1:B:51:PRO:HD2	2.02	0.41
1:C:18:ALA:HB3	1:C:150:VAL:CG2	2.51	0.41
1:C:131:ARG:H	1:C:131:ARG:HG2	1.49	0.41
1:D:55:LEU:HA	1:D:125:GLN:HA	2.03	0.41
1:E:69:CYS:HA	1:E:114:TRP:HE1	1.85	0.41
1:C:50:VAL:O	1:C:129:GLY:N	2.53	0.41
1:C:57:LEU:HD23	1:C:58:ILE:N	2.36	0.41
1:F:65:LYS:HB3	1:F:65:LYS:HE2	1.65	0.41
1:E:26:LEU:HD11	1:E:28:TRP:CH2	2.55	0.40
1:E:80:ILE:HA	1:E:133:SER:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:GLY:HA2	1:F:59:TYR:CE2	2.55	0.40
1:E:136:ILE:CD1	1:E:142:LEU:HD21	2.48	0.40
1:F:58:ILE:HG21	1:F:132:LEU:HD11	2.02	0.40
1:B:63:LEU:HD22	1:B:64:PHE:N	2.37	0.40
1:C:17:VAL:HG12	1:C:32:ARG:NH2	2.36	0.40
1:C:99:SER:HA	1:C:100:PRO:HD2	1.79	0.40
1:D:57:LEU:HB3	1:D:155:ILE:CG2	2.49	0.40
1:E:111:ALA:HB1	1:E:112:LYS:H	1.50	0.40
1:E:123:VAL:HG11	1:F:155:ILE:HG12	2.02	0.40
1:E:50:VAL:HG11	1:E:127:GLU:O	2.21	0.40
1:F:69:CYS:SG	1:F:114:TRP:NE1	2.95	0.40
1:B:74:VAL:O	1:B:75:LEU:HB2	2.22	0.40
1:C:69:CYS:HA	1:C:70:PRO:HD2	1.85	0.40
1:D:66:GLY:O	1:D:113:PRO:HA	2.21	0.40
1:D:150:VAL:HG13	1:D:150:VAL:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:OE2	1:D:86:SER:C[6_765]	2.03	0.17
1:A:42:GLU:OE2	1:D:86:SER:O[6_765]	2.04	0.16

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	149/157 (95%)	108 (72%)	28 (19%)	13 (9%)	0	4
1	B	149/157 (95%)	108 (72%)	30 (20%)	11 (7%)	1	5
1	C	149/157 (95%)	108 (72%)	25 (17%)	16 (11%)	0	2
1	D	149/157 (95%)	106 (71%)	27 (18%)	16 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	149/157 (95%)	106 (71%)	30 (20%)	13 (9%)	0	4
1	F	149/157 (95%)	108 (72%)	29 (20%)	12 (8%)	1	4
All	All	894/942 (95%)	644 (72%)	169 (19%)	81 (9%)	0	3

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	LEU
1	B	39	ASN
1	B	104	GLU
1	C	8	PRO
1	C	53	GLU
1	C	90	LYS
1	C	100	PRO
1	C	106	PRO
1	C	113	PRO
1	D	33	ALA
1	D	38	ALA
1	D	39	ASN
1	D	88	GLN
1	D	106	PRO
1	D	111	ALA
1	D	135	GLU
1	E	32	ARG
1	E	70	PRO
1	E	73	HIS
1	F	9	SER
1	F	52	SER
1	F	53	GLU
1	F	145	ALA
1	A	9	SER
1	A	33	ALA
1	A	70	PRO
1	A	109	ALA
1	B	33	ALA
1	B	109	ALA
1	C	52	SER
1	C	72	THR
1	C	103	ARG
1	D	66	GLY
1	D	72	THR

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Mol	Chain	Res	Type
1	D	147	SER
1	D	148	GLY
1	E	8	PRO
1	E	51	PRO
1	E	75	LEU
1	E	109	ALA
1	E	110	GLU
1	F	26	LEU
1	F	72	THR
1	A	39	ASN
1	A	51	PRO
1	A	86	SER
1	A	113	PRO
1	B	44	ARG
1	B	110	GLU
1	C	23	GLU
1	C	26	LEU
1	C	39	ASN
1	D	70	PRO
1	D	103	ARG
1	E	104	GLU
1	F	31	ARG
1	F	75	LEU
1	B	22	ALA
1	B	103	ARG
1	C	75	LEU
1	D	8	PRO
1	D	104	GLU
1	E	31	ARG
1	E	72	THR
1	E	106	PRO
1	F	105	THR
1	F	108	GLY
1	A	100	PRO
1	A	105	THR
1	B	88	GLN
1	C	111	ALA
1	E	84	VAL
1	A	72	THR
1	C	9	SER
1	C	147	SER
1	D	100	PRO

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Mol	Chain	Res	Type
1	B	155	ILE
1	F	51	PRO
1	F	100	PRO
1	A	155	ILE
1	B	8	PRO

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	128/134 (96%)	113 (88%)	15 (12%)	5	22
1	B	128/134 (96%)	117 (91%)	11 (9%)	10	34
1	C	128/134 (96%)	112 (88%)	16 (12%)	4	19
1	D	128/134 (96%)	116 (91%)	12 (9%)	8	31
1	E	128/134 (96%)	109 (85%)	19 (15%)	3	13
1	F	128/134 (96%)	113 (88%)	15 (12%)	5	22
All	All	768/804 (96%)	680 (88%)	88 (12%)	5	23

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	27	GLN
1	A	30	ASN
1	A	43	LEU
1	A	74	VAL
1	A	76	LEU
1	A	83	ILE
1	A	87	TYR
1	A	92	ASN
1	A	97	ILE
1	A	103	ARG
1	A	112	LYS
1	A	128	LYS

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Mol	Chain	Res	Type
1	A	151	TYR
1	A	157	LEU
1	B	19	ASN
1	B	23	GLU
1	B	25	GLN
1	B	30	ASN
1	B	42	GLU
1	B	45	ASP
1	B	61	GLN
1	B	73	HIS
1	B	136	ILE
1	B	140	ASP
1	B	142	LEU
1	C	17	VAL
1	C	29	LEU
1	C	36	LEU
1	C	53	GLU
1	C	61	GLN
1	C	67	GLN
1	C	76	LEU
1	C	87	TYR
1	C	100	PRO
1	C	104	GLU
1	C	106	PRO
1	C	112	LYS
1	C	113	PRO
1	C	140	ASP
1	C	143	LEU
1	C	146	GLU
1	D	17	VAL
1	D	21	GLN
1	D	48	LEU
1	D	51	PRO
1	D	76	LEU
1	D	83	ILE
1	D	106	PRO
1	D	107	GLU
1	D	112	LYS
1	D	128	LYS
1	D	143	LEU
1	D	149	GLN
1	E	10	ASP

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Mol	Chain	Res	Type
1	E	21	GLN
1	E	27	GLN
1	E	29	LEU
1	E	30	ASN
1	E	32	ARG
1	E	73	HIS
1	E	76	LEU
1	E	77	THR
1	E	79	THR
1	E	92	ASN
1	E	97	ILE
1	E	101	CYS
1	E	102	GLN
1	E	103	ARG
1	E	107	GLU
1	E	125	GLN
1	E	126	LEU
1	E	143	LEU
1	F	48	LEU
1	F	57	LEU
1	F	58	ILE
1	F	67	GLN
1	F	73	HIS
1	F	74	VAL
1	F	75	LEU
1	F	102	GLN
1	F	112	LYS
1	F	125	GLN
1	F	128	LYS
1	F	131	ARG
1	F	144	PHE
1	F	149	GLN
1	F	155	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	27	GLN
1	A	30	ASN
1	A	46	ASN
1	B	19	ASN

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Mol	Chain	Res	Type
1	B	21	GLN
1	B	25	GLN
1	B	92	ASN
1	C	19	ASN
1	C	21	GLN
1	C	61	GLN
1	D	27	GLN
1	D	46	ASN
1	D	47	GLN
1	D	61	GLN
1	D	92	ASN
1	E	30	ASN
1	E	34	ASN
1	E	39	ASN
1	E	73	HIS
1	E	88	GLN
1	E	92	ASN
1	E	125	GLN
1	F	25	GLN
1	F	46	ASN
1	F	73	HIS
1	F	102	GLN
1	F	149	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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.