



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:40 PM UTC

PDB ID : 1MLC / pdb_00001mlc
Title : MONOCLONAL ANTIBODY FAB D44.1 RAISED AGAINST CHICKEN EGG-WHITE LYSOZYME COMPLEXED WITH LYSOZYME
Authors : Braden, B.C.; Souchon, H.; Eisele, J.-L.; Bentley, G.A.; Bhat, T.N.; Navaza, J.; Poljak, R.J.
Deposited on : 1995-03-10
Resolution : 2.50 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

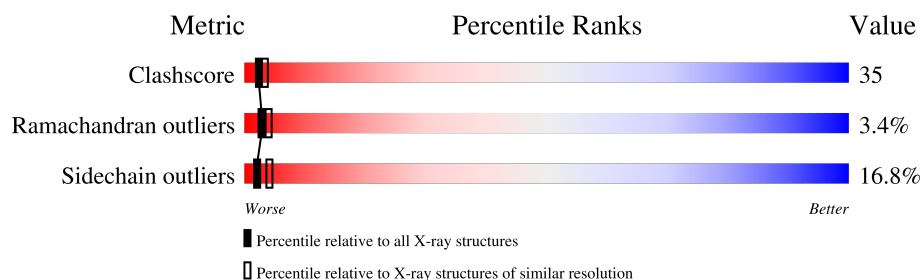
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	31% 45% 18% 6%
1	C	214	26% 44% 27% .
2	B	218	40% 39% 19% .
2	D	218	30% 52% 16% .
3	E	129	22% 50% 21% 6%
3	F	129	35% 43% 17% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8792 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 IGG1-KAPPA D44.1 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1658	1023	283	345	7			
1	C	214	Total	C	N	O	S	0	0	0
			1658	1023	283	345	7			

- Molecule 2 is a protein called IGG1-KAPPA D44.1 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1632	1029	266	329	8			
2	D	218	Total	C	N	O	S	0	0	0
			1632	1029	266	329	8			

- Molecule 3 is a protein called HEN EGG WHITE LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			
3	F	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	48	Total	O	0	0
			48	48		
4	C	35	Total	O	0	0
			35	35		
4	D	35	Total	O	0	0
			35	35		

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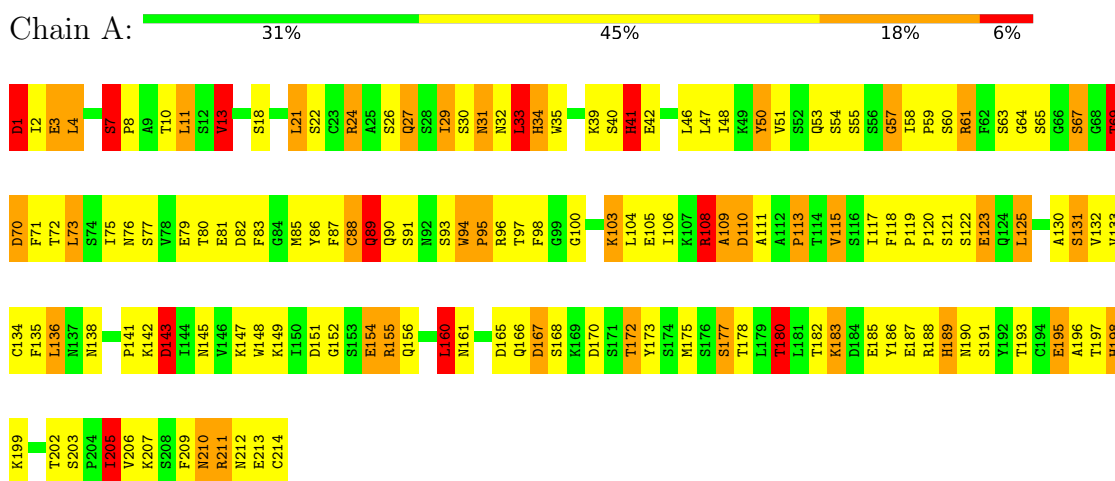
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	22	Total 22	O 22	0	0
4	F	23	Total 23	O 23	0	0

3 Residue-property plots

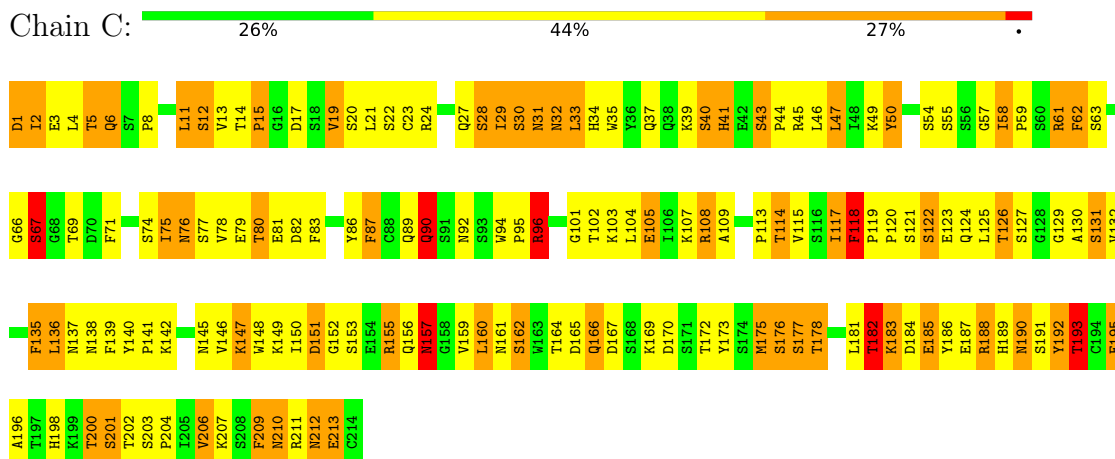
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: IGG1-KAPPA D44.1 FAB (LIGHT CHAIN)

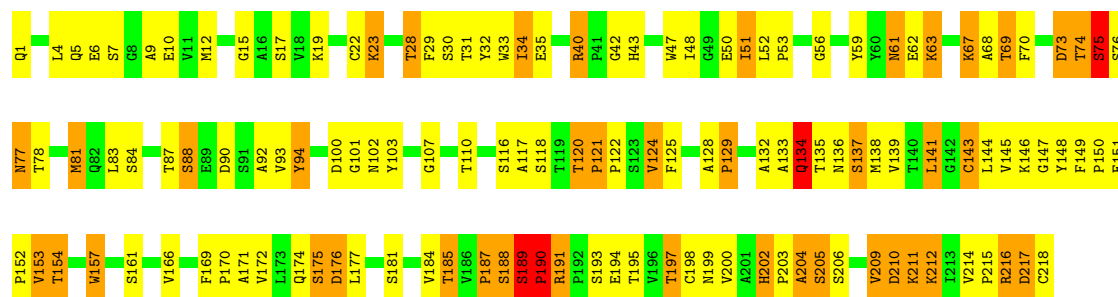


• Molecule 1: IGG1-KAPPA D44.1 FAB (LIGHT CHAIN)

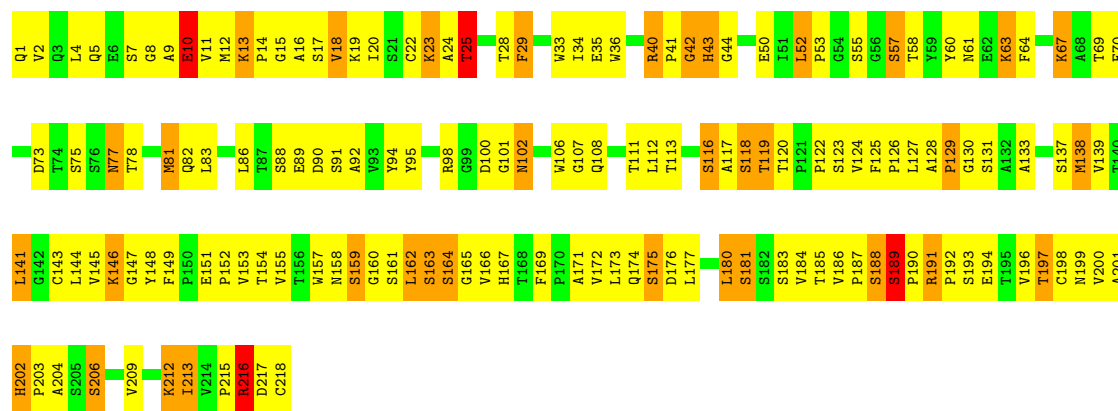


• Molecule 2: IGG1-KAPPA D44.1 FAB (HEAVY CHAIN)

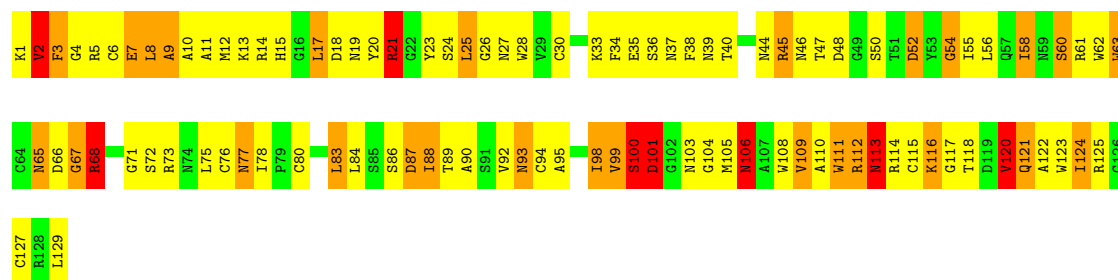




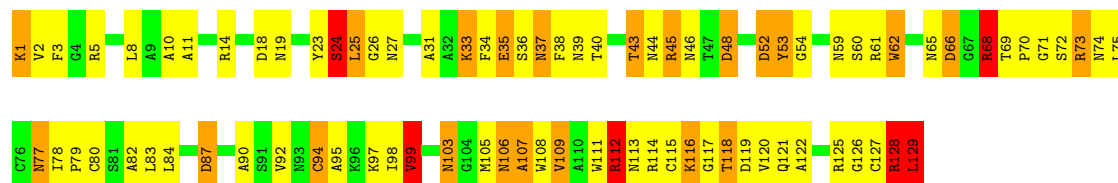
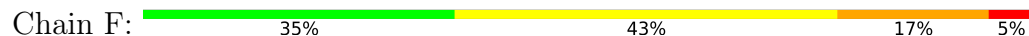
• Molecule 2: IGG1-KAPPA D44.1 FAB (HEAVY CHAIN)



• Molecule 3: HEN EGG WHITE LYSOZYME



• Molecule 3: HEN EGG WHITE LYSOZYME



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.70Å 167.30Å 84.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.184 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8792	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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	1.28	2/1695 (0.1%)	2.38	103/2298 (4.5%)
1	C	1.24	1/1695 (0.1%)	2.34	101/2298 (4.4%)
2	B	1.38	1/1676 (0.1%)	2.43	115/2290 (5.0%)
2	D	1.26	3/1676 (0.2%)	2.23	83/2290 (3.6%)
3	E	1.14	0/1021	2.23	50/1379 (3.6%)
3	F	1.24	1/1021 (0.1%)	2.44	72/1379 (5.2%)
All	All	1.27	8/8784 (0.1%)	2.35	524/11934 (4.4%)

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	A	0	1
3	E	0	1
3	F	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	101	GLY	N-CA	7.89	1.56	1.45
2	B	101	GLY	N-CA	7.26	1.55	1.45
3	F	103	ASN	N-CA	6.31	1.51	1.46
1	C	31	ASN	N-CA	5.62	1.52	1.46
1	A	31	ASN	N-CA	5.60	1.52	1.46
1	A	91	SER	CA-CB	-5.29	1.46	1.53
2	D	42	GLY	N-CA	5.01	1.52	1.45
2	D	44	GLY	N-CA	5.00	1.52	1.45

All (524) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	ASP	CA-CB-CG	19.41	132.01	112.60
1	A	165	ASP	CA-CB-CG	14.07	126.67	112.60
3	E	103	ASN	N-CA-C	-13.79	97.38	114.75
3	F	113	ASN	OD1-CG-ND2	11.46	134.06	122.60
1	A	210	ASN	CA-C-O	-10.47	109.40	120.40
2	B	120	THR	O-C-N	10.37	131.63	121.57
2	B	83	LEU	CA-C-O	-10.32	109.21	120.36
1	A	143	ASP	CA-CB-CG	10.28	122.88	112.60
1	C	30	SER	CB-CA-C	-10.07	103.53	117.23
1	C	44	PRO	CB-CA-C	9.96	123.97	111.12
2	D	83	LEU	CA-C-O	-9.73	110.19	120.70
3	E	113	ASN	CA-CB-CG	9.69	122.29	112.60
1	A	205	ILE	N-CA-CB	9.69	121.28	110.72
2	D	167	HIS	CA-CB-CG	-9.59	104.21	113.80
1	A	145	ASN	CA-C-O	-9.51	110.16	120.24
3	F	3	PHE	O-C-N	9.31	133.41	122.79
1	A	58	ILE	CB-CA-C	9.29	119.58	110.94
2	B	23	LYS	CA-C-O	-9.21	110.14	120.54
1	C	87	PHE	CA-CB-CG	9.16	122.96	113.80
1	C	6	GLN	OE1-CD-NE2	9.12	131.72	122.60
1	A	165	ASP	N-CA-C	-9.07	98.55	110.43
1	A	189	HIS	CA-CB-CG	-9.05	104.75	113.80
2	B	40	ARG	NE-CZ-NH1	9.02	130.52	121.50
1	A	94	TRP	CA-C-O	-8.87	109.50	120.23
1	A	96	ARG	N-CA-C	-8.81	97.44	110.48
1	A	94	TRP	O-C-N	8.70	130.25	121.72
2	B	187	PRO	CA-C-O	-8.58	111.21	121.67
3	E	68	ARG	NE-CZ-NH1	8.30	129.80	121.50
1	A	1	ASP	CA-CB-CG	-8.29	104.31	112.60
3	E	68	ARG	CG-CD-NE	8.28	130.22	112.00
3	F	24	SER	CA-C-O	-8.25	112.58	121.99
2	B	9	ALA	CA-C-O	-8.23	112.82	121.55
3	F	69	THR	O-C-N	8.21	128.91	121.19
2	B	216	ARG	NE-CZ-NH1	-8.13	113.37	121.50
1	C	62	PHE	CA-CB-CG	8.12	121.92	113.80
2	D	107	GLY	N-CA-C	-8.12	100.18	112.60
3	F	11	ALA	CA-C-O	8.09	128.99	120.42
1	A	211	ARG	NE-CZ-NH2	-8.08	111.93	119.20
2	B	211	LYS	CA-C-O	-8.02	111.88	120.46
2	B	61	ASN	CA-CB-CG	7.95	120.55	112.60
3	E	103	ASN	CB-CA-C	7.92	119.37	109.16
1	A	31	ASN	N-CA-CB	-7.88	99.09	111.39
3	F	39	ASN	OD1-CG-ND2	-7.88	114.72	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	45	ARG	NE-CZ-NH1	-7.87	113.63	121.50
2	B	62	GLU	CA-C-N	7.84	131.43	120.29
2	B	62	GLU	C-N-CA	7.84	131.43	120.29
2	D	73	ASP	O-C-N	7.78	132.94	122.59
1	A	29	ILE	N-CA-C	-7.77	103.69	111.77
2	D	16	ALA	CA-C-O	-7.76	113.86	122.01
3	E	68	ARG	NE-CZ-NH2	-7.76	112.22	119.20
1	C	201	SER	CA-C-N	7.76	136.36	121.54
1	C	201	SER	C-N-CA	7.76	136.36	121.54
1	A	69	THR	CA-CB-OG1	-7.73	98.01	109.60
1	C	63	SER	CA-C-O	-7.73	112.67	121.40
2	D	20	ILE	CA-CB-CG2	7.70	123.59	110.50
3	E	103	ASN	O-C-N	7.69	131.10	121.64
2	B	197	THR	CA-CB-OG1	-7.69	98.07	109.60
1	C	31	ASN	CB-CA-C	7.61	123.35	111.02
1	C	162	SER	O-C-N	7.60	132.15	123.48
2	B	93	VAL	CA-C-O	-7.58	112.45	120.48
1	C	19	VAL	N-CA-CB	-7.56	99.73	112.44
2	B	153	VAL	CA-C-O	-7.55	111.81	121.40
2	D	40	ARG	NE-CZ-NH2	7.54	125.98	119.20
3	E	54	GLY	CA-C-N	7.53	135.53	121.97
3	E	54	GLY	C-N-CA	7.53	135.53	121.97
2	B	216	ARG	NE-CZ-NH2	7.51	125.96	119.20
1	C	74	SER	CA-C-O	-7.50	112.27	120.36
3	F	36	SER	CA-C-O	-7.49	110.64	119.48
3	E	71	GLY	CA-C-N	7.48	132.20	121.50
3	E	71	GLY	C-N-CA	7.48	132.20	121.50
2	D	40	ARG	CD-NE-CZ	-7.40	114.04	124.40
1	A	191	SER	N-CA-C	7.39	120.97	109.07
2	D	44	GLY	N-CA-C	-7.37	95.71	113.18
1	C	209	PHE	CA-CB-CG	7.37	121.17	113.80
3	E	65	ASN	CA-C-O	-7.37	112.42	120.30
2	B	176	ASP	CA-CB-CG	-7.36	105.24	112.60
1	A	195	GLU	CA-C-O	-7.36	112.64	120.80
3	F	99	VAL	N-CA-C	7.35	118.11	110.62
1	C	117	ILE	CA-C-O	-7.33	112.60	120.59
2	B	102	ASN	N-CA-C	-7.31	101.42	110.41
3	F	118	THR	CA-CB-OG1	-7.30	98.64	109.60
1	C	114	THR	CA-C-O	-7.27	112.68	120.46
3	F	112	ARG	CD-NE-CZ	-7.27	114.22	124.40
3	F	128	ARG	CD-NE-CZ	7.23	134.53	124.40
2	B	81	MET	CA-C-O	-7.21	112.31	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	PHE	O-C-N	7.21	131.47	123.33
2	B	161	SER	O-C-N	7.20	129.49	122.07
1	C	118	PHE	CA-CB-CG	7.19	120.99	113.80
2	B	206	SER	CA-C-N	7.18	130.91	120.71
2	B	206	SER	C-N-CA	7.18	130.91	120.71
3	F	1	LYS	CA-C-O	-7.18	108.60	120.80
1	C	108	ARG	CA-C-O	7.16	128.51	121.14
1	C	136	LEU	CB-CA-C	7.15	122.26	110.74
3	E	112	ARG	O-C-N	7.15	132.10	122.59
3	F	118	THR	CA-CB-CG2	7.15	122.65	110.50
1	C	58	ILE	O-C-N	7.14	129.78	121.57
2	B	61	ASN	N-CA-C	-7.14	98.41	109.76
2	D	18	VAL	CA-C-O	-7.12	114.41	121.67
1	A	111	ALA	CA-C-O	-7.10	112.08	120.60
1	C	96	ARG	CD-NE-CZ	-7.10	114.46	124.40
2	B	194	GLU	CA-C-N	7.08	130.93	120.87
2	B	194	GLU	C-N-CA	7.08	130.93	120.87
3	E	111	TRP	CA-C-N	7.08	135.06	121.54
3	E	111	TRP	C-N-CA	7.08	135.06	121.54
2	B	189	SER	O-C-N	7.02	127.31	120.71
2	D	201	ALA	CA-C-N	7.00	128.44	122.28
2	D	201	ALA	C-N-CA	7.00	128.44	122.28
1	A	108	ARG	N-CA-CB	-7.00	100.68	111.46
1	C	12	SER	CA-C-O	-6.99	112.63	120.32
3	F	52	ASP	CA-C-O	-6.98	113.31	120.71
3	F	1	LYS	N-CA-CB	6.97	122.35	110.50
3	E	83	LEU	N-CA-C	-6.96	104.77	113.20
3	E	100	SER	CA-C-N	6.96	134.82	121.54
3	E	100	SER	C-N-CA	6.96	134.82	121.54
1	A	82	ASP	CA-CB-CG	-6.95	105.65	112.60
1	C	45	ARG	CD-NE-CZ	-6.95	114.68	124.40
1	C	32	ASN	CA-CB-CG	6.93	119.53	112.60
1	A	96	ARG	CA-C-O	-6.92	113.51	121.47
1	C	92	ASN	CA-C-O	6.92	127.83	120.70
3	E	73	ARG	NE-CZ-NH2	6.92	125.42	119.20
1	A	58	ILE	CA-C-O	6.91	125.13	119.47
1	A	50	TYR	CA-C-N	6.87	134.34	121.97
1	A	50	TYR	C-N-CA	6.87	134.34	121.97
1	C	105	GLU	CB-CG-CD	6.86	124.26	112.60
1	C	43	SER	O-C-N	6.86	128.87	121.60
2	D	86	LEU	CA-C-O	-6.86	113.48	121.16
2	D	98	ARG	CD-NE-CZ	-6.86	114.80	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ASP	CA-C-N	6.85	130.47	120.82
1	A	165	ASP	C-N-CA	6.85	130.47	120.82
2	D	217	ASP	CA-C-O	6.83	127.77	120.46
2	B	110	THR	CA-C-O	-6.79	111.93	120.28
2	B	7	SER	O-C-N	-6.78	114.32	122.65
3	E	111	TRP	CA-C-O	6.78	128.00	120.89
2	D	25	THR	CA-CB-OG1	-6.77	99.44	109.60
2	D	10	GLU	CB-CA-C	-6.77	98.01	109.72
3	F	1	LYS	O-C-N	6.77	133.83	123.00
2	D	19	LYS	CA-C-O	-6.76	112.82	120.32
1	A	91	SER	CA-CB-OG	6.75	124.61	111.10
2	B	40	ARG	NE-CZ-NH2	-6.75	113.12	119.20
3	F	66	ASP	CA-CB-CG	6.74	119.34	112.60
3	F	128	ARG	CA-C-O	-6.74	113.33	120.40
3	F	46	ASN	CA-C-O	6.71	128.34	120.89
2	D	102	ASN	OD1-CG-ND2	-6.68	115.92	122.60
2	B	171	ALA	CA-C-O	-6.66	112.76	120.49
1	A	190	ASN	OD1-CG-ND2	6.66	129.26	122.60
2	B	125	PHE	O-C-N	6.65	127.31	121.39
2	D	82	GLN	CA-C-O	-6.64	113.14	120.38
2	D	11	VAL	CB-CA-C	6.63	120.71	110.83
1	C	50	TYR	CA-C-N	6.61	133.87	121.97
1	C	50	TYR	C-N-CA	6.61	133.87	121.97
1	C	203	SER	O-C-N	6.61	128.92	121.32
1	C	54	SER	N-CA-CB	6.59	120.47	110.45
3	F	45	ARG	NE-CZ-NH2	6.58	125.12	119.20
1	C	190	ASN	CA-CB-CG	-6.58	106.02	112.60
2	D	29	PHE	CA-CB-CG	6.58	120.38	113.80
2	D	189	SER	CA-C-N	6.57	126.51	119.28
2	D	189	SER	C-N-CA	6.57	126.51	119.28
2	D	44	GLY	O-C-N	6.56	131.23	122.70
3	F	74	ASN	OD1-CG-ND2	-6.56	116.04	122.60
3	F	68	ARG	NE-CZ-NH1	6.56	128.06	121.50
3	E	68	ARG	CD-NE-CZ	6.54	133.56	124.40
1	C	76	ASN	CA-CB-CG	-6.54	106.06	112.60
2	B	161	SER	N-CA-C	-6.53	104.08	111.07
1	C	164	THR	N-CA-C	-6.53	101.12	110.59
2	B	129	PRO	O-C-N	6.53	130.52	123.01
2	D	11	VAL	CA-C-O	-6.52	113.57	120.48
1	A	35	TRP	CA-C-O	-6.51	113.67	120.70
2	D	69	THR	CA-C-O	-6.51	112.27	120.28
2	B	216	ARG	CA-C-N	6.51	130.61	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	216	ARG	C-N-CA	6.51	130.61	121.24
1	A	57	GLY	N-CA-C	-6.50	106.19	113.79
2	B	101	GLY	N-CA-C	-6.49	97.80	113.18
2	D	57	SER	O-C-N	6.49	130.93	123.27
3	F	3	PHE	CA-C-O	-6.49	114.34	121.87
1	C	27	GLN	OE1-CD-NE2	6.49	129.09	122.60
1	C	22	SER	O-C-N	6.48	130.56	123.10
1	A	95	PRO	N-CD-CG	-6.48	96.03	103.80
1	A	130	ALA	CA-C-O	-6.47	112.30	120.20
1	C	138	ASN	CA-C-O	-6.47	114.05	122.45
1	C	192	TYR	N-CA-C	6.46	120.81	112.41
2	B	74	THR	CA-C-O	6.45	127.39	120.10
1	C	200	THR	CA-C-O	6.45	127.52	119.59
3	F	53	TYR	CA-C-O	6.45	127.66	120.70
1	C	105	GLU	CA-CB-CG	6.44	126.99	114.10
1	C	74	SER	O-C-N	6.44	130.97	123.30
3	E	17	LEU	CB-CA-C	6.43	122.06	109.72
3	F	107	ALA	O-C-N	6.41	130.16	122.27
3	F	120	VAL	CA-C-O	-6.41	113.66	120.64
3	E	66	ASP	CA-CB-CG	6.40	119.00	112.60
1	C	190	ASN	OD1-CG-ND2	6.40	129.00	122.60
1	C	87	PHE	CA-C-O	-6.39	112.93	120.60
1	A	41	HIS	CA-CB-CG	-6.39	107.41	113.80
1	A	103	LYS	N-CA-CB	-6.38	99.45	110.17
2	D	7	SER	CA-C-O	-6.38	113.59	121.88
2	B	1	GLN	CA-C-O	-6.37	109.98	120.80
2	B	56	GLY	CA-C-N	6.35	131.15	122.19
2	B	56	GLY	C-N-CA	6.35	131.15	122.19
2	D	155	VAL	CA-C-N	6.35	132.50	122.21
2	D	155	VAL	C-N-CA	6.35	132.50	122.21
1	A	61	ARG	CD-NE-CZ	-6.35	115.51	124.40
1	A	24	ARG	O-C-N	6.35	130.85	123.30
1	A	198	HIS	CA-C-N	6.33	129.62	120.38
1	A	198	HIS	C-N-CA	6.33	129.62	120.38
3	E	7	GLU	CB-CG-CD	6.31	123.33	112.60
3	F	116	LYS	N-CA-C	-6.31	100.70	110.10
3	F	27	ASN	OD1-CG-ND2	6.30	128.90	122.60
1	A	75	ILE	O-C-N	6.28	130.33	122.66
2	D	163	SER	CA-C-N	6.27	133.51	121.54
2	D	163	SER	C-N-CA	6.27	133.51	121.54
1	A	96	ARG	NE-CZ-NH2	6.27	124.84	119.20
1	C	6	GLN	O-C-N	6.27	130.76	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	46	ASN	CA-CB-CG	6.26	118.86	112.60
1	A	65	SER	O-C-N	6.23	129.66	122.99
3	F	77	ASN	CA-C-N	6.23	133.65	122.13
3	F	77	ASN	C-N-CA	6.23	133.65	122.13
3	E	60	SER	CA-C-N	-6.22	112.17	120.63
3	E	60	SER	C-N-CA	-6.22	112.17	120.63
3	F	68	ARG	O-C-N	6.22	129.18	121.84
1	C	29	ILE	CA-C-N	-6.22	113.96	123.04
1	C	29	ILE	C-N-CA	-6.22	113.96	123.04
1	C	155	ARG	NE-CZ-NH1	6.19	127.69	121.50
3	E	63	TRP	N-CA-C	6.18	119.22	111.24
2	D	100	ASP	CA-CB-CG	6.17	118.77	112.60
3	F	53	TYR	O-C-N	-6.16	115.22	123.23
1	A	115	VAL	N-CA-CB	-6.16	103.61	110.99
1	C	209	PHE	CA-C-O	-6.15	114.10	120.99
1	C	80	THR	CA-CB-OG1	-6.15	100.38	109.60
2	B	189	SER	CA-C-O	-6.15	112.38	118.34
2	B	129	PRO	CA-C-O	-6.14	114.66	121.23
2	D	20	ILE	CB-CA-C	6.13	119.96	111.19
1	A	113	PRO	CA-C-O	-6.12	114.13	121.48
2	B	210	ASP	O-C-N	6.12	130.83	123.36
3	F	87	ASP	CB-CA-C	6.11	120.09	110.19
3	F	48	ASP	CA-CB-CG	-6.11	106.49	112.60
1	A	26	SER	N-CA-C	-6.11	105.79	113.18
1	C	69	THR	O-C-N	6.10	128.57	122.10
1	A	118	PHE	O-C-N	6.10	127.04	121.80
1	C	11	LEU	CA-C-O	-6.09	112.79	120.28
1	C	37	GLN	O-C-N	6.09	130.70	123.27
2	B	144	LEU	CA-C-O	-6.08	113.63	120.32
2	B	42	GLY	N-CA-C	-6.08	107.25	114.48
2	D	123	SER	CA-C-O	-6.07	114.05	121.58
3	F	90	ALA	CA-C-N	6.07	129.53	120.31
3	F	90	ALA	C-N-CA	6.07	129.53	120.31
1	C	164	THR	CA-C-O	-6.06	114.80	121.89
2	B	88	SER	CA-CB-OG	-6.06	98.98	111.10
3	E	2	VAL	N-CA-C	6.04	115.05	106.53
1	C	63	SER	O-C-N	6.04	130.47	123.17
1	A	188	ARG	NE-CZ-NH2	-6.03	113.77	119.20
1	C	193	THR	CA-C-N	6.03	131.88	123.07
1	C	193	THR	C-N-CA	6.03	131.88	123.07
3	E	52	ASP	CA-CB-CG	-6.02	106.58	112.60
2	D	77	ASN	CA-CB-CG	-6.01	106.59	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	27	GLN	CB-CG-CD	-6.01	102.38	112.60
1	A	145	ASN	O-C-N	6.00	130.29	123.27
2	B	73	ASP	CA-C-N	6.00	128.92	120.28
2	B	73	ASP	C-N-CA	6.00	128.92	120.28
1	A	64	GLY	O-C-N	-6.00	118.00	123.57
3	F	34	PHE	CA-CB-CG	-5.99	107.81	113.80
3	F	113	ASN	CA-CB-CG	-5.99	106.61	112.60
2	D	58	THR	CA-CB-OG1	-5.97	100.64	109.60
1	A	151	ASP	CA-CB-CG	5.97	118.57	112.60
1	C	210	ASN	CB-CA-C	5.97	120.29	109.37
3	F	65	ASN	CA-C-O	-5.96	113.92	120.24
1	A	64	GLY	CA-C-O	5.95	128.00	121.63
1	C	63	SER	N-CA-C	-5.95	100.26	109.24
1	A	27	GLN	O-C-N	5.94	129.34	123.46
1	C	54	SER	O-C-N	5.93	129.61	122.85
2	B	68	ALA	CA-C-O	-5.93	114.43	121.66
2	B	157	TRP	O-C-N	5.93	130.24	123.31
2	B	52	LEU	CB-CA-C	5.92	115.77	110.44
2	D	16	ALA	CA-C-N	5.92	131.86	122.62
2	D	16	ALA	C-N-CA	5.92	131.86	122.62
1	C	58	ILE	CA-C-O	-5.92	114.62	119.47
2	B	28	THR	O-C-N	5.91	130.52	122.48
2	D	102	ASN	CA-C-O	-5.89	114.86	121.81
2	B	100	ASP	CA-CB-CG	5.88	118.48	112.60
2	B	194	GLU	O-C-N	-5.88	116.48	123.06
3	F	117	GLY	CA-C-N	5.87	132.75	121.54
3	F	117	GLY	C-N-CA	5.87	132.75	121.54
2	D	28	THR	CA-CB-OG1	-5.87	100.80	109.60
1	A	88	CYS	CA-C-O	-5.87	114.49	120.71
1	A	70	ASP	O-C-N	5.85	130.11	123.27
1	A	145	ASN	CA-CB-CG	-5.85	106.75	112.60
1	A	210	ASN	CA-CB-CG	-5.85	106.75	112.60
2	B	137	SER	N-CA-C	5.84	120.48	113.23
1	C	19	VAL	CB-CA-C	5.84	119.43	110.55
1	C	129	GLY	CA-C-O	-5.84	115.02	120.57
2	B	170	PRO	CB-CA-C	5.84	118.99	111.46
2	B	195	THR	CA-CB-OG1	-5.83	100.86	109.60
2	B	205	SER	O-C-N	5.83	128.75	122.05
1	C	146	VAL	N-CA-C	5.82	116.67	108.17
3	E	34	PHE	CA-CB-CG	-5.82	107.98	113.80
1	C	15	PRO	CB-CA-C	5.82	119.03	111.64
2	B	161	SER	CA-C-O	-5.81	114.72	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	THR	N-CA-C	-5.80	100.72	109.95
1	A	13	VAL	CB-CA-C	5.79	119.42	110.50
1	C	210	ASN	N-CA-C	-5.78	100.76	109.95
3	F	60	SER	CA-C-O	-5.77	112.31	119.18
3	E	73	ARG	CD-NE-CZ	-5.77	116.32	124.40
2	B	124	VAL	CA-C-O	5.77	127.40	120.65
2	B	110	THR	O-C-N	5.76	130.39	123.36
1	C	182	THR	CB-CA-C	5.76	119.24	109.50
1	A	110	ASP	CA-C-O	-5.75	115.45	121.55
2	D	146	LYS	O-C-N	5.75	130.67	123.19
2	D	116	SER	CA-C-O	-5.74	112.95	119.78
2	B	151	GLU	CB-CG-CD	-5.74	102.84	112.60
3	F	98	ILE	CA-C-O	-5.73	114.53	121.18
2	D	10	GLU	CA-C-O	-5.73	114.13	120.38
1	A	135	PHE	CA-C-O	-5.72	114.45	120.80
1	A	31	ASN	CB-CA-C	5.70	120.29	111.28
3	F	53	TYR	N-CA-C	5.70	118.70	109.40
1	C	176	SER	CA-C-N	5.70	130.37	121.76
1	C	176	SER	C-N-CA	5.70	130.37	121.76
2	B	125	PHE	CA-C-O	-5.70	113.88	119.69
3	F	62	TRP	N-CA-C	5.69	120.24	112.04
1	A	34	HIS	CA-CB-CG	-5.68	108.12	113.80
1	C	90	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	A	11	LEU	N-CA-CB	-5.67	101.23	110.59
1	C	3	GLU	CA-C-N	5.66	129.93	121.72
1	C	3	GLU	C-N-CA	5.66	129.93	121.72
2	B	144	LEU	CA-C-N	5.66	131.03	123.10
2	B	144	LEU	C-N-CA	5.66	131.03	123.10
3	F	94	CYS	CB-CA-C	5.66	120.92	110.56
2	B	171	ALA	O-C-N	5.65	129.97	123.02
2	B	78	THR	CA-CB-OG1	-5.64	101.14	109.60
2	B	136	ASN	CA-C-O	-5.64	115.60	121.98
1	C	31	ASN	N-CA-CB	-5.64	101.89	111.20
1	C	122	SER	O-C-N	5.64	127.95	122.09
1	C	210	ASN	CA-C-O	-5.63	114.80	121.16
2	B	121	PRO	O-C-N	5.62	128.09	121.46
2	B	212	LYS	N-CA-CB	5.62	118.55	110.06
3	E	47	THR	CA-CB-OG1	-5.62	101.17	109.60
2	B	128	ALA	CB-CA-C	5.62	117.20	108.61
1	A	209	PHE	CA-CB-CG	-5.61	108.19	113.80
2	D	169	PHE	CB-CA-C	5.59	116.91	108.86
3	F	126	GLY	N-CA-C	-5.58	107.33	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	202	HIS	CA-C-N	5.58	125.04	119.24
2	D	202	HIS	C-N-CA	5.58	125.04	119.24
1	A	212	ASN	CA-C-O	-5.58	112.53	119.28
2	B	154	THR	CA-C-O	-5.58	114.34	120.36
2	D	198	CYS	O-C-N	5.57	130.97	123.34
2	B	19	LYS	CA-C-N	5.57	129.56	122.37
2	B	19	LYS	C-N-CA	5.57	129.56	122.37
1	A	190	ASN	CA-C-O	-5.55	111.89	120.16
1	A	123	GLU	N-CA-CB	5.54	118.10	110.07
2	D	41	PRO	CA-C-O	-5.54	114.44	120.92
3	F	24	SER	N-CA-C	-5.54	103.60	110.41
1	A	91	SER	CB-CA-C	5.53	119.98	111.02
3	E	94	CYS	CA-C-O	-5.53	114.63	120.55
2	B	35	GLU	CB-CG-CD	5.52	121.99	112.60
1	A	160	LEU	CA-C-O	-5.51	114.39	120.24
3	F	48	ASP	O-C-N	5.51	127.53	121.85
2	B	69	THR	O-C-N	5.51	129.97	123.36
2	D	61	ASN	N-CA-C	-5.51	101.76	109.96
2	D	106	TRP	CA-C-O	-5.50	114.74	121.78
2	B	134	GLN	CA-C-N	5.49	128.40	120.38
2	B	134	GLN	C-N-CA	5.49	128.40	120.38
1	C	195	GLU	CB-CG-CD	5.49	121.94	112.60
3	E	87	ASP	N-CA-CB	-5.49	103.16	110.57
1	C	192	TYR	CA-C-N	5.49	132.02	121.54
1	C	192	TYR	C-N-CA	5.49	132.02	121.54
2	D	111	THR	CA-C-O	-5.48	114.35	120.54
3	F	109	VAL	CA-C-O	-5.48	114.71	120.57
2	D	7	SER	CB-CA-C	5.47	122.55	111.60
2	D	42	GLY	N-CA-C	-5.47	107.81	114.92
2	B	176	ASP	O-C-N	5.47	129.86	122.59
2	B	7	SER	N-CA-CB	-5.46	102.63	110.44
1	C	135	PHE	CA-CB-CG	5.46	119.26	113.80
2	D	113	THR	CA-C-O	-5.46	114.45	120.30
3	F	27	ASN	CA-CB-CG	-5.46	107.14	112.60
2	D	57	SER	N-CA-C	-5.46	99.62	108.52
1	A	73	LEU	N-CA-C	-5.46	100.34	109.24
1	C	57	GLY	N-CA-C	-5.46	107.99	114.48
1	C	157	ASN	OD1-CG-ND2	5.45	128.05	122.60
1	A	122	SER	O-C-N	5.45	127.90	122.12
1	A	209	PHE	CA-C-O	-5.44	112.86	120.21
2	B	31	THR	CA-C-O	-5.44	113.51	120.31
1	C	47	LEU	CA-C-N	5.44	130.50	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	LEU	C-N-CA	5.44	130.50	122.94
2	B	34	ILE	CA-C-O	-5.43	114.76	120.57
3	F	106	ASN	OD1-CG-ND2	5.42	128.02	122.60
3	E	39	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	C	17	ASP	N-CA-CB	5.42	118.52	110.29
1	A	33	LEU	CA-C-O	-5.41	114.44	120.66
2	B	103	TYR	CA-C-N	5.40	127.14	120.34
2	B	103	TYR	C-N-CA	5.40	127.14	120.34
1	C	41	HIS	CA-CB-CG	-5.38	108.42	113.80
1	C	76	ASN	OD1-CG-ND2	5.38	127.98	122.60
1	C	92	ASN	O-C-N	-5.38	116.28	122.09
2	B	92	ALA	O-C-N	5.38	128.63	123.04
2	D	113	THR	O-C-N	5.38	129.51	123.27
2	B	31	THR	O-C-N	5.37	129.55	122.30
2	B	125	PHE	N-CA-C	-5.37	100.81	109.40
3	E	21	ARG	CA-C-N	5.37	128.89	121.26
3	E	21	ARG	C-N-CA	5.37	128.89	121.26
2	D	77	ASN	CA-C-O	-5.37	112.83	120.51
1	A	39	LYS	N-CA-C	-5.36	102.58	110.52
2	B	15	GLY	N-CA-C	-5.36	107.61	114.37
3	E	67	GLY	CA-C-O	-5.36	113.64	118.95
1	C	178	THR	CA-CB-OG1	-5.36	101.56	109.60
3	E	106	ASN	CA-CB-CG	5.36	117.96	112.60
1	A	138	ASN	OD1-CG-ND2	-5.36	117.25	122.60
2	D	42	GLY	CA-C-O	5.35	125.07	119.07
1	A	117	ILE	CA-C-O	-5.35	114.60	121.40
2	B	146	LYS	N-CA-C	5.35	117.82	109.52
1	A	73	LEU	CA-C-O	-5.35	114.60	120.43
1	A	109	ALA	CA-C-O	-5.35	115.73	121.56
1	A	155	ARG	NE-CZ-NH2	5.34	124.01	119.20
3	E	98	ILE	O-C-N	5.34	127.28	121.94
1	A	166	GLN	CA-C-O	5.34	127.00	120.92
2	D	7	SER	N-CA-C	-5.34	102.11	110.17
3	F	65	ASN	N-CA-CB	-5.33	102.41	110.77
2	B	195	THR	CA-CB-CG2	5.33	119.56	110.50
1	C	190	ASN	O-C-N	5.33	129.67	122.59
3	E	62	TRP	CA-C-N	5.33	129.51	120.88
3	E	62	TRP	C-N-CA	5.33	129.51	120.88
1	A	132	VAL	CA-C-O	-5.32	114.70	120.71
3	F	94	CYS	N-CA-C	-5.32	104.39	112.04
1	C	105	GLU	N-CA-CB	5.31	119.34	110.85
2	D	67	LYS	CA-C-O	-5.31	112.92	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	106	ASN	CA-CB-CG	-5.31	107.29	112.60
1	A	118	PHE	CA-C-O	-5.30	114.47	120.46
2	D	113	THR	CB-CA-C	-5.29	101.39	110.16
3	E	75	LEU	CB-CA-C	5.28	119.83	110.85
1	C	155	ARG	NE-CZ-NH2	-5.28	114.45	119.20
2	B	197	THR	CA-CB-CG2	5.28	119.47	110.50
3	F	37	ASN	CA-C-N	5.28	129.84	122.08
3	F	37	ASN	C-N-CA	5.28	129.84	122.08
3	F	129	LEU	CA-CB-CG	5.28	134.76	116.30
1	A	167	ASP	CA-C-N	5.27	127.78	120.29
1	A	167	ASP	C-N-CA	5.27	127.78	120.29
2	D	60	TYR	N-CA-C	5.27	118.08	109.59
2	D	40	ARG	NE-CZ-NH1	-5.27	116.23	121.50
3	F	98	ILE	CB-CA-C	5.27	118.67	111.87
3	E	58	ILE	N-CA-C	-5.27	102.19	110.09
2	B	61	ASN	CB-CA-C	5.26	118.41	109.84
2	D	35	GLU	CB-CG-CD	5.26	121.54	112.60
2	D	63	LYS	CB-CA-C	-5.25	99.33	110.31
1	C	17	ASP	CB-CG-OD1	5.25	130.47	118.40
1	A	180	THR	CA-CB-OG1	-5.25	101.73	109.60
1	A	96	ARG	O-C-N	5.24	128.88	122.96
1	C	19	VAL	CA-CB-CG2	5.23	119.30	110.40
1	C	160	LEU	CA-C-O	-5.23	115.25	121.16
1	A	67	SER	O-C-N	5.23	129.55	122.59
2	B	199	ASN	CA-CB-CG	-5.23	107.37	112.60
2	B	118	SER	CA-C-O	-5.23	115.34	121.46
2	D	64	PHE	CA-CB-CG	-5.23	108.57	113.80
2	B	63	LYS	CA-C-N	5.22	131.43	122.09
2	B	63	LYS	C-N-CA	5.22	131.43	122.09
2	B	75	SER	CA-C-N	5.22	129.43	120.72
2	B	75	SER	C-N-CA	5.22	129.43	120.72
1	C	11	LEU	N-CA-CB	-5.22	102.05	110.81
1	A	100	GLY	CA-C-N	5.21	131.62	121.41
1	A	100	GLY	C-N-CA	5.21	131.62	121.41
3	E	98	ILE	CA-C-O	-5.21	115.86	121.27
2	B	190	PRO	CA-C-O	-5.20	111.13	120.60
3	E	104	GLY	O-C-N	5.20	128.39	122.67
3	F	43	THR	CA-CB-OG1	-5.19	101.81	109.60
2	B	29	PHE	CA-CB-CG	5.19	118.99	113.80
1	C	33	LEU	O-C-N	5.19	129.82	123.44
2	D	34	ILE	N-CA-C	-5.19	100.94	108.36
2	D	41	PRO	O-C-N	5.19	128.53	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	LEU	N-CA-CB	-5.18	101.62	111.00
1	A	61	ARG	CA-CB-CG	5.18	124.46	114.10
2	B	153	VAL	N-CA-C	-5.18	101.02	108.89
3	F	48	ASP	N-CA-C	-5.17	106.50	114.16
1	A	61	ARG	N-CA-CB	-5.17	102.25	110.22
1	C	166	GLN	CB-CA-C	5.17	118.27	109.84
2	D	117	ALA	O-C-N	5.16	128.74	122.85
2	B	59	TYR	CB-CA-C	5.16	118.57	109.80
2	B	87	THR	CA-CB-CG2	5.15	119.26	110.50
1	A	89	GLN	OE1-CD-NE2	-5.15	117.45	122.60
2	D	101	GLY	N-CA-C	-5.13	101.03	113.18
2	D	188	SER	CA-C-O	5.13	125.87	119.97
3	F	2	VAL	N-CA-CB	-5.13	105.21	111.67
2	B	185	THR	CA-CB-OG1	-5.12	101.91	109.60
2	B	169	PHE	CA-CB-CG	-5.12	108.68	113.80
2	D	35	GLU	CA-C-O	-5.12	115.33	121.11
1	A	131	SER	CA-C-O	-5.12	114.89	120.36
2	B	63	LYS	N-CA-CB	-5.11	102.60	110.16
1	A	172	THR	CA-C-N	5.11	132.19	123.05
1	A	172	THR	C-N-CA	5.11	132.19	123.05
2	B	209	VAL	O-C-N	5.11	128.71	123.04
2	D	24	ALA	CA-C-O	-5.11	115.26	121.28
3	E	18	ASP	CA-CB-CG	-5.11	107.49	112.60
2	B	94	TYR	CA-C-O	-5.10	115.40	121.16
3	F	92	VAL	CB-CA-C	5.09	118.71	112.04
2	D	146	LYS	CA-C-N	5.09	131.38	121.41
2	D	146	LYS	C-N-CA	5.09	131.38	121.41
2	B	202	HIS	CA-C-N	5.08	124.69	119.05
2	B	202	HIS	C-N-CA	5.08	124.69	119.05
2	D	201	ALA	N-CA-C	-5.08	102.54	110.42
3	E	45	ARG	O-C-N	5.08	129.56	123.16
3	E	2	VAL	N-CA-CB	-5.08	106.46	112.40
2	B	51	ILE	CA-CB-CG2	5.08	119.13	110.50
1	A	61	ARG	CA-C-N	5.07	129.52	122.77
1	A	61	ARG	C-N-CA	5.07	129.52	122.77
2	D	201	ALA	O-C-N	5.07	128.76	123.03
2	B	22	CYS	O-C-N	5.07	129.62	123.14
1	A	31	ASN	OD1-CG-ND2	5.06	127.66	122.60
1	A	203	SER	O-C-N	5.06	124.95	121.71
2	D	14	PRO	CA-C-N	5.06	130.55	122.25
2	D	14	PRO	C-N-CA	5.06	130.55	122.25
3	F	14	ARG	CD-NE-CZ	-5.06	117.31	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	24	SER	O-C-N	5.06	128.82	122.65
3	F	35	GLU	CG-CD-OE2	5.06	130.04	118.40
3	F	84	LEU	N-CA-CB	-5.06	102.85	111.20
3	F	10	ALA	CA-C-O	-5.06	115.25	120.92
2	D	15	GLY	N-CA-C	-5.05	108.14	115.27
3	E	3	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	7	SER	CA-CB-OG	-5.05	101.00	111.10
2	B	139	VAL	CB-CA-C	5.05	118.27	110.50
1	A	73	LEU	O-C-N	5.04	128.97	123.27
1	C	204	PRO	N-CA-C	5.04	118.97	111.41
3	F	69	THR	CA-CB-OG1	-5.04	102.04	109.60
2	B	212	LYS	CA-CB-CG	5.03	124.16	114.10
1	A	210	ASN	OD1-CG-ND2	5.02	127.62	122.60
2	D	102	ASN	N-CA-C	-5.02	103.77	110.55
1	C	213	GLU	CB-CG-CD	5.02	121.13	112.60
3	F	73	ARG	NE-CZ-NH2	-5.01	114.69	119.20
2	B	63	LYS	N-CA-C	5.01	116.82	111.36
3	F	43	THR	CA-CB-CG2	5.01	119.01	110.50
2	B	81	MET	O-C-N	5.00	129.16	123.31

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
3	E	68	ARG	Sidechain
3	F	5	ARG	Sidechain

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	1658	0	1572	94	0
1	C	1658	0	1572	171	0
2	B	1632	0	1576	73	0
2	D	1632	0	1576	115	0
3	E	1001	0	959	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1001	0	959	53	0
4	A	47	0	0	3	0
4	B	48	0	0	3	0
4	C	35	0	0	2	0
4	D	35	0	0	3	0
4	E	22	0	0	0	0
4	F	23	0	0	2	0
All	All	8792	0	8214	589	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 35.

All (589) 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:187:GLU:HA	1:C:211:ARG:NH1	1.60	1.15
1:A:195:GLU:HG2	1:A:206:VAL:HG22	1.29	1.09
1:A:115:VAL:HG12	1:A:207:LYS:HG3	1.25	1.08
3:E:121:GLN:HA	3:E:124:ILE:HD11	1.38	1.05
2:D:187:PRO:HD2	2:D:190:PRO:HG2	1.37	1.04
2:D:191:ARG:HG3	2:D:191:ARG:HH11	1.17	1.04
1:C:155:ARG:HG2	1:C:156:GLN:H	1.24	1.03
1:C:11:LEU:HD23	1:C:104:LEU:HD13	1.43	1.00
2:D:10:GLU:HG3	2:D:18:VAL:HG21	1.44	1.00
2:D:70:PHE:CE1	2:D:81:MET:HG3	1.99	0.98
2:D:70:PHE:HE1	2:D:81:MET:HG3	1.24	0.98
3:E:26:GLY:HA3	3:E:120:VAL:HG23	1.46	0.97
2:D:189:SER:HB2	2:D:190:PRO:HD3	1.46	0.97
3:F:62:TRP:CZ3	3:F:73:ARG:HD3	2.02	0.94
2:B:197:THR:OG1	2:B:212:LYS:HD2	1.72	0.89
1:A:115:VAL:CG1	1:A:207:LYS:HG3	2.03	0.89
1:A:83:PHE:CE2	1:A:106:ILE:HG12	2.08	0.88
1:C:187:GLU:HA	1:C:211:ARG:HH12	1.22	0.88
1:A:133:VAL:HG22	1:A:178:THR:HG23	1.56	0.87
1:C:113:PRO:HB3	1:C:139:PHE:HB3	1.56	0.87
1:C:124:GLN:HE22	1:C:131:SER:HB2	1.38	0.86
1:C:151:ASP:HA	1:C:191:SER:OG	1.76	0.86
2:D:175:SER:O	2:D:176:ASP:HB2	1.73	0.85
3:E:121:GLN:HA	3:E:124:ILE:CD1	2.08	0.83
3:E:121:GLN:O	3:E:124:ILE:HG13	1.78	0.83
1:C:150:ILE:HG12	1:C:192:TYR:CE1	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ASN:ND2	1:C:147:LYS:HZ3	1.76	0.83
2:D:10:GLU:HG3	2:D:18:VAL:CG2	2.09	0.82
1:A:30:SER:OG	1:A:31:ASN:N	2.08	0.82
1:C:115:VAL:HG22	1:C:136:LEU:HG	1.61	0.82
2:B:187:PRO:HB2	2:B:190:PRO:HD2	1.61	0.82
1:C:155:ARG:HG2	1:C:156:GLN:N	1.93	0.81
2:B:166:VAL:HG22	2:B:184:VAL:HG23	1.61	0.81
3:E:106:ASN:ND2	3:E:111:TRP:HZ3	1.76	0.81
2:B:70:PHE:HE1	2:B:81:MET:HE3	1.46	0.80
1:A:213:GLU:O	1:A:214:CYS:HB3	1.81	0.80
1:A:80:THR:HA	1:A:83:PHE:CE2	2.17	0.80
3:F:62:TRP:HZ3	3:F:73:ARG:HD3	1.41	0.79
1:A:40:SER:O	1:A:41:HIS:HB2	1.80	0.79
2:D:197:THR:HG23	2:D:212:LYS:HE3	1.64	0.79
1:C:187:GLU:CA	1:C:211:ARG:HH12	1.95	0.79
1:C:150:ILE:HA	1:C:191:SER:O	1.83	0.78
1:A:54:SER:HA	4:A:1618:HOH:O	1.83	0.78
1:C:66:GLY:O	1:C:67:SER:HB2	1.83	0.78
2:B:48:ILE:HG21	2:B:81:MET:CE	2.12	0.78
1:C:11:LEU:HD23	1:C:104:LEU:CD1	2.13	0.78
1:C:195:GLU:HB2	1:C:206:VAL:HG13	1.64	0.77
3:F:68:ARG:HD2	4:F:2109:HOH:O	1.83	0.77
1:C:90:GLN:HE21	1:C:90:GLN:C	1.92	0.77
3:F:121:GLN:HG3	3:F:122:ALA:N	1.99	0.77
2:D:23:LYS:HB3	2:D:23:LYS:NZ	2.00	0.76
3:E:106:ASN:HD22	3:E:111:TRP:HZ3	1.32	0.76
1:A:2:ILE:HD11	1:A:27:GLN:HE21	1.51	0.76
2:D:145:VAL:HG11	2:D:153:VAL:HG21	1.67	0.76
2:D:189:SER:HB2	2:D:190:PRO:CD	2.16	0.76
3:E:21:ARG:HG3	3:E:21:ARG:HH11	1.50	0.75
2:D:138:MET:HG2	2:D:185:THR:HG22	1.69	0.75
3:E:10:ALA:CB	3:E:14:ARG:HH21	2.00	0.74
2:B:48:ILE:HD12	2:B:81:MET:HE1	1.69	0.74
1:C:166:GLN:HB2	1:C:173:TYR:CE1	2.23	0.74
1:C:181:LEU:HD13	1:C:186:TYR:HA	1.68	0.74
3:F:119:ASP:OD2	3:F:125:ARG:NH2	2.21	0.73
1:C:115:VAL:HG12	1:C:207:LYS:HG3	1.70	0.73
1:C:8:PRO:HG3	1:C:11:LEU:HD13	1.71	0.73
3:E:106:ASN:HD21	3:E:116:LYS:HE3	1.52	0.72
1:A:80:THR:HA	1:A:83:PHE:HE2	1.53	0.72
1:C:136:LEU:C	1:C:137:ASN:HD22	1.98	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:36:SER:OG	3:E:55:ILE:HA	1.90	0.71
2:D:191:ARG:HG3	2:D:191:ARG:NH1	1.93	0.71
1:A:160:LEU:HD21	2:B:172:VAL:HG23	1.71	0.71
2:D:138:MET:HG3	2:D:186:VAL:C	2.15	0.71
3:E:21:ARG:HH11	3:E:21:ARG:CG	2.04	0.70
1:C:150:ILE:O	1:C:151:ASP:C	2.34	0.70
2:D:191:ARG:HH11	2:D:191:ARG:CG	1.97	0.70
3:E:10:ALA:O	3:E:13:LYS:HG2	1.91	0.70
3:F:111:TRP:CZ3	3:F:116:LYS:HE2	2.25	0.70
1:C:11:LEU:HD22	1:C:21:LEU:HD21	1.72	0.70
3:E:98:ILE:O	3:E:101:ASP:HB2	1.92	0.70
1:C:11:LEU:CD2	1:C:21:LEU:HD21	2.22	0.69
3:E:108:TRP:O	3:E:109:VAL:C	2.35	0.69
2:D:13:LYS:HD2	2:D:116:SER:HA	1.75	0.69
2:D:159:SER:O	2:D:161:SER:N	2.26	0.69
1:C:212:ASN:N	1:C:212:ASN:OD1	2.25	0.68
2:D:191:ARG:HD2	2:D:192:PRO:HA	1.74	0.68
2:D:129:PRO:HG3	2:D:141:LEU:HD12	1.74	0.68
1:A:119:PRO:HD2	2:B:216:ARG:NH2	2.08	0.68
2:D:146:LYS:NZ	2:D:174:GLN:HE21	1.92	0.68
3:E:87:ASP:O	3:E:89:THR:N	2.27	0.68
2:D:161:SER:O	2:D:163:SER:N	2.26	0.68
3:E:17:LEU:HD11	3:E:92:VAL:HG13	1.76	0.68
3:E:116:LYS:O	3:E:118:THR:HG23	1.94	0.67
1:C:11:LEU:HD21	1:C:19:VAL:HG22	1.76	0.67
2:B:203:PRO:O	2:B:205:SER:N	2.28	0.67
3:E:33:LYS:HG2	3:E:123:TRP:CH2	2.29	0.66
1:C:125:LEU:O	1:C:183:LYS:HD2	1.95	0.66
1:A:47:LEU:C	1:A:48:ILE:HG12	2.21	0.66
1:C:108:ARG:NE	1:C:109:ALA:O	2.26	0.66
3:E:4:GLY:O	3:E:8:LEU:HB2	1.96	0.66
2:D:23:LYS:HB3	2:D:23:LYS:HZ2	1.60	0.65
3:E:108:TRP:O	3:E:111:TRP:N	2.23	0.65
1:A:2:ILE:CD1	1:A:27:GLN:HE21	2.09	0.65
1:C:124:GLN:NE2	1:C:131:SER:HB2	2.10	0.65
1:C:145:ASN:ND2	1:C:147:LYS:NZ	2.45	0.65
1:C:148:TRP:O	1:C:149:LYS:HG3	1.97	0.65
2:B:48:ILE:HG21	2:B:81:MET:HE2	1.77	0.65
1:C:181:LEU:HD12	1:C:186:TYR:HD1	1.62	0.65
1:A:24:ARG:HA	1:A:69:THR:O	1.98	0.64
1:C:8:PRO:CG	1:C:11:LEU:HD13	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:191:ARG:NH1	2:D:191:ARG:CG	2.60	0.64
1:A:29:ILE:HD11	1:A:71:PHE:CE1	2.32	0.64
3:E:10:ALA:HB1	3:E:14:ARG:HH21	1.61	0.64
1:A:185:GLU:O	1:A:189:HIS:HD2	1.80	0.64
3:E:80:CYS:O	3:E:83:LEU:HB2	1.97	0.64
1:C:136:LEU:HD13	1:C:175:MET:HE2	1.79	0.64
3:E:26:GLY:CA	3:E:120:VAL:HG23	2.25	0.64
3:F:52:ASP:OD1	3:F:59:ASN:ND2	2.30	0.64
1:C:150:ILE:HG12	1:C:192:TYR:CD1	2.32	0.64
3:E:20:TYR:O	3:E:23:TYR:HB2	1.98	0.63
3:E:56:LEU:HD13	3:E:95:ALA:HB2	1.79	0.63
2:B:48:ILE:CD1	2:B:81:MET:HE1	2.27	0.63
3:F:61:ARG:NH1	3:F:71:GLY:HA3	2.14	0.63
1:C:47:LEU:HD23	1:C:58:ILE:HD12	1.79	0.63
3:E:27:ASN:ND2	3:E:120:VAL:HG11	2.14	0.63
2:D:122:PRO:HB3	2:D:148:TYR:HB3	1.81	0.63
2:D:139:VAL:N	2:D:186:VAL:O	2.26	0.62
3:E:52:ASP:HA	3:E:58:ILE:O	1.99	0.62
1:C:184:ASP:OD1	1:C:185:GLU:N	2.32	0.62
1:C:11:LEU:HB3	1:C:104:LEU:HD12	1.81	0.62
1:C:183:LYS:O	1:C:186:TYR:HB3	1.99	0.62
2:D:187:PRO:CD	2:D:190:PRO:HG2	2.22	0.62
2:D:52:LEU:HB3	2:D:55:SER:OG	2.00	0.62
2:D:192:PRO:HB3	2:D:215:PRO:HG3	1.81	0.62
1:C:115:VAL:CG1	1:C:207:LYS:HG3	2.29	0.62
1:A:205:ILE:HD12	1:A:205:ILE:N	2.15	0.62
3:E:13:LYS:HD3	3:E:129:LEU:HD22	1.82	0.62
1:A:85:MET:HG2	1:A:87:PHE:CZ	2.34	0.62
1:A:161:ASN:HB3	1:A:175:MET:HE1	1.81	0.62
3:E:15:HIS:HB3	3:E:92:VAL:HG11	1.81	0.62
2:B:70:PHE:CE1	2:B:81:MET:HE3	2.32	0.61
1:C:34:HIS:ND1	2:D:102:ASN:HB3	2.15	0.61
2:D:187:PRO:C	2:D:190:PRO:HD2	2.25	0.61
3:E:8:LEU:O	3:E:11:ALA:N	2.33	0.61
1:A:89:GLN:HG2	1:A:90:GLN:N	2.14	0.61
3:E:3:PHE:CZ	3:E:88:ILE:HG23	2.35	0.61
1:C:166:GLN:HB2	1:C:173:TYR:CZ	2.35	0.61
1:C:2:ILE:HG21	1:C:29:ILE:HG22	1.82	0.61
2:D:138:MET:HA	2:D:187:PRO:HA	1.83	0.61
3:E:37:ASN:O	3:E:38:PHE:HB2	2.00	0.61
2:D:180:LEU:HD23	2:D:181:SER:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LYS:HG2	1:A:154:GLU:HA	1.83	0.61
1:C:80:THR:O	1:C:83:PHE:CD2	2.54	0.61
1:C:150:ILE:HG23	1:C:189:HIS:HB3	1.83	0.61
3:E:83:LEU:HD23	3:E:90:ALA:HB1	1.83	0.61
1:C:61:ARG:HG3	1:C:61:ARG:HH11	1.65	0.60
1:C:198:HIS:O	1:C:201:SER:HB2	2.02	0.60
2:D:137:SER:O	2:D:187:PRO:HA	2.01	0.60
1:A:83:PHE:CD2	1:A:106:ILE:CG1	2.84	0.60
2:D:197:THR:CG2	2:D:212:LYS:HE3	2.31	0.60
1:C:71:PHE:HB3	4:C:1813:HOH:O	1.99	0.60
1:C:182:THR:O	1:C:183:LYS:C	2.44	0.60
1:C:188:ARG:HG2	1:C:189:HIS:CE1	2.37	0.60
1:A:79:GLU:O	1:A:83:PHE:CE2	2.55	0.60
3:E:30:CYS:O	3:E:33:LYS:HB3	2.02	0.60
1:C:181:LEU:CD1	1:C:186:TYR:HD1	2.15	0.59
2:B:48:ILE:HG21	2:B:81:MET:HE1	1.83	0.59
1:A:160:LEU:CD2	2:B:172:VAL:HG23	2.32	0.59
3:E:124:ILE:HA	3:E:127:CYS:SG	2.42	0.59
1:C:145:ASN:HD22	1:C:147:LYS:NZ	2.01	0.59
2:D:193:SER:HB2	2:D:194:GLU:OE1	2.03	0.59
3:F:121:GLN:CG	3:F:122:ALA:N	2.66	0.59
3:F:31:ALA:O	3:F:35:GLU:HG2	2.03	0.58
3:F:121:GLN:CD	3:F:125:ARG:NH1	2.61	0.58
1:C:28:SER:C	1:C:30:SER:H	2.10	0.58
1:A:115:VAL:CG1	1:A:207:LYS:CG	2.79	0.58
1:A:119:PRO:HD2	2:B:216:ARG:CZ	2.34	0.58
3:E:106:ASN:CG	3:E:112:ARG:HG3	2.29	0.58
1:A:115:VAL:HG12	1:A:207:LYS:CG	2.17	0.58
1:C:59:PRO:HG2	1:C:62:PHE:CE2	2.39	0.58
1:C:150:ILE:CD1	1:C:192:TYR:HE1	2.16	0.58
2:D:193:SER:CB	2:D:194:GLU:OE1	2.52	0.58
3:E:13:LYS:CD	3:E:129:LEU:HB3	2.33	0.58
3:F:111:TRP:CH2	3:F:116:LYS:HE2	2.39	0.57
1:A:47:LEU:HD11	1:A:86:TYR:HE2	1.68	0.57
2:D:189:SER:CB	2:D:190:PRO:CD	2.82	0.57
2:D:158:ASN:OD1	2:D:196:VAL:HA	2.04	0.57
3:F:61:ARG:O	3:F:72:SER:HA	2.04	0.57
2:B:203:PRO:C	2:B:205:SER:N	2.62	0.57
2:D:138:MET:HG3	2:D:186:VAL:O	2.05	0.57
1:C:29:ILE:HD11	1:C:33:LEU:HD12	1.87	0.57
1:C:34:HIS:CE1	2:D:102:ASN:HB3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ILE:HG21	1:C:189:HIS:CG	2.40	0.57
3:E:20:TYR:O	3:E:23:TYR:CD2	2.58	0.57
2:D:216:ARG:HA	2:D:216:ARG:CZ	2.35	0.56
3:E:20:TYR:O	3:E:23:TYR:HD2	1.87	0.56
1:A:47:LEU:HD11	1:A:86:TYR:CE2	2.40	0.56
1:A:121:SER:O	1:A:125:LEU:HD22	2.05	0.56
3:F:78:ILE:HG13	3:F:79:PRO:HD2	1.86	0.56
1:A:83:PHE:CD2	1:A:106:ILE:HG12	2.40	0.56
2:B:40:ARG:HB3	2:B:43:HIS:HD2	1.71	0.56
1:C:182:THR:OG1	1:C:185:GLU:HB2	2.06	0.56
1:C:29:ILE:HD11	1:C:33:LEU:HB2	1.86	0.56
3:E:9:ALA:HB1	3:E:129:LEU:HD11	1.88	0.56
2:B:40:ARG:HB3	2:B:43:HIS:CD2	2.42	0.55
1:C:124:GLN:HG3	2:D:125:PHE:CE2	2.40	0.55
2:B:10:GLU:HG2	4:B:1708:HOH:O	2.05	0.55
1:C:32:ASN:ND2	3:F:70:PRO:HG3	2.21	0.55
2:D:43:HIS:ND1	2:D:43:HIS:N	2.53	0.55
2:D:90:ASP:O	2:D:94:TYR:OH	2.16	0.55
3:E:113:ASN:HD22	3:E:114:ARG:HG2	1.71	0.55
2:B:217:ASP:O	2:B:218:CYS:SG	2.65	0.55
3:E:61:ARG:HG3	3:E:61:ARG:NH1	2.20	0.55
3:E:124:ILE:O	3:E:125:ARG:C	2.47	0.55
2:B:217:ASP:O	2:B:218:CYS:CB	2.55	0.55
3:E:10:ALA:HB3	3:E:14:ARG:HH21	1.70	0.54
3:F:8:LEU:CD2	3:F:38:PHE:HD1	2.20	0.54
1:C:29:ILE:HD11	1:C:33:LEU:CD1	2.36	0.54
1:C:32:ASN:HD21	3:F:70:PRO:HG3	1.72	0.54
2:D:10:GLU:HA	2:D:10:GLU:OE1	2.08	0.54
2:B:147:GLY:HA2	2:B:177:LEU:HB3	1.90	0.54
2:B:209:VAL:HG12	2:B:210:ASP:N	2.22	0.54
2:B:67:LYS:NZ	2:B:90:ASP:OD2	2.41	0.54
3:E:12:MET:HE1	3:E:28:TRP:HB3	1.90	0.54
2:B:203:PRO:C	2:B:205:SER:H	2.15	0.54
2:D:146:LYS:HZ1	2:D:174:GLN:HE21	1.54	0.54
3:F:94:CYS:O	3:F:97:LYS:N	2.39	0.54
3:E:8:LEU:O	3:E:10:ALA:N	2.41	0.53
1:A:110:ASP:OD2	1:A:199:LYS:NZ	2.25	0.53
1:C:66:GLY:O	1:C:67:SER:CB	2.54	0.53
3:E:13:LYS:HD3	3:E:129:LEU:HD13	1.89	0.53
3:E:113:ASN:C	3:E:114:ARG:HG2	2.34	0.53
1:C:108:ARG:HH21	1:C:109:ALA:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:204:ALA:HB2	4:D:1912:HOH:O	2.09	0.53
1:A:81:GLU:OE1	1:A:81:GLU:N	2.41	0.53
1:C:113:PRO:HB3	1:C:139:PHE:CD2	2.44	0.53
3:E:10:ALA:O	3:E:14:ARG:HG3	2.09	0.53
1:C:15:PRO:HA	1:C:78:VAL:O	2.08	0.53
1:C:124:GLN:O	1:C:127:SER:HB2	2.09	0.53
1:A:29:ILE:O	1:A:32:ASN:HB2	2.09	0.53
1:C:175:MET:HG3	1:C:176:SER:O	2.08	0.53
1:A:2:ILE:HG12	1:A:27:GLN:NE2	2.22	0.53
1:C:21:LEU:HD22	1:C:102:THR:HG21	1.90	0.53
1:C:125:LEU:HD23	1:C:183:LYS:HG3	1.91	0.53
1:C:147:LYS:HE3	1:C:195:GLU:HG2	1.90	0.53
2:D:189:SER:O	2:D:193:SER:OG	2.15	0.53
3:E:89:THR:O	3:E:93:ASN:HB2	2.09	0.53
2:D:129:PRO:HG3	2:D:141:LEU:CD1	2.39	0.52
3:F:8:LEU:HD22	3:F:38:PHE:HD1	1.73	0.52
1:A:4:LEU:HD22	1:A:4:LEU:N	2.24	0.52
2:B:10:GLU:CG	4:B:1708:HOH:O	2.56	0.52
3:E:1:LYS:HG2	3:E:86:SER:HB3	1.91	0.52
1:C:2:ILE:HG21	1:C:29:ILE:CG2	2.39	0.52
1:C:115:VAL:HA	1:C:135:PHE:O	2.10	0.52
3:F:109:VAL:HG22	3:F:112:ARG:NH2	2.24	0.52
3:E:106:ASN:ND2	3:E:111:TRP:CZ3	2.62	0.52
2:D:157:TRP:O	2:D:162:LEU:HB3	2.10	0.52
1:A:50:TYR:HB2	1:A:53:GLN:HE21	1.74	0.52
2:B:117:ALA:HB2	2:B:176:ASP:HB3	1.91	0.52
2:D:8:GLY:O	2:D:9:ALA:C	2.51	0.52
1:A:61:ARG:HG3	1:A:76:ASN:O	2.10	0.52
1:A:1:ASP:OD1	1:A:1:ASP:N	2.32	0.52
3:F:23:TYR:CE2	3:F:105:MET:HG3	2.45	0.52
2:D:118:SER:O	2:D:119:THR:C	2.51	0.51
2:B:147:GLY:O	2:B:177:LEU:HD13	2.10	0.51
1:C:71:PHE:N	1:C:71:PHE:CD1	2.77	0.51
2:D:91:SER:O	2:D:92:ALA:HB2	2.08	0.51
3:E:3:PHE:HB2	3:E:8:LEU:HG	1.93	0.51
3:F:111:TRP:CD1	3:F:115:CYS:HB2	2.46	0.51
3:F:103:ASN:O	3:F:106:ASN:HB2	2.10	0.51
1:A:18:SER:OG	3:F:128:ARG:HG3	2.10	0.51
1:A:193:THR:CG2	1:A:206:VAL:HG13	2.41	0.51
1:C:11:LEU:HD21	1:C:19:VAL:CG2	2.41	0.51
2:B:73:ASP:OD1	2:B:75:SER:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ILE:HD12	1:A:205:ILE:H	1.76	0.51
2:B:17:SER:HB3	2:B:84:SER:HA	1.93	0.51
1:C:150:ILE:CG1	1:C:192:TYR:CE1	2.92	0.51
1:C:181:LEU:HD12	1:C:186:TYR:CD1	2.44	0.51
1:C:117:ILE:HG22	1:C:207:LYS:HB3	1.93	0.50
1:C:190:ASN:O	1:C:210:ASN:HA	2.11	0.50
1:C:11:LEU:HD22	1:C:21:LEU:CD2	2.40	0.50
3:E:7:GLU:O	3:E:7:GLU:HG2	2.10	0.50
1:A:70:ASP:HB3	4:A:1616:HOH:O	2.10	0.50
2:B:28:THR:HG22	2:B:30:SER:OG	2.11	0.50
1:C:62:PHE:CD1	1:C:75:ILE:HG12	2.46	0.50
1:C:79:GLU:O	1:C:82:ASP:HB2	2.11	0.50
1:C:136:LEU:HD21	1:C:196:ALA:HB2	1.93	0.50
2:B:132:ALA:O	2:B:134:GLN:N	2.41	0.50
2:B:203:PRO:O	2:B:204:ALA:C	2.53	0.50
1:C:148:TRP:C	1:C:149:LYS:HG3	2.37	0.50
3:E:27:ASN:HB3	3:E:105:MET:SD	2.52	0.50
3:E:87:ASP:C	3:E:89:THR:H	2.20	0.50
2:B:150:PRO:HD2	2:B:204:ALA:HB1	1.93	0.50
1:C:122:SER:OG	1:C:123:GLU:OE1	2.28	0.50
3:F:1:LYS:HB3	3:F:40:THR:OG1	2.11	0.50
3:F:33:LYS:NZ	3:F:37:ASN:OD1	2.30	0.50
3:F:62:TRP:HZ3	3:F:73:ARG:CD	2.20	0.50
1:A:213:GLU:CG	1:A:214:CYS:N	2.72	0.50
2:B:137:SER:HA	2:B:188:SER:OG	2.11	0.50
2:D:187:PRO:O	2:D:190:PRO:HD2	2.12	0.50
1:A:195:GLU:HA	1:A:205:ILE:O	2.12	0.50
1:C:28:SER:C	1:C:30:SER:N	2.70	0.50
2:D:139:VAL:HG13	2:D:186:VAL:HG22	1.94	0.50
1:C:94:TRP:HA	1:C:95:PRO:C	2.37	0.50
2:D:146:LYS:NZ	2:D:174:GLN:NE2	2.60	0.50
3:E:27:ASN:HD22	3:E:111:TRP:HE1	1.60	0.50
3:E:121:GLN:HA	3:E:124:ILE:CG1	2.42	0.49
1:A:119:PRO:HB2	1:A:120:PRO:HD2	1.93	0.49
2:B:73:ASP:HB3	2:B:76:SER:OG	2.13	0.49
1:C:40:SER:O	1:C:41:HIS:HB2	2.11	0.49
1:C:49:LYS:O	1:C:50:TYR:C	2.56	0.49
1:C:187:GLU:C	1:C:189:HIS:H	2.20	0.49
2:D:157:TRP:C	2:D:159:SER:H	2.21	0.49
3:E:112:ARG:O	3:E:113:ASN:HB2	2.11	0.49
1:A:154:GLU:HG3	1:A:155:ARG:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:PRO:HD2	2:B:204:ALA:CB	2.43	0.49
2:B:187:PRO:HD2	2:B:190:PRO:HG2	1.95	0.49
1:C:170:ASP:OD1	1:C:170:ASP:C	2.56	0.49
3:F:25:LEU:O	3:F:26:GLY:C	2.56	0.49
3:F:94:CYS:O	3:F:95:ALA:C	2.55	0.49
1:C:13:VAL:HG21	1:C:104:LEU:HD11	1.95	0.49
1:C:198:HIS:HD2	1:C:200:THR:H	1.60	0.49
2:D:52:LEU:O	2:D:53:PRO:C	2.56	0.49
1:A:210:ASN:HB2	1:A:213:GLU:HB3	1.94	0.49
2:B:143:CYS:O	2:B:181:SER:HA	2.13	0.49
1:C:183:LYS:HG2	1:C:187:GLU:OE1	2.12	0.49
1:C:125:LEU:CD2	1:C:183:LYS:HG3	2.43	0.49
1:C:162:SER:O	1:C:175:MET:HA	2.12	0.49
2:D:180:LEU:HD23	2:D:180:LEU:C	2.38	0.49
1:A:141:PRO:HG3	1:A:199:LYS:HD2	1.95	0.48
2:D:202:HIS:CE1	2:D:204:ALA:HB3	2.47	0.48
3:E:36:SER:OG	3:E:55:ILE:O	2.24	0.48
2:B:190:PRO:HD3	4:B:1934:HOH:O	2.12	0.48
1:C:61:ARG:HH11	1:C:61:ARG:CG	2.23	0.48
2:D:50:GLU:OE2	3:F:45:ARG:NH2	2.43	0.48
3:E:110:ALA:O	3:E:114:ARG:HB2	2.12	0.48
1:A:183:LYS:NZ	1:A:187:GLU:OE1	2.47	0.48
1:C:1:ASP:HB3	4:C:1816:HOH:O	2.13	0.48
3:E:61:ARG:O	3:E:72:SER:HA	2.13	0.48
3:F:43:THR:HA	3:F:52:ASP:O	2.13	0.48
1:C:29:ILE:O	1:C:30:SER:HB3	2.13	0.48
1:C:125:LEU:C	1:C:127:SER:H	2.20	0.48
2:D:173:LEU:HD23	2:D:177:LEU:O	2.14	0.48
3:F:23:TYR:CD2	3:F:105:MET:HG3	2.48	0.48
1:A:161:ASN:HB3	1:A:175:MET:CE	2.43	0.48
1:C:94:TRP:CE3	3:F:45:ARG:HB3	2.48	0.48
2:D:157:TRP:C	2:D:159:SER:N	2.72	0.48
1:A:161:ASN:OD1	1:A:177:SER:HB2	2.14	0.48
2:D:187:PRO:HB2	2:D:190:PRO:HD2	1.94	0.48
2:B:150:PRO:O	2:B:202:HIS:NE2	2.44	0.48
1:A:40:SER:O	1:A:41:HIS:CB	2.56	0.48
2:D:157:TRP:O	2:D:158:ASN:HB2	2.13	0.48
1:C:8:PRO:HG3	1:C:11:LEU:CD1	2.42	0.48
1:C:149:LYS:N	1:C:193:THR:O	2.41	0.48
2:D:10:GLU:HB3	2:D:112:LEU:HD12	1.95	0.48
1:C:170:ASP:OD1	1:C:172:THR:OG1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:192:PRO:CB	2:D:215:PRO:HG3	2.42	0.47
3:E:112:ARG:O	3:E:112:ARG:HD2	2.13	0.47
1:C:155:ARG:CG	1:C:156:GLN:N	2.72	0.47
2:D:146:LYS:HZ1	2:D:174:GLN:NE2	2.12	0.47
1:A:83:PHE:CE2	1:A:106:ILE:CG1	2.88	0.47
3:E:21:ARG:CG	3:E:21:ARG:NH1	2.73	0.47
3:E:77:ASN:OD1	3:E:77:ASN:C	2.56	0.47
3:E:99:VAL:O	3:E:100:SER:C	2.58	0.47
1:C:13:VAL:CG2	1:C:104:LEU:HD11	2.45	0.47
1:C:188:ARG:CG	1:C:189:HIS:CE1	2.96	0.47
3:E:8:LEU:HD12	3:E:38:PHE:CD1	2.49	0.47
2:D:29:PHE:CE2	2:D:53:PRO:HB3	2.50	0.47
1:C:33:LEU:HA	1:C:89:GLN:O	2.14	0.47
1:C:58:ILE:HA	1:C:59:PRO:HD2	1.81	0.47
1:C:61:ARG:O	1:C:75:ILE:HA	2.15	0.47
2:D:33:TRP:CH2	3:F:45:ARG:NH2	2.81	0.47
2:D:139:VAL:O	2:D:185:THR:HA	2.14	0.47
3:E:99:VAL:O	3:E:101:ASP:N	2.47	0.47
1:A:170:ASP:OD1	1:A:172:THR:OG1	2.26	0.47
2:B:6:GLU:OE2	2:B:107:GLY:HA3	2.14	0.47
3:E:10:ALA:HB3	3:E:14:ARG:NH2	2.30	0.47
1:A:94:TRP:HA	1:A:95:PRO:C	2.40	0.47
1:A:175:MET:HE3	1:A:175:MET:HB2	1.73	0.47
2:D:139:VAL:HG12	2:D:186:VAL:O	2.14	0.47
1:A:31:ASN:OD1	1:A:31:ASN:O	2.32	0.47
1:A:80:THR:HA	1:A:83:PHE:CD2	2.50	0.47
3:E:8:LEU:C	3:E:10:ALA:N	2.73	0.46
2:B:138:MET:HB3	2:B:185:THR:HG22	1.97	0.46
1:C:142:LYS:O	1:C:142:LYS:HG2	2.14	0.46
1:C:86:TYR:O	1:C:101:GLY:HA2	2.15	0.46
3:E:58:ILE:HG22	3:E:63:TRP:HB2	1.96	0.46
3:F:48:ASP:N	3:F:48:ASP:OD1	2.48	0.46
1:A:21:LEU:HD23	1:A:73:LEU:HD23	1.97	0.46
1:A:33:LEU:HD22	1:A:71:PHE:CG	2.50	0.46
1:A:34:HIS:O	1:A:88:CYS:HA	2.15	0.46
1:A:193:THR:HG23	1:A:206:VAL:HG13	1.96	0.46
1:C:140:TYR:CD1	1:C:141:PRO:HA	2.51	0.46
2:D:153:VAL:CG1	2:D:180:LEU:HD13	2.44	0.46
3:E:13:LYS:HD2	3:E:129:LEU:HB3	1.97	0.46
3:F:8:LEU:CD2	3:F:38:PHE:CD1	2.97	0.46
1:A:57:GLY:O	1:A:59:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:VAL:HG22	2:D:141:LEU:CD1	2.46	0.46
3:E:109:VAL:O	3:E:113:ASN:HB3	2.15	0.46
1:A:11:LEU:HD23	1:A:104:LEU:HD12	1.96	0.46
1:C:39:LYS:HE2	1:C:83:PHE:CE1	2.50	0.46
3:E:25:LEU:HD22	3:E:25:LEU:HA	1.63	0.46
1:C:124:GLN:HE22	1:C:131:SER:CB	2.21	0.46
3:F:80:CYS:O	3:F:83:LEU:HB2	2.16	0.46
2:B:124:VAL:HG21	2:B:200:VAL:HG21	1.98	0.46
3:E:17:LEU:CD1	3:E:92:VAL:HG13	2.44	0.46
1:A:142:LYS:HB2	1:A:173:TYR:CE2	2.51	0.46
2:B:50:GLU:CD	3:E:68:ARG:HH22	2.23	0.46
2:B:145:VAL:HG11	2:B:153:VAL:HG21	1.98	0.46
2:B:147:GLY:C	2:B:177:LEU:HD13	2.41	0.46
1:C:151:ASP:N	1:C:191:SER:O	2.46	0.45
2:D:12:MET:HB3	2:D:12:MET:HE3	1.60	0.45
3:E:10:ALA:CB	3:E:14:ARG:NH2	2.76	0.45
1:C:113:PRO:CB	1:C:139:PHE:HB3	2.36	0.45
2:D:91:SER:HA	2:D:112:LEU:O	2.17	0.45
2:D:138:MET:HG2	2:D:185:THR:CG2	2.44	0.45
2:D:151:GLU:OE2	2:D:171:ALA:HB3	2.17	0.45
1:A:21:LEU:O	1:A:72:THR:HA	2.16	0.45
1:A:30:SER:HG	1:A:31:ASN:H	1.60	0.45
3:F:121:GLN:OE1	3:F:125:ARG:NH1	2.49	0.45
3:E:8:LEU:O	3:E:9:ALA:C	2.60	0.45
1:A:134:CYS:HB2	1:A:148:TRP:CZ2	2.52	0.45
1:C:61:ARG:NH1	1:C:82:ASP:OD2	2.29	0.45
3:E:121:GLN:C	3:E:124:ILE:HG13	2.41	0.45
2:B:47:TRP:O	2:B:61:ASN:ND2	2.46	0.45
1:C:89:GLN:HG2	1:C:90:GLN:N	2.31	0.45
1:C:167:ASP:HB3	1:C:170:ASP:OD1	2.17	0.45
1:C:13:VAL:HG21	1:C:19:VAL:HG21	1.97	0.45
2:D:23:LYS:NZ	2:D:23:LYS:CB	2.76	0.45
3:E:8:LEU:HD12	3:E:38:PHE:CE1	2.52	0.45
3:F:114:ARG:HH11	3:F:114:ARG:HD2	1.68	0.45
3:E:3:PHE:CZ	3:E:88:ILE:CG2	3.00	0.45
3:E:111:TRP:HE3	3:E:112:ARG:HB2	1.82	0.45
3:F:99:VAL:HG13	3:F:108:TRP:HZ3	1.81	0.45
1:A:131:SER:OG	1:A:180:THR:HG23	2.17	0.45
1:C:125:LEU:C	1:C:127:SER:N	2.75	0.44
2:D:203:PRO:O	2:D:204:ALA:C	2.59	0.44
3:F:105:MET:C	3:F:107:ALA:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASP:HB3	1:A:170:ASP:OD1	2.17	0.44
1:C:119:PRO:HB3	1:C:209:PHE:CE1	2.52	0.44
3:E:48:ASP:OD1	3:E:50:SER:OG	2.33	0.44
2:B:122:PRO:HB3	2:B:148:TYR:HB3	1.99	0.44
2:D:139:VAL:HG22	2:D:141:LEU:HD12	1.98	0.44
2:D:166:VAL:HG12	2:D:184:VAL:HG23	1.99	0.44
1:A:119:PRO:HD2	2:B:216:ARG:HH21	1.79	0.44
1:C:61:ARG:HB2	1:C:76:ASN:O	2.17	0.44
2:D:23:LYS:HG3	4:D:1918:HOH:O	2.17	0.44
2:D:120:THR:HG21	2:D:177:LEU:CD1	2.47	0.44
2:D:148:TYR:O	2:D:149:PHE:HB2	2.18	0.44
2:D:193:SER:HB3	2:D:194:GLU:OE1	2.17	0.44
1:C:113:PRO:HB3	1:C:139:PHE:CB	2.37	0.44
1:C:132:VAL:HG12	1:C:148:TRP:CH2	2.52	0.44
1:C:160:LEU:HD11	2:D:174:GLN:OE1	2.16	0.44
1:C:193:THR:HG23	1:C:206:VAL:HG12	1.99	0.44
3:E:13:LYS:HD3	3:E:129:LEU:HB3	1.98	0.44
3:E:113:ASN:O	3:E:114:ARG:HG2	2.18	0.44
1:A:89:GLN:HA	1:A:97:THR:O	2.17	0.44
1:A:160:LEU:CD2	2:B:172:VAL:CG2	2.95	0.44
1:C:39:LYS:HE3	1:C:81:GLU:O	2.17	0.44
3:E:6:CYS:C	3:E:8:LEU:N	2.73	0.44
3:E:117:GLY:O	3:E:118:THR:C	2.59	0.44
1:A:109:ALA:N	4:A:1627:HOH:O	2.51	0.44
2:D:188:SER:O	2:D:191:ARG:O	2.35	0.44
3:E:19:ASN:HD22	3:E:19:ASN:HA	1.35	0.44
2:B:175:SER:O	2:B:176:ASP:HB2	2.18	0.44
1:C:118:PHE:CD2	2:D:127:LEU:CB	3.01	0.44
2:B:124:VAL:CG2	2:B:200:VAL:HG21	2.48	0.43
2:B:197:THR:CG2	2:B:210:ASP:HB3	2.48	0.43
2:D:4:LEU:HD22	2:D:22:CYS:SG	2.58	0.43
1:A:143:ASP:O	1:A:198:HIS:HD2	2.00	0.43
2:B:51:ILE:O	2:B:53:PRO:HD3	2.18	0.43
2:B:137:SER:C	2:B:188:SER:OG	2.61	0.43
1:C:47:LEU:CD2	1:C:58:ILE:HD12	2.46	0.43
1:C:96:ARG:HH11	1:C:96:ARG:HD2	1.59	0.43
1:C:151:ASP:CA	1:C:191:SER:OG	2.59	0.43
2:D:108:GLN:OE1	2:D:108:GLN:N	2.49	0.43
3:E:3:PHE:HE1	3:E:40:THR:CG2	2.31	0.43
1:C:23:CYS:HB2	1:C:35:TRP:CH2	2.54	0.43
2:D:120:THR:HG21	2:D:177:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:146:LYS:HZ3	2:D:174:GLN:HE21	1.65	0.43
3:E:20:TYR:O	3:E:23:TYR:CB	2.66	0.43
3:F:8:LEU:HD22	3:F:38:PHE:CD1	2.52	0.43
2:B:50:GLU:OE1	3:E:68:ARG:NH2	2.51	0.43
3:E:4:GLY:O	3:E:5:ARG:C	2.62	0.43
3:E:27:ASN:ND2	3:E:111:TRP:HE1	2.15	0.43
3:E:95:ALA:HA	3:E:98:ILE:HD12	1.99	0.43
2:B:132:ALA:O	2:B:133:ALA:HB3	2.19	0.43
1:C:189:HIS:O	1:C:211:ARG:HD3	2.19	0.43
1:A:195:GLU:HG2	1:A:206:VAL:CG2	2.22	0.43
1:C:186:TYR:CE1	1:C:192:TYR:CE2	3.06	0.43
1:C:6:GLN:OE1	1:C:87:PHE:HA	2.18	0.43
1:C:59:PRO:HG2	1:C:62:PHE:CD2	2.54	0.43
2:D:36:TRP:HA	2:D:95:TYR:O	2.18	0.43
2:B:33:TRP:CE3	2:B:50:GLU:HG3	2.54	0.43
2:D:40:ARG:HB2	4:D:1929:HOH:O	2.18	0.43
3:F:35:GLU:OE1	3:F:35:GLU:HA	2.19	0.42
2:D:88:SER:C	2:D:90:ASP:H	2.27	0.42
2:D:120:THR:O	2:D:148:TYR:HA	2.19	0.42
2:D:153:VAL:HG11	2:D:180:LEU:HD13	2.00	0.42
3:E:76:CYS:O	3:E:77:ASN:C	2.62	0.42
2:B:10:GLU:OE1	2:B:12:MET:HE3	2.19	0.42
1:C:159:VAL:HA	1:C:178:THR:O	2.20	0.42
2:D:2:VAL:HA	2:D:25:THR:O	2.19	0.42
1:A:136:LEU:HD21	1:A:196:ALA:HB2	2.00	0.42
1:C:12:SER:HB3	1:C:107:LYS:HB2	2.02	0.42
3:E:120:VAL:C	3:E:122:ALA:N	2.77	0.42
1:A:113:PRO:HB2	1:A:136:LEU:HB3	2.01	0.42
1:C:29:ILE:CD1	1:C:33:LEU:HD12	2.48	0.42
1:C:33:LEU:HD13	1:C:71:PHE:CD1	2.54	0.42
1:C:136:LEU:C	1:C:137:ASN:ND2	2.74	0.42
2:D:165:GLY:O	2:D:184:VAL:HA	2.19	0.42
3:F:62:TRP:O	3:F:75:LEU:HB2	2.20	0.42
1:A:121:SER:O	1:A:125:LEU:CD2	2.67	0.42
2:B:76:SER:O	2:B:77:ASN:HB2	2.19	0.42
1:C:29:ILE:HG21	1:C:29:ILE:HD13	1.80	0.42
2:D:120:THR:HG22	2:D:147:GLY:O	2.19	0.42
3:E:121:GLN:O	3:E:122:ALA:C	2.62	0.42
1:A:185:GLU:O	1:A:189:HIS:CD2	2.66	0.42
3:F:23:TYR:C	3:F:24:SER:O	2.62	0.42
1:A:136:LEU:CD2	1:A:196:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:GLY:O	2:D:177:LEU:HD13	2.19	0.42
3:E:27:ASN:N	3:E:120:VAL:HG21	2.35	0.42
3:E:106:ASN:O	3:E:112:ARG:NE	2.37	0.42
3:F:18:ASP:O	3:F:19:ASN:HB2	2.19	0.42
2:B:174:GLN:C	2:B:175:SER:OG	2.63	0.41
2:B:189:SER:HB2	2:B:190:PRO:HD3	2.01	0.41
1:C:150:ILE:HD11	1:C:192:TYR:HE1	1.83	0.41
2:D:40:ARG:HG3	2:D:92:ALA:HB2	2.02	0.41
2:B:149:PHE:HA	2:B:150:PRO:HA	1.85	0.41
1:C:5:THR:N	1:C:24:ARG:O	2.38	0.41
1:C:184:ASP:O	1:C:185:GLU:C	2.62	0.41
1:C:189:HIS:HB2	1:C:192:TYR:CZ	2.54	0.41
1:C:198:HIS:CD2	1:C:200:THR:H	2.38	0.41
2:D:124:VAL:HG21	2:D:209:VAL:HB	2.02	0.41
2:B:90:ASP:O	2:B:94:TYR:OH	2.29	0.41
2:B:133:ALA:O	2:B:134:GLN:C	2.63	0.41
1:A:2:ILE:C	1:A:3:GLU:OE1	2.63	0.41
1:C:187:GLU:C	1:C:211:ARG:HH12	2.27	0.41
1:C:61:ARG:CG	1:C:61:ARG:NH1	2.83	0.41
1:C:90:GLN:C	1:C:90:GLN:NE2	2.72	0.41
1:C:150:ILE:O	1:C:153:SER:N	2.54	0.41
1:C:188:ARG:O	1:C:188:ARG:HG3	2.20	0.41
3:F:127:CYS:HB2	3:F:129:LEU:HD13	2.02	0.41
1:A:2:ILE:CG1	1:A:27:GLN:NE2	2.83	0.41
2:B:191:ARG:HE	2:B:191:ARG:HB3	1.40	0.41
3:E:12:MET:HE2	3:E:17:LEU:CD1	2.51	0.41
2:B:73:ASP:O	2:B:77:ASN:N	2.53	0.41
2:B:214:VAL:HA	2:B:215:PRO:HD3	1.90	0.41
1:C:29:ILE:O	1:C:30:SER:CB	2.67	0.41
3:F:40:THR:O	3:F:54:GLY:HA2	2.21	0.41
1:A:89:GLN:HB2	1:A:98:PHE:CD1	2.56	0.41
2:B:129:PRO:HD3	2:B:141:LEU:HD12	2.02	0.41
1:C:11:LEU:HA	1:C:11:LEU:HD12	1.82	0.41
1:C:13:VAL:CG2	1:C:19:VAL:HG21	2.51	0.41
2:D:186:VAL:HG23	2:D:187:PRO:O	2.20	0.41
3:E:108:TRP:O	3:E:110:ALA:N	2.52	0.41
1:A:13:VAL:HG13	1:A:83:PHE:HE1	1.85	0.41
1:A:94:TRP:CE3	3:E:45:ARG:HB3	2.55	0.41
1:A:186:TYR:CZ	1:A:211:ARG:HD3	2.56	0.41
2:B:157:TRP:HA	2:B:197:THR:O	2.21	0.41
1:C:14:THR:O	1:C:15:PRO:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LYS:HA	1:C:153:SER:O	2.21	0.41
2:D:10:GLU:HB3	2:D:112:LEU:CD1	2.50	0.41
1:A:7:SER:HA	1:A:8:PRO:HA	1.83	0.40
2:B:120:THR:HA	2:B:121:PRO:HD3	1.80	0.40
1:C:77:SER:O	1:C:78:VAL:C	2.63	0.40
1:C:118:PHE:HA	1:C:119:PRO:HD3	1.79	0.40
1:C:123:GLU:O	1:C:126:THR:OG1	2.28	0.40
1:C:161:ASN:HD22	1:C:177:SER:HA	1.86	0.40
2:D:42:GLY:C	2:D:43:HIS:ND1	2.79	0.40
3:F:121:GLN:O	3:F:122:ALA:C	2.64	0.40
1:A:83:PHE:CD2	1:A:106:ILE:HG13	2.55	0.40
1:A:213:GLU:HG3	1:A:214:CYS:N	2.37	0.40
1:C:121:SER:HB2	2:D:125:PHE:HB3	2.03	0.40
3:F:19:ASN:N	3:F:23:TYR:O	2.54	0.40
3:F:80:CYS:C	3:F:82:ALA:N	2.79	0.40
3:F:87:ASP:HA	4:F:2112:HOH:O	2.22	0.40
1:C:155:ARG:HD3	1:C:157:ASN:O	2.22	0.40
1:C:198:HIS:HD2	1:C:200:THR:OG1	2.04	0.40
2:D:77:ASN:H	2:D:77:ASN:HD22	1.70	0.40
2:D:23:LYS:HG2	2:D:78:THR:OG1	2.21	0.40
2:D:128:ALA:O	2:D:129:PRO:C	2.64	0.40
2:D:138:MET:HA	2:D:186:VAL:O	2.22	0.40
2:D:154:THR:O	2:D:200:VAL:HA	2.21	0.40
2:D:213:ILE:O	2:D:215:PRO:HD3	2.22	0.40
3:E:1:LYS:HD2	3:E:2:VAL:N	2.37	0.40
3:E:6:CYS:O	3:E:7:GLU:C	2.65	0.40
2:B:32:TYR:CE1	3:E:67:GLY:HA3	2.57	0.40
1:C:124:GLN:OE1	1:C:130:ALA:HA	2.22	0.40
1:C:150:ILE:O	1:C:152:GLY:N	2.54	0.40
3:F:53:TYR:OH	3:F:66:ASP:OD2	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	212/214 (99%)	199 (94%)	7 (3%)	6 (3%)	4	6
1	C	212/214 (99%)	180 (85%)	26 (12%)	6 (3%)	4	6
2	B	216/218 (99%)	194 (90%)	19 (9%)	3 (1%)	9	17
2	D	216/218 (99%)	175 (81%)	30 (14%)	11 (5%)	1	2
3	E	127/129 (98%)	99 (78%)	18 (14%)	10 (8%)	1	0
3	F	127/129 (98%)	111 (87%)	14 (11%)	2 (2%)	7	14
All	All	1110/1122 (99%)	958 (86%)	114 (10%)	38 (3%)	3	4

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
2	B	134	GLN
1	C	67	SER
1	C	213	GLU
2	D	160	GLY
2	D	162	LEU
2	D	164	SER
3	E	88	ILE
3	E	100	SER
3	E	113	ASN
3	F	118	THR
1	A	51	VAL
1	A	60	SER
1	A	67	SER
2	B	190	PRO
2	B	204	ALA
1	C	151	ASP
2	D	130	GLY
2	D	159	SER
2	D	216	ARG
3	E	9	ALA
3	E	109	VAL
1	C	120	PRO
2	D	129	PRO
2	D	131	SER
2	D	133	ALA
2	D	206	SER

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Mol	Chain	Res	Type
3	F	77	ASN
1	A	77	SER
1	C	28	SER
3	E	54	GLY
3	E	77	ASN
3	E	101	ASP
3	E	120	VAL
1	C	193	THR
3	E	35	GLU
1	A	152	GLY
2	D	126	PRO

5.3.2 Protein sidechains [i](#)

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	194/194 (100%)	160 (82%)	34 (18%)	2	3
1	C	194/194 (100%)	160 (82%)	34 (18%)	2	3
2	B	184/184 (100%)	158 (86%)	26 (14%)	3	7
2	D	184/184 (100%)	147 (80%)	37 (20%)	1	2
3	E	105/105 (100%)	83 (79%)	22 (21%)	1	2
3	F	105/105 (100%)	96 (91%)	9 (9%)	10	21
All	All	966/966 (100%)	804 (83%)	162 (17%)	2	4

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	3	GLU
1	A	4	LEU
1	A	7	SER
1	A	10	THR
1	A	13	VAL
1	A	21	LEU

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Mol	Chain	Res	Type
1	A	22	SER
1	A	33	LEU
1	A	42	GLU
1	A	46	LEU
1	A	55	SER
1	A	63	SER
1	A	69	THR
1	A	89	GLN
1	A	93	SER
1	A	103	LYS
1	A	105	GLU
1	A	108	ARG
1	A	123	GLU
1	A	125	LEU
1	A	136	LEU
1	A	143	ASP
1	A	147	LYS
1	A	154	GLU
1	A	156	GLN
1	A	160	LEU
1	A	168	SER
1	A	177	SER
1	A	180	THR
1	A	183	LYS
1	A	197	THR
1	A	202	THR
1	A	205	ILE
2	B	4	LEU
2	B	5	GLN
2	B	23	LYS
2	B	34	ILE
2	B	63	LYS
2	B	67	LYS
2	B	69	THR
2	B	74	THR
2	B	75	SER
2	B	77	ASN
2	B	88	SER
2	B	116	SER
2	B	135	THR
2	B	141	LEU
2	B	143	CYS

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Mol	Chain	Res	Type
2	B	152	PRO
2	B	154	THR
2	B	175	SER
2	B	188	SER
2	B	189	SER
2	B	190	PRO
2	B	191	ARG
2	B	193	SER
2	B	198	CYS
2	B	211	LYS
2	B	217	ASP
1	C	1	ASP
1	C	2	ILE
1	C	4	LEU
1	C	5	THR
1	C	20	SER
1	C	31	ASN
1	C	40	SER
1	C	43	SER
1	C	46	LEU
1	C	55	SER
1	C	61	ARG
1	C	67	SER
1	C	75	ILE
1	C	90	GLN
1	C	96	ARG
1	C	103	LYS
1	C	105	GLU
1	C	114	THR
1	C	118	PHE
1	C	126	THR
1	C	131	SER
1	C	147	LYS
1	C	157	ASN
1	C	165	ASP
1	C	169	LYS
1	C	175	MET
1	C	177	SER
1	C	182	THR
1	C	183	LYS
1	C	185	GLU
1	C	188	ARG

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Mol	Chain	Res	Type
1	C	202	THR
1	C	206	VAL
1	C	212	ASN
2	D	1	GLN
2	D	5	GLN
2	D	10	GLU
2	D	13	LYS
2	D	17	SER
2	D	23	LYS
2	D	25	THR
2	D	43	HIS
2	D	52	LEU
2	D	57	SER
2	D	63	LYS
2	D	67	LYS
2	D	75	SER
2	D	81	MET
2	D	89	GLU
2	D	118	SER
2	D	119	THR
2	D	138	MET
2	D	141	LEU
2	D	143	CYS
2	D	144	LEU
2	D	152	PRO
2	D	164	SER
2	D	172	VAL
2	D	175	SER
2	D	180	LEU
2	D	181	SER
2	D	183	SER
2	D	189	SER
2	D	191	ARG
2	D	197	THR
2	D	199	ASN
2	D	206	SER
2	D	212	LYS
2	D	213	ILE
2	D	216	ARG
2	D	218	CYS
3	E	2	VAL
3	E	8	LEU

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Mol	Chain	Res	Type
3	E	21	ARG
3	E	24	SER
3	E	25	LEU
3	E	44	ASN
3	E	46	ASN
3	E	60	SER
3	E	65	ASN
3	E	68	ARG
3	E	78	ILE
3	E	84	LEU
3	E	93	ASN
3	E	99	VAL
3	E	101	ASP
3	E	106	ASN
3	E	113	ASN
3	E	115	CYS
3	E	116	LYS
3	E	120	VAL
3	E	121	GLN
3	E	124	ILE
3	F	24	SER
3	F	25	LEU
3	F	33	LYS
3	F	44	ASN
3	F	68	ARG
3	F	99	VAL
3	F	112	ARG
3	F	128	ARG
3	F	129	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	32	ASN
1	A	53	GLN
1	A	145	ASN
1	A	189	HIS
1	A	210	ASN
2	B	43	HIS
2	B	77	ASN
2	B	134	GLN

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Mol	Chain	Res	Type
1	C	32	ASN
1	C	53	GLN
1	C	76	ASN
1	C	92	ASN
1	C	137	ASN
1	C	145	ASN
1	C	157	ASN
1	C	161	ASN
1	C	198	HIS
1	C	210	ASN
2	D	77	ASN
2	D	174	GLN
3	E	19	ASN
3	E	27	ASN
3	E	57	GLN
3	E	106	ASN
3	E	113	ASN
3	F	41	GLN
3	F	46	ASN
3	F	93	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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.