



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:53 AM UTC

PDB ID : 1AHW / pdb_00001ahw
Title : A COMPLEX OF EXTRACELLULAR DOMAIN OF TISSUE FACTOR
WITH AN INHIBITORY FAB (5G9)
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Deposited on : 1997-04-10
Resolution : 3.00 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

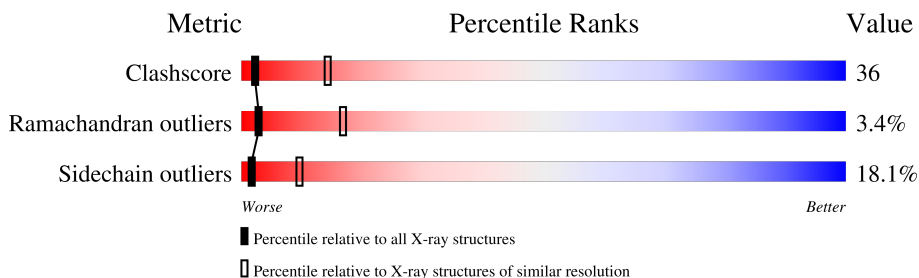
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	35% 43% 20% .
1	D	214	34% 43% 21% .
2	B	214	36% 45% 17% .
2	E	214	40% 45% 14%
3	C	219	32% 42% 16% . 9%
3	F	219	33% 44% 13% . 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9830 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 IMMUNOGLOBULIN FAB 5G9 (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1672	1040	278	346	8			
1	D	214	Total	C	N	O	S	0	0	0
			1672	1040	278	346	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ARG	TYR	conflict	UNP P01837
A	31	LYS	SER	conflict	UNP P01837
A	34	ASN	SER	conflict	UNP P01837
A	36	TYR	PHE	conflict	UNP P01837
A	41	TRP	GLY	conflict	UNP P01837
A	50	TYR	ARG	conflict	UNP P01837
A	52	THR	ASN	conflict	UNP P01837
A	53	SER	ARG	conflict	UNP P01837
A	55	ALA	VAL	conflict	UNP P01837
A	80	SER	TYR	conflict	UNP P01837
A	81	ASP	GLU	conflict	UNP P01837
A	83	THR	LEU	conflict	UNP P01837
A	84	ALA	GLY	conflict	UNP P01837
A	85	THR	ILE	conflict	UNP P01837
A	91	HIS	PHE	conflict	UNP P01837
A	92	GLY	ASP	conflict	UNP P01837
A	94	SER	PHE	conflict	UNP P01837
A	107	ASN	LYS	conflict	UNP P01837
D	30	ARG	TYR	conflict	UNP P01837
D	31	LYS	SER	conflict	UNP P01837
D	34	ASN	SER	conflict	UNP P01837
D	36	TYR	PHE	conflict	UNP P01837
D	41	TRP	GLY	conflict	UNP P01837
D	50	TYR	ARG	conflict	UNP P01837
D	52	THR	ASN	conflict	UNP P01837

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Chain	Residue	Modelled	Actual	Comment	Reference
D	53	SER	ARG	conflict	UNP P01837
D	55	ALA	VAL	conflict	UNP P01837
D	80	SER	TYR	conflict	UNP P01837
D	81	ASP	GLU	conflict	UNP P01837
D	83	THR	LEU	conflict	UNP P01837
D	84	ALA	GLY	conflict	UNP P01837
D	85	THR	ILE	conflict	UNP P01837
D	91	HIS	PHE	conflict	UNP P01837
D	92	GLY	ASP	conflict	UNP P01837
D	94	SER	PHE	conflict	UNP P01837
D	107	ASN	LYS	conflict	UNP P01837

- Molecule 2 is a protein called IMMUNOGLOBULIN FAB 5G9 (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1632	1034	263	329	6			
2	E	214	Total	C	N	O	S	0	0	0
			1632	1034	263	329	6			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLU	-	insertion	PIR S49220
B	2	ILE	-	insertion	PIR S49220
B	?	-	VAL	deletion	PIR S49220
B	?	-	LYS	deletion	PIR S49220
B	5	GLN	LEU	conflict	PIR S49220
B	6	GLN	GLU	conflict	PIR S49220
B	13	ARG	LYS	conflict	PIR S49220
B	14	PRO	SER	conflict	PIR S49220
B	17	LEU	SER	conflict	PIR S49220
B	23	LYS	THR	conflict	PIR S49220
B	32	TYR	THR	conflict	PIR S49220
B	50	LEU	ARG	conflict	PIR S49220
B	54	GLU	ALA	conflict	PIR S49220
B	57	ASN	GLU	conflict	PIR S49220
B	58	THR	ILE	conflict	PIR S49220
B	59	ILE	LYS	conflict	PIR S49220
B	67	LYS	THR	conflict	PIR S49220
B	69	SER	THR	conflict	PIR S49220
B	76	SER	THR	conflict	PIR S49220

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Chain	Residue	Modelled	Actual	Comment	Reference
B	97	ALA	VAL	conflict	PIR S49220
B	?	-	ARG	deletion	PIR S49220
B	?	-	GLY	deletion	PIR S49220
B	99	ASP	TYR	conflict	PIR S49220
B	100	ASN	GLY	conflict	PIR S49220
B	102	TYR	SER	conflict	PIR S49220
B	103	TYR	GLN	conflict	PIR S49220
B	104	PHE	GLU	conflict	PIR S49220
B	105	ASP	PRO	conflict	PIR S49220
E	1	GLU	-	insertion	PIR S49220
E	2	ILE	-	insertion	PIR S49220
E	?	-	VAL	deletion	PIR S49220
E	?	-	LYS	deletion	PIR S49220
E	5	GLN	LEU	conflict	PIR S49220
E	6	GLN	GLU	conflict	PIR S49220
E	13	ARG	LYS	conflict	PIR S49220
E	14	PRO	SER	conflict	PIR S49220
E	17	LEU	SER	conflict	PIR S49220
E	23	LYS	THR	conflict	PIR S49220
E	32	TYR	THR	conflict	PIR S49220
E	50	LEU	ARG	conflict	PIR S49220
E	54	GLU	ALA	conflict	PIR S49220
E	57	ASN	GLU	conflict	PIR S49220
E	58	THR	ILE	conflict	PIR S49220
E	59	ILE	LYS	conflict	PIR S49220
E	67	LYS	THR	conflict	PIR S49220
E	69	SER	THR	conflict	PIR S49220
E	76	SER	THR	conflict	PIR S49220
E	97	ALA	VAL	conflict	PIR S49220
E	?	-	ARG	deletion	PIR S49220
E	?	-	GLY	deletion	PIR S49220
E	99	ASP	TYR	conflict	PIR S49220
E	100	ASN	GLY	conflict	PIR S49220
E	102	TYR	SER	conflict	PIR S49220
E	103	TYR	GLN	conflict	PIR S49220
E	104	PHE	GLU	conflict	PIR S49220
E	105	ASP	PRO	conflict	PIR S49220

- Molecule 3 is a protein called TISSUE FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	200	Total	C	N	O	S	0	0	0
			1611	1021	262	323	5			

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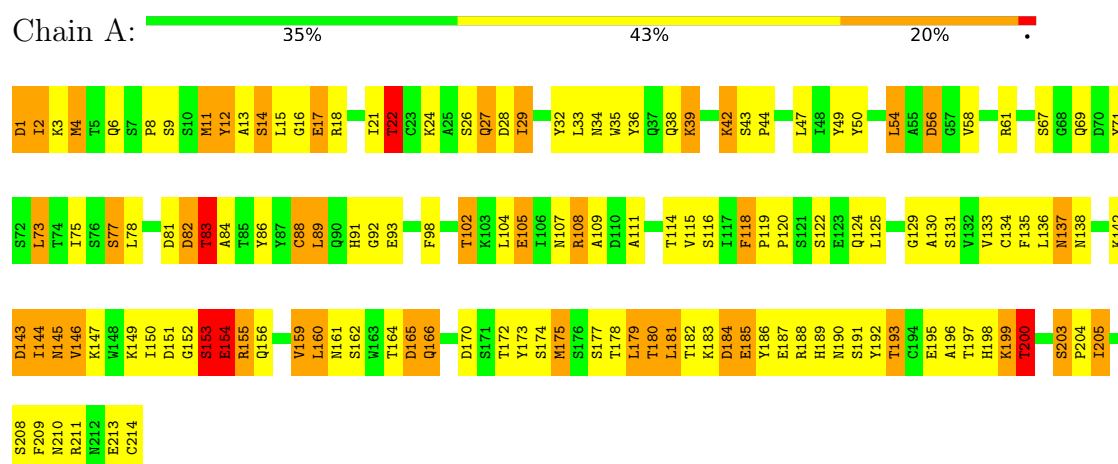
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	200	Total	C	N	O	S	0	0	0
			1611	1021	262	323	5			

3 Residue-property plots

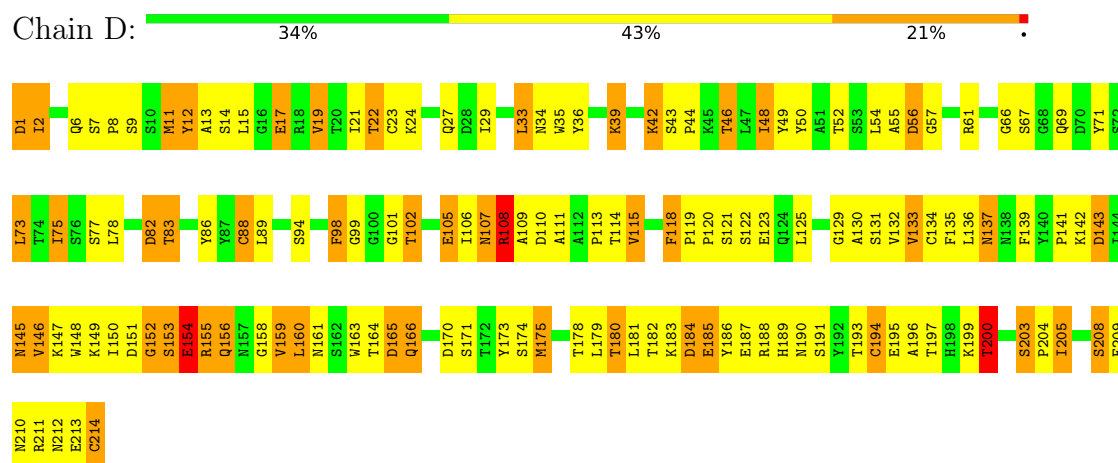
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: IMMUNOGLOBULIN FAB 5G9 (LIGHT CHAIN)



• Molecule 1: IMMUNOGLOBULIN FAB 5G9 (LIGHT CHAIN)



• Molecule 2: IMMUNOGLOBULIN FAB 5G9 (HEAVY CHAIN)





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.30Å 73.31Å 115.83Å 90.00° 90.89° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00	Depositor
% Data completeness (in resolution range)	78.1 (7.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.217 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9830	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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	1.07	1/1711 (0.1%)	1.39	23/2321 (1.0%)
1	D	1.01	2/1711 (0.1%)	1.34	21/2321 (0.9%)
2	B	1.10	3/1675 (0.2%)	1.46	30/2292 (1.3%)
2	E	0.94	1/1675 (0.1%)	1.37	20/2292 (0.9%)
3	C	0.97	2/1646 (0.1%)	1.31	26/2239 (1.2%)
3	F	0.85	0/1646	1.27	15/2239 (0.7%)
All	All	0.99	9/10064 (0.1%)	1.36	135/13704 (1.0%)

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
2	E	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	115	VAL	CA-CB	6.42	1.61	1.54
3	C	123	VAL	CA-CB	6.11	1.60	1.53
3	C	193	ILE	CA-C	5.99	1.57	1.53
2	E	39	GLN	CA-C	5.63	1.59	1.53
1	D	46	THR	CA-CB	5.34	1.59	1.52
2	B	169	THR	CA-CB	-5.33	1.45	1.53
1	A	4	MET	SD-CE	-5.32	1.66	1.79
2	B	37	VAL	C-O	-5.17	1.18	1.24
1	D	114	THR	CA-CB	5.03	1.59	1.53

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	GLN	N-CA-C	11.23	123.06	108.34
1	D	158	GLY	N-CA-C	-10.15	99.53	115.67
1	A	200	THR	N-CA-C	-9.42	101.92	113.50
2	E	213	LYS	N-CA-C	-9.23	94.20	109.24
2	B	203	HIS	CA-C-N	8.93	129.50	119.32
2	B	203	HIS	C-N-CA	8.93	129.50	119.32
2	E	147	LYS	N-CA-C	8.83	123.80	109.85
1	D	200	THR	N-CA-C	-8.73	102.07	112.89
2	E	138	SER	N-CA-C	-8.68	101.30	112.23
2	B	109	GLN	N-CA-C	-8.42	99.75	110.19
1	D	156	GLN	N-CA-C	8.36	119.27	108.24
1	A	138	ASN	N-CA-C	8.16	122.64	111.39
3	C	193	ILE	N-CA-C	-8.15	100.14	107.56
2	B	86	LEU	N-CA-C	8.12	122.20	110.10
2	E	86	LEU	N-CA-C	8.00	122.31	110.30
2	B	96	CYS	N-CA-C	-7.99	96.38	109.40
1	D	54	LEU	N-CA-C	-7.92	98.75	110.48
3	F	43	GLY	N-CA-C	7.86	123.81	111.08
2	B	170	PHE	CA-C-N	7.78	127.79	119.78
2	B	170	PHE	C-N-CA	7.78	127.79	119.78
2	E	103	TYR	N-CA-C	7.72	119.87	108.14
3	F	200	ARG	N-CA-C	7.65	119.70	111.36
2	E	117	SER	N-CA-C	-7.57	103.11	113.18
1	A	83	THR	N-CA-C	-7.33	98.60	109.15
1	D	98	PHE	N-CA-C	-7.30	98.71	110.32
3	C	50	PHE	N-CA-C	7.25	120.90	110.10
1	A	32	TYR	N-CA-C	-7.20	101.58	110.65
1	A	43	SER	N-CA-C	-7.20	99.84	110.20
1	D	43	SER	N-CA-C	-7.17	100.18	110.08
1	D	52	THR	N-CA-C	7.09	122.93	112.94
1	A	39	LYS	N-CA-C	-7.09	99.89	110.24
2	B	55	ASN	N-CA-C	-7.06	99.08	109.11
3	C	162	SER	N-CA-C	7.02	120.06	109.95
2	B	138	SER	N-CA-C	-7.01	102.85	111.40
2	B	108	GLY	N-CA-C	-7.00	103.58	112.54
3	F	165	LYS	N-CA-C	6.91	120.80	109.94
2	E	109	GLN	CA-C-N	-6.91	114.12	121.45
2	E	109	GLN	C-N-CA	-6.91	114.12	121.45
1	A	82	ASP	N-CA-C	-6.90	103.26	113.61
3	F	198	VAL	N-CA-C	6.81	123.50	109.34
3	C	101	THR	CA-C-N	6.72	128.24	119.84
3	C	101	THR	C-N-CA	6.72	128.24	119.84
1	D	82	ASP	N-CA-C	-6.66	105.72	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	LYS	N-CA-C	6.64	120.69	110.20
2	B	213	LYS	N-CA-C	-6.63	98.39	109.07
3	C	60	THR	N-CA-C	6.62	119.05	111.11
2	B	167	VAL	N-CA-C	6.55	118.59	109.55
3	C	43	GLY	N-CA-C	6.55	120.68	111.19
3	C	143	LEU	N-CA-C	-6.51	104.10	111.07
3	F	28	LYS	N-CA-C	-6.49	100.82	109.84
3	F	50	PHE	N-CA-C	6.44	119.10	109.25
3	C	16	SER	N-CA-C	6.39	118.12	108.46
2	B	201	VAL	N-CA-C	6.38	117.30	107.99
2	B	105	ASP	N-CA-C	6.36	119.96	112.72
1	A	88	CYS	N-CA-C	-6.28	99.47	109.59
1	A	114	THR	N-CA-C	-6.28	98.49	108.73
2	B	56	GLY	N-CA-C	6.27	128.04	113.18
1	A	54	LEU	N-CA-C	-6.27	101.21	110.48
1	D	99	GLY	N-CA-C	-6.25	102.54	112.66
2	B	61	ASP	N-CA-C	-6.21	101.94	109.83
2	E	203	HIS	CA-C-N	6.21	126.67	119.47
2	E	203	HIS	C-N-CA	6.21	126.67	119.47
3	C	6	THR	N-CA-C	-6.21	97.69	107.93
2	E	181	LEU	N-CA-C	-6.19	101.03	109.95
3	F	12	LEU	N-CA-C	-6.18	99.13	108.96
2	E	108	GLY	N-CA-C	-6.12	102.03	111.64
1	D	75	ILE	N-CA-C	-6.11	99.79	108.58
1	D	108	ARG	N-CA-C	6.11	117.51	108.60
2	B	147	LYS	N-CA-C	6.08	118.65	109.23
1	A	137	ASN	N-CA-C	6.07	118.74	110.55
1	D	88	CYS	N-CA-C	-6.07	99.82	109.59
2	B	181	LEU	N-CA-C	-6.06	101.23	109.95
3	C	192	VAL	CA-C-N	-6.04	118.50	122.60
3	C	192	VAL	C-N-CA	-6.04	118.50	122.60
1	A	118	PHE	CA-C-N	5.95	126.51	120.38
1	A	118	PHE	C-N-CA	5.95	126.51	120.38
3	C	21	THR	N-CA-C	5.88	118.83	109.24
1	A	22	THR	N-CA-C	5.86	118.76	109.50
3	F	125	VAL	CB-CA-C	-5.83	103.68	110.91
3	C	165	LYS	N-CA-C	5.83	118.88	109.79
3	F	98	PRO	N-CA-C	-5.82	102.73	111.57
2	B	159	ASN	N-CA-C	-5.80	103.40	111.52
3	F	137	ASN	CB-CA-C	-5.80	108.24	115.89
1	D	208	SER	N-CA-C	5.78	118.48	109.52
2	B	84	SER	N-CA-C	5.75	116.99	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	61	ASP	N-CA-C	-5.73	101.08	109.50
1	D	137	ASN	N-CA-C	5.71	118.98	110.52
3	F	201	LYS	N-CA-C	5.69	118.76	110.17
2	B	5	GLN	N-CA-C	5.69	118.75	109.59
2	B	43	GLN	N-CA-C	5.63	117.74	109.24
1	D	203	SER	CA-C-N	5.63	126.88	119.84
1	D	203	SER	C-N-CA	5.63	126.88	119.84
3	C	172	THR	N-CA-C	-5.56	98.96	110.80
2	E	165	SER	N-CA-C	5.55	122.63	110.80
3	C	28	LYS	N-CA-C	-5.54	102.60	109.64
1	D	115	VAL	N-CA-C	5.54	117.88	109.12
2	B	109	GLN	CA-C-N	-5.53	113.66	121.13
2	B	109	GLN	C-N-CA	-5.53	113.66	121.13
3	C	195	SER	N-CA-C	5.52	118.06	111.71
2	B	158	TRP	N-CA-C	5.52	117.51	108.52
1	A	180	THR	N-CA-C	5.51	118.18	107.71
2	B	117	SER	N-CA-C	-5.50	107.12	113.88
1	D	39	LYS	N-CA-C	-5.49	102.51	110.08
1	D	52	THR	CB-CA-C	-5.46	101.25	110.64
2	E	96	CYS	N-CA-C	-5.45	100.52	109.40
2	E	140	VAL	N-CA-C	5.42	117.61	109.20
2	B	40	ARG	CA-C-N	5.41	126.61	119.84
2	B	40	ARG	C-N-CA	5.41	126.61	119.84
2	E	164	SER	N-CA-C	5.41	119.87	112.68
3	C	78	TYR	CA-C-N	5.39	125.56	119.90
3	C	78	TYR	C-N-CA	5.39	125.56	119.90
2	B	118	ALA	N-CA-C	-5.36	102.85	110.35
3	F	16	SER	N-CA-C	5.35	117.90	108.75
3	C	7	VAL	CB-CA-C	-5.29	104.33	111.63
2	B	141	THR	CB-CA-C	-5.28	102.19	110.79
3	F	172	THR	N-CA-C	-5.27	99.57	110.80
3	F	147	PHE	N-CA-C	5.26	118.16	111.69
3	C	156	TYR	N-CA-C	-5.25	100.68	109.24
2	E	119	LYS	N-CA-C	5.24	118.64	110.32
1	A	179	LEU	N-CA-C	-5.18	101.26	109.76
3	C	110	GLN	CA-C-N	5.17	125.17	120.21
3	C	110	GLN	C-N-CA	5.17	125.17	120.21
1	D	118	PHE	CA-C-O	5.17	123.62	119.59
1	A	203	SER	CA-C-N	5.15	126.28	119.84
1	A	203	SER	C-N-CA	5.15	126.28	119.84
2	E	167	VAL	N-CA-C	5.14	116.37	108.71
1	A	21	ILE	N-CA-C	-5.12	101.04	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	180	THR	N-CA-C	5.11	117.43	107.71
3	C	35	THR	N-CA-C	-5.10	100.72	109.24
1	A	193	THR	N-CA-C	5.09	117.46	108.75
3	F	106	THR	N-CA-C	-5.09	102.32	109.96
2	E	129	ALA	N-CA-C	-5.05	103.83	110.39
1	A	73	LEU	N-CA-C	-5.04	101.47	109.59
3	C	53	THR	N-CA-C	-5.03	105.95	113.89
3	C	178	ASP	N-CA-C	-5.02	103.90	110.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	TYR	Sidechain
2	E	94	TYR	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	1672	0	1590	128	0
1	D	1672	0	1590	139	0
2	B	1632	0	1580	110	0
2	E	1632	0	1580	114	0
3	C	1611	0	1564	113	0
3	F	1611	0	1564	133	0
All	All	9830	0	9468	702	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 36.

All (702) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:THR:HG23	2:E:114:THR:HA	1.35	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:136:ARG:HB3	3:F:141:LEU:HD11	1.35	1.05
1:D:6:GLN:HE21	1:D:102:THR:HG23	1.29	0.94
1:D:196:ALA:HB3	1:D:205:ILE:HB	1.51	0.92
2:E:4:LEU:HD23	2:E:22:CYS:SG	2.11	0.90
1:D:34:ASN:HD22	1:D:49:TYR:HA	1.39	0.87
1:D:149:LYS:HG2	1:D:155:ARG:HB3	1.56	0.87
1:D:147:LYS:HB2	1:D:195:GLU:HB2	1.56	0.87
3:F:136:ARG:HD2	3:F:141:LEU:HD21	1.55	0.86
1:D:6:GLN:NE2	1:D:102:THR:HG23	1.93	0.83
3:C:135:ARG:NH2	3:C:138:ASN:HA	1.94	0.83
3:C:13:THR:HG21	3:C:15:LYS:HE2	1.60	0.81
3:F:11:ASN:HB2	3:F:26:GLU:HG3	1.62	0.81
1:A:8:PRO:O	1:A:102:THR:HB	1.81	0.81
1:D:149:LYS:HA	1:D:155:ARG:HA	1.61	0.80
3:F:183:GLU:HB2	3:F:185:TYR:HE1	1.46	0.80
2:E:60:TYR:OH	2:E:69:SER:HA	1.82	0.80
1:D:136:LEU:HD11	1:D:146:VAL:HG21	1.64	0.79
3:F:33:VAL:HG12	3:F:53:THR:HG23	1.65	0.79
2:B:142:LEU:HD22	2:B:214:ILE:HD12	1.64	0.78
1:D:193:THR:HB	1:D:208:SER:CB	2.13	0.78
1:D:34:ASN:ND2	1:D:49:TYR:HA	1.97	0.78
3:C:149:LYS:HG3	3:C:171:ASN:HD22	1.48	0.78
3:C:136:ARG:HB3	3:C:141:LEU:HD21	1.64	0.77
1:A:29:ILE:HD11	1:A:71:TYR:CE2	2.19	0.77
1:D:188:ARG:HB3	1:D:189:HIS:CD2	2.19	0.77
1:A:147:LYS:HD3	1:A:155:ARG:HH12	1.49	0.77
2:E:86:LEU:HD13	2:E:115:VAL:HG22	1.67	0.76
3:F:152:ILE:HD13	3:F:171:ASN:HB3	1.66	0.76
2:B:4:LEU:HD23	2:B:22:CYS:SG	2.25	0.76
1:D:111:ALA:C	1:D:200:THR:HG21	2.10	0.76
1:D:187:GLU:HA	1:D:211:ARG:CZ	2.16	0.75
1:D:150:ILE:HD12	1:D:156:GLN:OE1	1.87	0.75
2:E:35:HIS:CD2	2:E:99:ASP:HB2	2.22	0.75
1:A:193:THR:HB	1:A:208:SER:HB2	1.68	0.74
3:F:149:LYS:HG3	3:F:171:ASN:HD22	1.52	0.74
1:D:150:ILE:HD13	1:D:181:LEU:HD21	1.68	0.74
3:F:8:ALA:HB2	3:F:93:LEU:HD12	1.69	0.74
1:A:129:GLY:HA2	1:A:182:THR:HA	1.67	0.74
3:F:57:CYS:SG	3:F:59:LEU:HD21	2.27	0.74
3:F:10:TYR:O	3:F:26:GLU:HB2	1.86	0.74
1:D:193:THR:HB	1:D:208:SER:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LYS:O	1:A:187:GLU:HG3	1.89	0.73
1:D:75:ILE:HG21	1:D:78:LEU:HD12	1.69	0.73
1:D:190:ASN:O	1:D:210:ASN:HA	1.89	0.73
3:C:194:PRO:HA	3:C:200:ARG:NH2	2.04	0.73
1:A:33:LEU:HD22	1:A:71:TYR:CG	2.24	0.72
2:B:145:LEU:HD21	2:B:147:LYS:HD2	1.71	0.72
3:F:32:GLN:HB2	3:F:78:TYR:O	1.90	0.71
1:A:181:LEU:HG	1:A:185:GLU:HG2	1.70	0.71
2:B:4:LEU:HD21	2:B:34:MET:HE1	1.73	0.71
1:A:108:ARG:HG2	1:A:109:ALA:N	2.06	0.70
1:D:185:GLU:O	1:D:189:HIS:HD2	1.73	0.70
1:D:24:LYS:HA	1:D:69:GLN:O	1.91	0.70
1:A:150:ILE:HD13	1:A:181:LEU:HD21	1.73	0.70
1:A:188:ARG:HB3	1:A:189:HIS:CD2	2.26	0.70
1:D:6:GLN:HB2	1:D:23:CYS:SG	2.32	0.70
2:B:29:ILE:H	2:B:77:ASN:HD21	1.39	0.70
3:F:11:ASN:O	3:F:25:TRP:HA	1.92	0.70
1:D:39:LYS:O	1:D:42:LYS:HB2	1.92	0.70
3:C:149:LYS:HB2	3:C:149:LYS:NZ	2.07	0.69
3:C:38:ILE:HD12	3:C:59:LEU:HD13	1.72	0.69
3:C:135:ARG:CZ	3:C:138:ASN:HA	2.22	0.69
3:F:141:LEU:HB3	3:F:145:ASP:HB2	1.72	0.69
1:A:115:VAL:O	2:B:136:THR:HG21	1.92	0.69
1:A:150:ILE:CD1	1:A:181:LEU:HD21	2.21	0.69
1:A:39:LYS:O	1:A:42:LYS:HB2	1.93	0.69
2:E:6:GLN:HE21	2:E:108:GLY:HA3	1.56	0.68
3:F:78:TYR:HE1	3:F:92:PRO:HG3	1.59	0.68
1:A:160:LEU:HG	2:B:173:VAL:HG11	1.74	0.68
1:A:149:LYS:HG2	1:A:155:ARG:HB3	1.75	0.68
3:F:93:LEU:HD23	3:F:93:LEU:H	1.59	0.67
3:F:167:THR:HG22	3:F:168:ALA:H	1.58	0.67
3:F:37:GLN:HG2	3:F:45:TRP:HB3	1.77	0.67
3:C:180:ASP:HB2	3:C:183:GLU:HG3	1.76	0.67
1:D:14:SER:O	1:D:17:GLU:HB2	1.94	0.67
1:D:136:LEU:CD1	1:D:146:VAL:HG21	2.23	0.67
1:A:185:GLU:O	1:A:189:HIS:HD2	1.78	0.67
2:B:142:LEU:HD13	2:B:214:ILE:HD11	1.77	0.67
1:D:108:ARG:HG3	1:D:108:ARG:HH11	1.59	0.67
2:E:181:LEU:HD23	2:E:182:SER:N	2.10	0.66
2:B:199:CYS:O	2:B:199:CYS:SG	2.52	0.66
3:C:149:LYS:HG3	3:C:171:ASN:ND2	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:THR:HG21	1:D:166:GLN:HB3	1.76	0.66
1:A:6:GLN:HA	1:A:22:THR:O	1.93	0.66
3:C:74:ARG:NE	3:C:94:TYR:CE2	2.63	0.66
1:D:19:VAL:HG23	1:D:75:ILE:HB	1.77	0.66
2:E:157:THR:HG23	2:E:200:ASN:OD1	1.96	0.66
2:E:130:PRO:HD2	2:E:192:TRP:CH2	2.30	0.66
2:E:130:PRO:HB2	2:E:132:SER:O	1.97	0.65
3:F:136:ARG:HD2	3:F:141:LEU:CD2	2.26	0.65
2:B:196:THR:HG23	2:B:213:LYS:HE3	1.78	0.65
2:B:175:GLN:O	2:B:176:SER:HB3	1.97	0.65
1:D:8:PRO:O	1:D:102:THR:HB	1.95	0.65
1:D:134:CYS:HB2	1:D:148:TRP:CZ2	2.32	0.65
1:A:39:LYS:HZ3	1:A:81:ASP:C	2.05	0.65
3:F:152:ILE:CD1	3:F:171:ASN:HB3	2.27	0.65
1:A:149:LYS:HA	1:A:155:ARG:HA	1.78	0.65
3:C:156:TYR:HB3	3:C:165:LYS:NZ	2.11	0.65
2:B:29:ILE:HG12	2:B:77:ASN:ND2	2.11	0.64
1:A:12:TYR:CD1	1:A:12:TYR:N	2.65	0.64
2:B:127:PRO:CB	2:B:214:ILE:HG22	2.28	0.64
3:C:122:LYS:HG2	3:C:178:ASP:OD1	1.97	0.64
1:D:147:LYS:HD3	1:D:155:ARG:HH12	1.63	0.64
2:B:127:PRO:HB2	2:B:214:ILE:HG22	1.79	0.64
2:E:29:ILE:H	2:E:77:ASN:HD21	1.44	0.64
3:F:32:GLN:HA	3:F:80:ALA:N	2.12	0.64
3:C:26:GLU:HB3	3:C:27:PRO:HA	1.80	0.64
3:F:23:LEU:HD12	3:F:24:GLU:N	2.12	0.64
3:F:149:LYS:HG3	3:F:171:ASN:ND2	2.13	0.63
1:A:2:ILE:HD13	1:A:27:GLN:HG2	1.79	0.63
1:D:160:LEU:HG	2:E:173:VAL:HG11	1.79	0.63
2:E:5:GLN:CG	2:E:23:LYS:HB3	2.29	0.63
3:C:13:THR:CG2	3:C:15:LYS:HE2	2.28	0.63
1:A:2:ILE:C	1:A:2:ILE:HD12	2.24	0.63
3:F:136:ARG:CD	3:F:141:LEU:HD21	2.28	0.63
1:A:91:HIS:HD2	3:C:169:LYS:NZ	1.97	0.63
3:C:177:ILE:HG13	3:C:177:ILE:O	1.98	0.63
1:A:153:SER:O	1:A:155:ARG:N	2.31	0.63
3:F:39:SER:HB3	3:F:45:TRP:HA	1.81	0.63
1:A:193:THR:HB	1:A:208:SER:CB	2.29	0.62
1:D:12:TYR:N	1:D:12:TYR:CD1	2.67	0.62
1:A:185:GLU:HA	1:A:188:ARG:HE	1.65	0.62
2:B:147:LYS:HB3	2:B:180:THR:HG23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:51:ILE:O	2:E:53:PRO:HD3	1.98	0.62
2:E:142:LEU:HB3	2:E:214:ILE:HD12	1.82	0.62
2:B:59:ILE:O	2:B:60:TYR:HD1	1.83	0.62
1:A:33:LEU:HD22	1:A:71:TYR:CB	2.30	0.62
2:E:9:ALA:O	2:E:10:GLU:HB2	2.00	0.62
1:D:145:ASN:HB3	1:D:197:THR:OG1	1.99	0.62
3:C:11:ASN:HB2	3:C:26:GLU:HG3	1.82	0.62
1:D:2:ILE:HD13	1:D:27:GLN:HG2	1.81	0.62
2:B:20:LEU:HD12	2:B:81:LEU:HD12	1.83	0.61
3:C:147:PHE:CD2	3:C:193:ILE:HD12	2.35	0.61
1:D:66:GLY:HA3	1:D:71:TYR:CD1	2.35	0.61
1:D:135:PHE:CE2	2:E:184:SER:HB3	2.34	0.61
3:F:141:LEU:HB3	3:F:145:ASP:CB	2.30	0.61
1:A:147:LYS:HG2	1:A:155:ARG:HH22	1.65	0.61
1:A:6:GLN:HE21	1:A:102:THR:HG23	1.65	0.61
2:B:39:GLN:O	2:B:92:ALA:HB1	2.01	0.61
1:D:108:ARG:HH21	1:D:111:ALA:HB2	1.64	0.61
1:A:170:ASP:O	1:A:172:THR:HG23	2.01	0.61
1:D:152:GLY:O	1:D:154:GLU:N	2.33	0.61
1:A:108:ARG:HH21	1:A:111:ALA:HB2	1.66	0.61
2:B:59:ILE:C	2:B:60:TYR:HD1	2.08	0.61
1:D:120:PRO:CG	1:D:130:ALA:HB1	2.31	0.61
2:E:6:GLN:NE2	2:E:96:CYS:SG	2.74	0.61
2:B:20:LEU:HD22	2:B:111:THR:HG21	1.83	0.60
2:E:196:THR:HG23	2:E:213:LYS:HE3	1.83	0.60
1:A:34:ASN:ND2	1:A:49:TYR:HA	2.15	0.60
1:A:196:ALA:HB3	1:A:205:ILE:HB	1.83	0.60
1:D:83:THR:HG21	1:D:166:GLN:CB	2.31	0.60
3:C:74:ARG:HB3	3:C:96:ASN:OD1	2.00	0.60
1:D:129:GLY:HA2	1:D:182:THR:HA	1.82	0.60
2:B:173:VAL:O	2:B:179:TYR:HA	2.02	0.60
3:C:35:THR:HG22	3:C:76:PHE:HB2	1.84	0.60
1:A:6:GLN:NE2	1:A:102:THR:HG23	2.16	0.59
3:C:67:VAL:O	3:C:102:PRO:HB2	2.02	0.59
1:D:44:PRO:HD2	2:E:107:TRP:CE3	2.37	0.59
3:F:32:GLN:HA	3:F:80:ALA:H	1.67	0.59
2:B:12:VAL:CG2	2:B:113:LEU:HD11	2.31	0.59
2:E:130:PRO:HD2	2:E:192:TRP:HH2	1.67	0.59
3:F:38:ILE:HD12	3:F:59:LEU:HD13	1.84	0.59
2:B:50:LEU:HD12	2:B:51:ILE:N	2.18	0.59
1:D:193:THR:HB	1:D:208:SER:OG	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:135:ARG:HG3	3:F:139:THR:O	2.02	0.59
1:A:199:LYS:HE3	3:F:133:LEU:O	2.01	0.59
3:C:48:LYS:NZ	3:C:48:LYS:HB3	2.18	0.59
2:B:91:THR:HG23	2:B:114:THR:HA	1.84	0.59
1:A:175:MET:O	2:B:170:PHE:CE1	2.56	0.59
2:E:145:LEU:HG	2:E:147:LYS:HD2	1.84	0.59
3:C:42:SER:H	3:C:72:LEU:HD12	1.67	0.58
2:E:18:VAL:O	2:E:82:GLN:HA	2.03	0.58
3:F:28:LYS:HG2	3:F:29:PRO:HD2	1.85	0.58
2:B:12:VAL:HG23	2:B:113:LEU:HD11	1.85	0.58
3:C:69:GLN:HG3	3:C:70:THR:N	2.18	0.58
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.85	0.58
2:B:100:ASN:O	2:B:101:SER:HB2	2.04	0.58
2:B:156:VAL:HG11	2:B:183:SER:HB2	1.84	0.58
1:D:120:PRO:HG2	1:D:130:ALA:HB1	1.85	0.58
3:F:167:THR:HG22	3:F:168:ALA:N	2.18	0.58
3:F:189:VAL:HG12	3:F:205:SER:OG	2.04	0.58
1:D:6:GLN:HA	1:D:22:THR:O	2.04	0.58
1:D:160:LEU:HD13	2:E:175:GLN:HE21	1.68	0.58
3:F:183:GLU:CB	3:F:185:TYR:HE1	2.17	0.57
1:A:187:GLU:HA	1:A:211:ARG:CZ	2.33	0.57
3:C:135:ARG:HH21	3:C:138:ASN:HA	1.69	0.57
1:D:108:ARG:HH11	1:D:108:ARG:CG	2.16	0.57
3:F:76:PHE:CD2	3:F:94:TYR:HB3	2.40	0.57
1:A:136:LEU:HD21	1:A:196:ALA:HB2	1.87	0.57
2:B:71:THR:O	2:B:80:TYR:N	2.38	0.57
2:E:142:LEU:HB3	2:E:214:ILE:CD1	2.34	0.57
3:F:114:GLN:HB2	3:F:128:GLU:HB2	1.87	0.57
1:A:18:ARG:HG3	1:A:75:ILE:O	2.05	0.57
2:E:13:ARG:HH11	2:E:116:SER:C	2.13	0.57
1:A:111:ALA:C	1:A:200:THR:HG21	2.29	0.57
2:B:38:LYS:HG3	2:B:39:GLN:N	2.20	0.57
1:A:147:LYS:CG	1:A:155:ARG:HH22	2.17	0.57
1:A:152:GLY:O	1:A:154:GLU:N	2.38	0.57
3:C:35:THR:CG2	3:C:78:TYR:HE2	2.17	0.57
1:D:6:GLN:HE21	1:D:102:THR:CG2	2.11	0.57
3:C:160:SER:OG	3:C:184:ASN:HB3	2.05	0.56
1:D:150:ILE:HD12	1:D:156:GLN:CD	2.30	0.56
1:D:153:SER:O	1:D:155:ARG:N	2.38	0.56
1:D:187:GLU:HA	1:D:211:ARG:NE	2.20	0.56
3:F:192:VAL:O	3:F:194:PRO:HD3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG12	1:A:116:SER:N	2.20	0.56
1:A:190:ASN:O	1:A:210:ASN:HA	2.06	0.56
3:C:150:ASP:OD1	3:C:195:SER:HB3	2.05	0.56
2:E:13:ARG:HD2	2:E:117:SER:HA	1.86	0.56
3:F:16:SER:HB3	3:F:21:THR:HA	1.87	0.56
3:F:13:THR:O	3:F:24:GLU:HG2	2.05	0.56
1:A:91:HIS:CD2	3:C:169:LYS:NZ	2.73	0.56
2:B:51:ILE:O	2:B:53:PRO:HD3	2.06	0.56
3:C:20:LYS:HD2	3:C:133:LEU:HD11	1.87	0.56
3:C:33:VAL:HG12	3:C:52:THR:O	2.05	0.56
2:E:100:ASN:O	2:E:101:SER:HB2	2.05	0.56
2:E:102:TYR:OH	3:F:149:LYS:HG2	2.06	0.56
3:F:41:LYS:HA	3:F:72:LEU:HD12	1.88	0.56
1:A:150:ILE:HD13	1:A:192:TYR:HE1	1.71	0.56
2:B:198:THR:HG23	2:B:212:LYS:O	2.06	0.56
3:F:35:THR:HG22	3:F:76:PHE:HB2	1.88	0.56
2:B:1:GLU:OE1	2:B:2:ILE:HG13	2.06	0.56
1:D:11:MET:HE1	1:D:19:VAL:HG12	1.88	0.56
1:D:34:ASN:ND2	1:D:50:TYR:H	2.04	0.56
1:A:162:SER:OG	2:B:171:PRO:HG2	2.06	0.56
1:A:191:SER:HA	1:A:210:ASN:OD1	2.06	0.56
2:E:34:MET:HB2	2:E:51:ILE:CG2	2.36	0.56
3:F:12:LEU:HD21	3:F:75:VAL:HG23	1.88	0.55
1:D:33:LEU:HD22	1:D:71:TYR:CB	2.36	0.55
1:A:91:HIS:CD2	3:C:169:LYS:HZ2	2.24	0.55
1:D:139:PHE:HE2	1:D:175:MET:HB2	1.72	0.55
2:E:86:LEU:HD13	2:E:115:VAL:CG2	2.35	0.55
1:A:61:ARG:HH21	1:A:82:ASP:CG	2.15	0.55
3:C:60:THR:O	3:C:64:VAL:HG22	2.07	0.55
2:E:28:ASN:ND2	2:E:30:LYS:HG2	2.22	0.55
3:C:70:THR:HA	3:C:100:PHE:O	2.06	0.55
3:F:10:TYR:CZ	3:F:26:GLU:HB3	2.41	0.55
1:A:137:ASN:HA	1:A:174:SER:HA	1.88	0.55
3:C:28:LYS:HD3	3:C:29:PRO:N	2.21	0.55
1:A:151:ASP:OD2	1:A:189:HIS:HB3	2.07	0.55
2:E:154:VAL:HG23	2:E:181:LEU:HD13	1.89	0.55
2:E:29:ILE:H	2:E:77:ASN:ND2	2.04	0.55
3:F:74:ARG:HH21	3:F:96:ASN:HD21	1.55	0.54
2:B:145:LEU:HG	2:B:145:LEU:O	2.06	0.54
2:E:55:ASN:O	2:E:57:ASN:N	2.40	0.54
2:B:31:ASP:O	3:C:200:ARG:HD3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:LEU:HG	1:D:181:LEU:HD13	1.89	0.54
2:E:33:TYR:HB2	2:E:99:ASP:HB3	1.87	0.54
1:A:164:THR:HG23	2:B:170:PHE:CD1	2.42	0.54
3:F:25:TRP:HH2	3:F:57:CYS:HB2	1.72	0.54
1:D:196:ALA:HB3	1:D:205:ILE:CB	2.32	0.54
3:C:110:GLN:NE2	3:C:206:PRO:HD3	2.23	0.54
1:D:136:LEU:HB2	1:D:175:MET:HB3	1.89	0.54
3:F:108:LEU:HD11	3:F:193:ILE:HG12	1.90	0.54
3:F:179:VAL:HB	3:F:185:TYR:CZ	2.42	0.54
2:E:31:ASP:HB3	3:F:200:ARG:CD	2.38	0.54
3:F:155:LEU:HD12	3:F:156:TYR:N	2.23	0.54
3:C:136:ARG:HB2	3:C:141:LEU:HD11	1.89	0.53
3:C:149:LYS:HB2	3:C:149:LYS:HZ3	1.73	0.53
1:D:164:THR:HG23	2:E:170:PHE:CD1	2.43	0.53
1:A:193:THR:CB	1:A:208:SER:HB2	2.37	0.53
2:E:5:GLN:HG2	2:E:23:LYS:HB3	1.90	0.53
3:C:39:SER:HB3	3:C:45:TRP:HA	1.90	0.53
3:C:115:SER:O	3:C:116:PHE:HB3	2.07	0.53
3:F:29:PRO:HG3	3:F:53:THR:O	2.08	0.53
3:F:191:ALA:HB3	3:F:202:SER:HB3	1.91	0.53
1:A:39:LYS:HD3	1:A:84:ALA:HB2	1.91	0.53
1:D:15:LEU:O	1:D:17:GLU:N	2.38	0.53
1:D:166:GLN:HE21	1:D:171:SER:HA	1.73	0.53
2:E:13:ARG:HA	2:E:116:SER:O	2.08	0.53
1:A:146:VAL:HA	1:A:195:GLU:O	2.09	0.53
1:D:34:ASN:HD21	1:D:50:TYR:H	1.56	0.53
1:D:148:TRP:HD1	1:D:159:VAL:HG21	1.73	0.53
2:E:164:SER:O	2:E:167:VAL:HG23	2.08	0.53
2:B:174:LEU:HD12	2:B:178:LEU:O	2.09	0.53
1:D:108:ARG:HG2	1:D:109:ALA:N	2.23	0.53
3:F:187:PHE:O	3:F:207:VAL:HA	2.08	0.53
1:A:159:VAL:HA	1:A:178:THR:O	2.09	0.53
2:B:11:LEU:HB2	2:B:151:PRO:HG3	1.91	0.53
1:A:61:ARG:HD2	1:A:77:SER:O	2.09	0.52
1:D:106:ILE:HB	1:D:166:GLN:HE22	1.73	0.52
2:B:2:ILE:HA	2:B:25:SER:O	2.08	0.52
3:C:28:LYS:HD3	3:C:28:LYS:C	2.33	0.52
3:C:18:ASN:HB3	3:C:132:THR:HG22	1.91	0.52
2:E:146:VAL:HG12	2:E:146:VAL:O	2.09	0.52
1:A:135:PHE:CE2	2:B:184:SER:HB3	2.44	0.52
1:A:161:ASN:HB3	1:A:175:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:LEU:HB3	2:B:214:ILE:CD1	2.40	0.52
1:A:124:GLN:HG3	2:B:126:TYR:CE2	2.44	0.52
2:B:52:ASP:O	2:B:54:GLU:N	2.42	0.52
3:C:41:LYS:HA	3:C:72:LEU:HD12	1.91	0.52
1:D:120:PRO:HD3	1:D:132:VAL:CG1	2.40	0.52
2:E:13:ARG:NH1	2:E:118:ALA:O	2.42	0.52
1:D:15:LEU:C	1:D:17:GLU:H	2.17	0.52
2:B:5:GLN:O	2:B:22:CYS:HA	2.10	0.52
2:B:50:LEU:HG	2:B:59:ILE:HB	1.91	0.52
2:B:94:TYR:N	2:B:94:TYR:CD1	2.77	0.52
3:F:153:TYR:HB2	3:F:170:THR:CG2	2.40	0.52
1:D:150:ILE:HD11	1:D:179:LEU:HD21	1.90	0.52
2:B:18:VAL:CG2	2:B:19:LYS:N	2.72	0.52
2:B:176:SER:C	2:B:178:LEU:H	2.18	0.52
1:D:139:PHE:HE1	1:D:142:LYS:HA	1.75	0.52
3:F:115:SER:O	3:F:116:PHE:HB3	2.10	0.52
1:A:39:LYS:HB2	1:A:42:LYS:HG3	1.92	0.52
1:A:183:LYS:HG2	1:A:187:GLU:OE1	2.10	0.52
2:B:54:GLU:HG3	2:B:55:ASN:N	2.25	0.52
3:C:35:THR:HG22	3:C:78:TYR:HE2	1.75	0.52
1:D:115:VAL:N	2:E:136:THR:HG21	2.25	0.52
3:F:25:TRP:CH2	3:F:57:CYS:HB2	2.45	0.52
2:B:135:GLN:C	2:B:135:GLN:CD	2.77	0.51
1:D:193:THR:CB	1:D:208:SER:HB2	2.38	0.51
2:E:42:GLU:O	2:E:43:GLN:HG3	2.10	0.51
1:A:145:ASN:HB3	1:A:197:THR:OG1	2.10	0.51
2:B:30:LYS:HA	2:B:53:PRO:HB2	1.93	0.51
1:D:19:VAL:CG2	1:D:75:ILE:HB	2.40	0.51
2:E:135:GLN:C	2:E:135:GLN:CD	2.78	0.51
3:F:28:LYS:HD3	3:F:29:PRO:N	2.25	0.51
1:D:150:ILE:O	1:D:151:ASP:HB2	2.10	0.51
2:B:174:LEU:HD13	2:B:179:TYR:CE2	2.46	0.51
2:E:51:ILE:HB	2:E:70:ILE:HG21	1.91	0.51
1:D:2:ILE:HD13	1:D:27:GLN:CG	2.41	0.51
1:D:150:ILE:CD1	1:D:181:LEU:HD21	2.39	0.51
1:D:163:TRP:CH2	1:D:175:MET:HE3	2.45	0.51
3:C:74:ARG:HD2	3:C:76:PHE:CZ	2.46	0.51
1:D:21:ILE:HG23	1:D:102:THR:HG21	1.93	0.51
3:F:154:THR:HG22	3:F:156:TYR:CE1	2.45	0.51
1:A:120:PRO:HD2	1:A:186:TYR:OH	2.11	0.51
2:B:200:ASN:HB3	2:B:211:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ALA:O	1:D:107:ASN:HB2	2.11	0.51
3:C:36:VAL:HG22	3:C:75:VAL:HG22	1.93	0.51
3:C:108:LEU:HD11	3:C:193:ILE:HG12	1.91	0.51
2:B:137:ASN:ND2	2:B:139:MET:SD	2.84	0.50
3:C:13:THR:HG21	3:C:15:LYS:CE	2.37	0.50
3:F:35:THR:OG1	3:F:50:PHE:HA	2.11	0.50
1:D:108:ARG:CG	1:D:108:ARG:NH1	2.73	0.50
1:A:4:MET:HE3	1:A:4:MET:HA	1.94	0.50
2:B:57:ASN:HD21	3:C:165:LYS:NZ	2.10	0.50
3:C:119:VAL:HG12	3:C:119:VAL:O	2.09	0.50
1:D:29:ILE:HD11	1:D:71:TYR:CE2	2.47	0.50
1:D:137:ASN:HA	1:D:174:SER:HA	1.93	0.50
2:E:62:PRO:HA	2:E:65:GLN:HG3	1.93	0.50
3:F:42:SER:H	3:F:72:LEU:CD1	2.24	0.50
2:B:156:VAL:HG22	2:B:201:VAL:HG22	1.93	0.50
2:B:30:LYS:HZ2	2:B:30:LYS:HB2	1.76	0.50
2:E:10:GLU:O	2:E:113:LEU:HD12	2.11	0.50
3:F:63:ILE:C	3:F:63:ILE:HD12	2.37	0.50
1:D:34:ASN:HA	1:D:48:ILE:O	2.11	0.50
3:F:135:ARG:HG3	3:F:139:THR:H	1.76	0.50
3:F:158:TRP:CE3	3:F:165:LYS:HG2	2.47	0.50
1:A:12:TYR:HA	1:A:105:GLU:O	2.11	0.49
1:A:33:LEU:HD22	1:A:71:TYR:HB3	1.94	0.49
3:C:144:ARG:NH2	3:C:172:THR:O	2.43	0.49
1:D:185:GLU:HA	1:D:188:ARG:HE	1.76	0.49
3:F:13:THR:CG2	3:F:15:LYS:HE2	2.41	0.49
3:F:78:TYR:CE1	3:F:92:PRO:HG3	2.43	0.49
1:D:55:ALA:O	1:D:57:GLY:N	2.44	0.49
2:E:51:ILE:HB	2:E:70:ILE:CG2	2.42	0.49
2:B:58:THR:C	2:B:59:ILE:HD12	2.38	0.49
2:E:5:GLN:C	2:E:6:GLN:HG2	2.37	0.49
2:B:38:LYS:CG	2:B:39:GLN:N	2.74	0.49
1:D:160:LEU:HD21	2:E:175:GLN:HG3	1.95	0.49
2:E:127:PRO:HB3	2:E:214:ILE:HG22	1.94	0.49
2:E:17:LEU:HD12	2:E:17:LEU:C	2.38	0.49
3:C:124:ASN:C	3:C:124:ASN:ND2	2.69	0.49
2:E:20:LEU:HD22	2:E:111:THR:HG21	1.94	0.49
2:B:60:TYR:OH	2:B:69:SER:HA	2.13	0.49
2:E:30:LYS:HA	2:E:53:PRO:HB2	1.95	0.49
1:A:199:LYS:NZ	3:F:135:ARG:HB3	2.28	0.49
3:C:42:SER:H	3:C:72:LEU:CD1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:THR:CG2	3:C:99:GLU:HB3	2.43	0.49
2:B:17:LEU:C	2:B:17:LEU:HD12	2.38	0.49
2:B:35:HIS:CD2	2:B:99:ASP:HB2	2.48	0.48
3:C:121:THR:O	3:C:121:THR:HG22	2.12	0.48
3:C:141:LEU:HB3	3:C:145:ASP:CB	2.43	0.48
1:D:134:CYS:HB2	1:D:148:TRP:CH2	2.48	0.48
1:A:61:ARG:NH2	1:A:82:ASP:OD1	2.43	0.48
3:C:4:THR:O	3:C:5:ASN:HB2	2.14	0.48
3:C:32:GLN:HE21	3:C:34:TYR:HE1	1.62	0.48
1:D:12:TYR:HD1	1:D:12:TYR:H	1.59	0.48
1:A:190:ASN:OD1	1:A:211:ARG:N	2.46	0.48
2:B:176:SER:O	2:B:178:LEU:N	2.46	0.48
3:F:74:ARG:HD3	3:F:76:PHE:CZ	2.49	0.48
1:A:147:LYS:CB	1:A:155:ARG:HH22	2.27	0.48
1:A:199:LYS:HZ3	3:F:135:ARG:HB3	1.77	0.48
2:E:127:PRO:CB	2:E:214:ILE:HG22	2.42	0.48
3:F:43:GLY:O	3:F:45:TRP:N	2.47	0.48
3:F:155:LEU:HD12	3:F:156:TYR:H	1.77	0.48
2:B:6:GLN:HB3	2:B:111:THR:OG1	2.14	0.48
2:B:181:LEU:HG	2:B:182:SER:H	1.79	0.48
2:E:150:PHE:CD1	2:E:150:PHE:C	2.92	0.48
3:F:16:SER:HG	3:F:100:PHE:HZ	1.61	0.48
1:A:83:THR:HG21	1:A:166:GLN:CB	2.44	0.48
1:A:130:ALA:N	1:A:181:LEU:O	2.45	0.48
2:E:17:LEU:HD12	2:E:18:VAL:N	2.28	0.48
3:F:10:TYR:CE1	3:F:27:PRO:HD3	2.48	0.48
3:F:33:VAL:HG21	3:F:51:TYR:HB3	1.95	0.48
3:F:38:ILE:HA	3:F:73:ALA:HA	1.95	0.48
3:F:78:TYR:HE1	3:F:92:PRO:CG	2.25	0.48
3:F:124:ASN:HD21	3:F:174:GLU:HB2	1.79	0.48
3:F:136:ARG:HG3	3:F:137:ASN:ND2	2.29	0.48
1:A:83:THR:HG21	1:A:166:GLN:HB2	1.95	0.48
3:F:136:ARG:NH1	3:F:141:LEU:HD13	2.29	0.48
1:D:125:LEU:HD22	1:D:183:LYS:HG3	1.96	0.48
2:E:137:ASN:HB3	2:E:139:MET:HG2	1.96	0.48
1:A:34:ASN:O	1:A:88:CYS:HA	2.14	0.48
1:A:119:PRO:HB3	1:A:209:PHE:CE2	2.49	0.48
3:C:149:LYS:HB2	3:C:149:LYS:HZ2	1.78	0.48
3:F:42:SER:H	3:F:72:LEU:HD12	1.79	0.48
3:F:196:ARG:HH11	3:F:199:ASN:HB3	1.79	0.48
2:B:167:VAL:HG12	2:B:168:HIS:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:THR:OG1	3:C:79:PRO:HB3	2.14	0.48
3:C:31:ASN:C	3:C:80:ALA:HB3	2.39	0.48
2:E:31:ASP:HB3	3:F:200:ARG:HD3	1.96	0.48
3:F:29:PRO:HB2	3:F:32:GLN:O	2.13	0.48
1:A:15:LEU:C	1:A:17:GLU:H	2.22	0.47
3:C:45:TRP:HZ3	3:C:73:ALA:HA	1.79	0.47
1:D:42:LYS:HB3	1:D:42:LYS:NZ	2.27	0.47
1:D:120:PRO:HD2	1:D:186:TYR:CZ	2.49	0.47
2:E:108:GLY:C	2:E:109:GLN:O	2.54	0.47
3:F:159:LYS:NZ	3:F:180:ASP:OD2	2.47	0.47
2:B:172:ALA:HB1	2:B:179:TYR:HB3	1.96	0.47
3:C:52:THR:OG1	3:C:53:THR:N	2.47	0.47
3:C:175:PHE:CD1	3:C:175:PHE:N	2.82	0.47
3:F:18:ASN:ND2	3:F:130:GLU:HG2	2.29	0.47
3:F:74:ARG:HH21	3:F:96:ASN:ND2	2.11	0.47
3:F:74:ARG:NE	3:F:94:TYR:CE2	2.82	0.47
2:B:6:GLN:HE21	2:B:108:GLY:HA3	1.79	0.47
2:B:2:ILE:O	2:B:3:GLN:HB3	2.14	0.47
3:C:10:TYR:CE1	3:C:27:PRO:HB3	2.50	0.47
1:A:14:SER:O	1:A:17:GLU:HB2	2.14	0.47
2:B:5:GLN:HG2	2:B:23:LYS:O	2.13	0.47
3:C:10:TYR:HE1	3:C:27:PRO:HB3	1.79	0.47
3:C:74:ARG:HD3	3:C:94:TYR:CD2	2.49	0.47
1:D:89:LEU:HD23	1:D:98:PHE:CD1	2.50	0.47
2:E:29:ILE:N	2:E:77:ASN:HD21	2.10	0.47
2:E:48:ILE:HG21	2:E:81:LEU:HD21	1.96	0.47
2:E:156:VAL:HG21	2:E:181:LEU:CD2	2.45	0.47
1:A:116:SER:HB2	1:A:135:PHE:HB2	1.97	0.47
1:D:160:LEU:HD13	2:E:175:GLN:NE2	2.29	0.47
2:E:17:LEU:HD13	2:E:82:GLN:CG	2.45	0.47
3:C:136:ARG:CB	3:C:141:LEU:HD11	2.44	0.47
1:D:12:TYR:HA	1:D:105:GLU:O	2.14	0.47
1:D:86:TYR:O	1:D:101:GLY:HA2	2.15	0.47
1:D:165:ASP:O	1:D:166:GLN:C	2.58	0.47
2:E:35:HIS:O	2:E:96:CYS:HA	2.15	0.47
2:E:137:ASN:CG	2:E:139:MET:SD	2.98	0.47
1:A:143:ASP:O	1:A:198:HIS:HD2	1.98	0.47
2:B:17:LEU:HD12	2:B:17:LEU:O	2.14	0.47
3:F:153:TYR:HB2	3:F:170:THR:HG23	1.95	0.47
2:E:100:ASN:O	2:E:101:SER:CB	2.62	0.47
2:E:181:LEU:HG	2:E:182:SER:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:186:CYS:HA	3:F:209:CYS:HA	1.97	0.47
1:A:1:ASP:CG	1:A:2:ILE:N	2.73	0.47
2:E:13:ARG:HD3	2:E:116:SER:O	2.15	0.47
1:A:39:LYS:NZ	1:A:81:ASP:C	2.71	0.46
1:A:170:ASP:OD1	1:A:170:ASP:C	2.58	0.46
1:D:151:ASP:OD2	1:D:189:HIS:HB3	2.14	0.46
2:B:18:VAL:HG12	2:B:86:LEU:HD11	1.97	0.46
2:B:185:VAL:O	2:B:185:VAL:HG13	2.15	0.46
3:C:40:THR:OG1	3:C:41:LYS:N	2.45	0.46
1:D:189:HIS:CD2	1:D:189:HIS:N	2.83	0.46
2:E:13:ARG:CD	2:E:116:SER:O	2.63	0.46
3:C:41:LYS:HE2	3:C:99:GLU:OE2	2.16	0.46
3:F:11:ASN:CB	3:F:26:GLU:HG3	2.37	0.46
2:B:7:SER:O	2:B:9:ALA:N	2.45	0.46
1:D:190:ASN:OD1	1:D:211:ARG:N	2.49	0.46
2:E:5:GLN:O	2:E:22:CYS:HA	2.15	0.46
2:B:156:VAL:HG11	2:B:183:SER:CB	2.45	0.46
2:E:14:PRO:HD2	2:E:116:SER:O	2.15	0.46
1:A:116:SER:HB3	1:A:118:PHE:CE1	2.51	0.46
1:A:142:LYS:HB2	1:A:173:TYR:CZ	2.50	0.46
1:D:35:TRP:CZ3	1:D:88:CYS:HB3	2.50	0.46
3:F:37:GLN:CG	3:F:45:TRP:HB3	2.44	0.46
2:E:153:PRO:O	2:E:204:PRO:HD2	2.16	0.46
3:F:23:LEU:HG	3:F:25:TRP:CE3	2.51	0.46
3:F:93:LEU:HD23	3:F:93:LEU:N	2.29	0.46
1:A:1:ASP:OD2	1:A:2:ILE:HG22	2.16	0.46
3:C:10:TYR:O	3:C:11:ASN:HB2	2.16	0.46
1:D:9:SER:O	1:D:102:THR:HA	2.15	0.46
2:B:11:LEU:HD21	2:B:13:ARG:HH12	1.81	0.46
3:C:46:LYS:HG2	3:C:48:LYS:HD3	1.97	0.46
2:E:123:PRO:HB3	2:E:149:TYR:HB3	1.98	0.46
3:F:75:VAL:O	3:F:94:TYR:HB2	2.15	0.46
1:A:47:LEU:HA	1:A:58:VAL:HG21	1.98	0.46
1:A:108:ARG:HG3	1:A:108:ARG:HH11	1.81	0.46
1:A:108:ARG:NH2	1:A:111:ALA:HB2	2.31	0.46
1:A:116:SER:HB3	1:A:118:PHE:HE1	1.80	0.46
2:B:128:LEU:HD12	2:B:143:GLY:C	2.41	0.46
3:C:41:LYS:HD2	3:C:72:LEU:HD11	1.97	0.46
2:E:2:ILE:HD13	2:E:98:ARG:NH1	2.30	0.46
3:F:10:TYR:HE1	3:F:27:PRO:HD3	1.79	0.46
1:A:4:MET:HE3	1:A:4:MET:CA	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASP:O	1:A:166:GLN:C	2.59	0.45
1:D:170:ASP:OD1	1:D:170:ASP:C	2.59	0.45
1:D:161:ASN:HB3	1:D:175:MET:HE2	1.98	0.45
2:B:84:SER:O	2:B:85:SER:C	2.59	0.45
3:C:141:LEU:HB3	3:C:145:ASP:HB2	1.97	0.45
1:D:115:VAL:O	2:E:136:THR:HG21	2.17	0.45
3:F:74:ARG:CZ	3:F:94:TYR:CE2	3.00	0.45
2:B:70:ILE:N	2:B:70:ILE:HD12	2.31	0.45
3:C:167:THR:HG22	3:C:168:ALA:N	2.32	0.45
3:C:210:MET:HB3	3:C:211:GLY:H	1.52	0.45
2:E:35:HIS:NE2	2:E:99:ASP:HB2	2.32	0.45
3:F:193:ILE:CG2	3:F:196:ARG:HG3	2.47	0.45
1:A:36:TYR:O	1:A:86:TYR:HA	2.16	0.45
1:D:118:PHE:HA	1:D:119:PRO:HD3	1.79	0.45
3:F:94:TYR:HE2	3:F:96:ASN:OD1	1.99	0.45
2:B:55:ASN:O	2:B:57:ASN:N	2.50	0.45
1:D:166:GLN:HG3	1:D:173:TYR:OH	2.16	0.45
2:E:4:LEU:HD21	2:E:34:MET:HE1	1.97	0.45
2:B:214:ILE:OXT	2:B:214:ILE:HG13	2.16	0.45
3:F:38:ILE:HD12	3:F:59:LEU:CD1	2.45	0.45
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.52	0.45
1:D:141:PRO:C	1:D:143:ASP:N	2.73	0.45
1:D:191:SER:HA	1:D:210:ASN:OD1	2.16	0.45
3:F:136:ARG:CG	3:F:141:LEU:HD21	2.46	0.45
1:A:29:ILE:HD11	1:A:71:TYR:CD2	2.52	0.45
2:B:18:VAL:O	2:B:82:GLN:HA	2.17	0.45
2:E:71:THR:O	2:E:80:TYR:N	2.48	0.45
1:A:9:SER:O	1:A:102:THR:HA	2.17	0.45
1:A:135:PHE:CZ	2:B:184:SER:HB3	2.52	0.44
1:D:34:ASN:ND2	1:D:49:TYR:CA	2.73	0.44
3:F:187:PHE:N	3:F:208:GLU:O	2.50	0.44
1:A:115:VAL:CG1	1:A:116:SER:N	2.80	0.44
2:B:5:GLN:HG3	2:B:23:LYS:HB3	1.99	0.44
1:D:14:SER:O	1:D:17:GLU:CB	2.63	0.44
1:D:61:ARG:NH2	1:D:82:ASP:OD1	2.49	0.44
1:D:108:ARG:NH2	1:D:111:ALA:HB2	2.30	0.44
2:E:2:ILE:HG22	2:E:3:GLN:N	2.31	0.44
2:E:90:ASP:O	2:E:91:THR:C	2.60	0.44
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.79	0.44
1:A:189:HIS:CD2	1:A:189:HIS:N	2.85	0.44
2:B:123:PRO:HB2	2:B:146:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:TYR:CZ	2:B:154:VAL:HG22	2.52	0.44
3:C:15:LYS:HG3	3:C:24:GLU:OE1	2.17	0.44
3:F:155:LEU:HG	3:F:157:TYR:HD2	1.82	0.44
3:C:10:TYR:HE1	3:C:27:PRO:CD	2.30	0.44
1:D:147:LYS:O	1:D:194:CYS:HA	2.17	0.44
1:A:26:SER:O	1:A:27:GLN:CB	2.65	0.44
1:A:149:LYS:HD2	1:A:153:SER:HA	1.99	0.44
3:C:143:LEU:HA	3:C:143:LEU:HD12	1.74	0.44
1:D:36:TYR:CE1	1:D:46:THR:HB	2.52	0.44
1:D:132:VAL:HG23	1:D:179:LEU:HB3	2.00	0.44
2:E:30:LYS:HZ2	2:E:30:LYS:HB2	1.82	0.44
1:A:24:LYS:HA	1:A:69:GLN:O	2.18	0.44
1:D:166:GLN:NE2	1:D:171:SER:HB3	2.32	0.44
1:A:27:GLN:O	1:A:28:ASP:C	2.60	0.44
2:B:117:SER:O	2:B:118:ALA:C	2.61	0.44
3:C:10:TYR:HE1	3:C:27:PRO:CB	2.30	0.44
3:C:135:ARG:NE	3:C:138:ASN:HA	2.32	0.44
2:E:145:LEU:CG	2:E:147:LYS:HD2	2.48	0.44
3:F:31:ASN:C	3:F:80:ALA:HB3	2.43	0.44
3:F:72:LEU:HD21	3:F:99:GLU:HG3	1.99	0.44
3:C:169:LYS:HB2	3:C:169:LYS:HE3	1.80	0.44
1:D:133:VAL:HG22	1:D:178:THR:OG1	2.18	0.44
1:D:148:TRP:CD1	1:D:159:VAL:HG21	2.52	0.44
1:D:212:ASN:C	1:D:214:CYS:SG	3.01	0.44
2:E:17:LEU:HD13	2:E:82:GLN:HG3	1.99	0.44
2:E:97:ALA:HA	2:E:106:TYR:O	2.18	0.44
3:C:124:ASN:HA	3:C:176:LEU:HD12	2.00	0.44
2:E:156:VAL:HG21	2:E:181:LEU:HD21	2.00	0.44
3:C:135:ARG:NH2	3:C:138:ASN:CA	2.75	0.43
3:C:198:VAL:HG23	3:C:199:ASN:H	1.82	0.43
1:D:35:TRP:CD2	1:D:73:LEU:HB2	2.53	0.43
1:A:13:ALA:HB3	1:A:78:LEU:CD2	2.48	0.43
1:A:50:TYR:HE2	3:C:149:LYS:HE3	1.83	0.43
1:D:36:TYR:O	1:D:86:TYR:HA	2.18	0.43
2:E:140:VAL:O	2:E:186:THR:HA	2.18	0.43
3:F:111:PRO:HB2	3:F:189:VAL:HG13	1.99	0.43
3:F:158:TRP:CE2	3:F:186:CYS:HB2	2.53	0.43
1:D:139:PHE:CD1	1:D:139:PHE:C	2.96	0.43
3:C:183:GLU:HB2	3:C:185:TYR:HE1	1.83	0.43
2:E:163:LEU:HG	2:E:185:VAL:HG21	2.00	0.43
1:A:134:CYS:HB3	1:A:177:SER:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ILE:O	1:D:150:ILE:HG22	2.18	0.43
1:A:50:TYR:CE2	3:C:149:LYS:HE3	2.54	0.43
3:C:43:GLY:O	3:C:45:TRP:CD1	2.71	0.43
3:C:125:VAL:HG12	3:C:126:THR:N	2.33	0.43
1:D:11:MET:HE1	1:D:19:VAL:CG1	2.48	0.43
2:E:33:TYR:HE1	3:F:156:TYR:OH	2.01	0.43
2:E:48:ILE:HD13	2:E:64:PHE:CE2	2.54	0.43
3:C:124:ASN:C	3:C:124:ASN:HD22	2.24	0.43
1:D:106:ILE:N	1:D:166:GLN:OE1	2.51	0.43
1:A:133:VAL:HG22	1:A:178:THR:OG1	2.19	0.43
1:D:121:SER:C	1:D:123:GLU:N	2.73	0.43
2:E:142:LEU:HD13	2:E:214:ILE:HD11	2.01	0.43
1:A:89:LEU:HG	1:A:98:PHE:CE1	2.54	0.43
2:B:118:ALA:HB3	2:B:150:PHE:CE2	2.54	0.43
2:B:174:LEU:HD13	2:B:179:TYR:CD2	2.54	0.43
1:D:113:PRO:HB3	1:D:139:PHE:HB3	2.01	0.43
3:F:152:ILE:HD13	3:F:152:ILE:HA	1.84	0.43
1:D:61:ARG:HH21	1:D:82:ASP:CG	2.27	0.42
3:F:37:GLN:HA	3:F:46:LYS:O	2.19	0.42
2:B:40:ARG:HG2	2:B:92:ALA:HB2	2.01	0.42
1:D:119:PRO:HG3	1:D:209:PHE:CG	2.55	0.42
3:F:135:ARG:HA	3:F:139:THR:O	2.19	0.42
3:C:32:GLN:HA	3:C:80:ALA:N	2.34	0.42
3:C:134:VAL:HG21	3:C:146:VAL:HG21	2.00	0.42
1:D:1:ASP:OD2	1:D:2:ILE:HG22	2.18	0.42
3:F:74:ARG:HG3	3:F:76:PHE:CE1	2.54	0.42
2:B:4:LEU:HD23	2:B:96:CYS:SG	2.58	0.42
2:B:38:LYS:HG3	2:B:39:GLN:H	1.83	0.42
1:D:11:MET:HB2	1:D:11:MET:HE3	1.67	0.42
2:E:39:GLN:HB2	2:E:45:LEU:HD23	2.01	0.42
3:F:16:SER:OG	3:F:100:PHE:HZ	2.02	0.42
1:A:38:GLN:HG3	1:A:44:PRO:HG3	2.02	0.42
3:C:12:LEU:HD21	3:C:75:VAL:HG23	2.00	0.42
3:C:155:LEU:HG	3:C:157:TYR:HD2	1.83	0.42
3:F:159:LYS:HA	3:F:185:TYR:HA	2.01	0.42
3:F:190:GLN:O	3:F:190:GLN:HG3	2.19	0.42
3:C:162:SER:OG	3:C:163:SER:N	2.53	0.42
3:F:185:TYR:O	3:F:209:CYS:HA	2.20	0.42
1:A:144:ILE:HG13	1:A:198:HIS:HB2	2.01	0.42
1:D:120:PRO:HD3	1:D:132:VAL:HG13	2.01	0.42
2:B:164:SER:O	2:B:167:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:152:ILE:HG13	3:C:194:PRO:HG2	2.02	0.42
2:E:5:GLN:HG3	2:E:23:LYS:HB3	2.01	0.42
3:F:186:CYS:HA	3:F:208:GLU:O	2.20	0.42
1:A:175:MET:O	2:B:170:PHE:CZ	2.73	0.42
2:B:139:MET:CB	2:B:188:PRO:HA	2.49	0.42
3:C:4:THR:HB	3:C:5:ASN:H	1.54	0.42
1:A:26:SER:O	1:A:27:GLN:HB3	2.20	0.42
3:C:156:TYR:HB3	3:C:165:LYS:HZ3	1.85	0.42
2:E:11:LEU:HD21	2:E:13:ARG:HH22	1.84	0.42
3:F:23:LEU:HD12	3:F:23:LEU:C	2.44	0.42
1:D:151:ASP:HA	1:D:191:SER:OG	2.20	0.41
2:E:142:LEU:O	2:E:184:SER:HA	2.20	0.41
3:C:106:THR:O	3:C:106:THR:CG2	2.67	0.41
1:A:44:PRO:HD2	2:B:107:TRP:CE3	2.55	0.41
3:C:63:ILE:HD12	3:C:63:ILE:C	2.46	0.41
1:D:119:PRO:HA	1:D:132:VAL:HG12	2.02	0.41
2:E:51:ILE:O	2:E:51:ILE:HG23	2.20	0.41
3:F:13:THR:HG21	3:F:15:LYS:HE2	2.02	0.41
3:F:38:ILE:HG13	3:F:72:LEU:O	2.20	0.41
3:F:48:LYS:HA	3:F:48:LYS:HD2	1.90	0.41
3:F:63:ILE:HD12	3:F:64:VAL:N	2.34	0.41
3:F:111:PRO:HD2	3:F:203:THR:O	2.19	0.41
2:E:2:ILE:O	2:E:3:GLN:HB3	2.19	0.41
3:F:157:TYR:CE1	3:F:166:LYS:HB2	2.55	0.41
1:A:89:LEU:HB2	1:A:98:PHE:CD1	2.55	0.41
1:A:131:SER:OG	1:A:180:THR:HG23	2.20	0.41
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.80	0.41
2:E:137:ASN:HB3	2:E:139:MET:O	2.20	0.41
3:F:180:ASP:HB2	3:F:185:TYR:OH	2.20	0.41
1:A:89:LEU:HD23	1:A:98:PHE:CD1	2.56	0.41
1:A:91:HIS:HD2	3:C:169:LYS:HZ3	1.69	0.41
2:B:59:ILE:C	2:B:60:TYR:CD1	2.93	0.41
2:B:156:VAL:HG21	2:B:181:LEU:CD2	2.50	0.41
1:D:152:GLY:C	1:D:154:GLU:N	2.78	0.41
2:E:93:VAL:HA	2:E:111:THR:O	2.20	0.41
2:E:149:TYR:CE1	2:E:179:TYR:HB2	2.56	0.41
3:F:19:PHE:O	3:F:63:ILE:HD11	2.21	0.41
3:F:51:TYR:HE1	3:F:78:TYR:CE2	2.38	0.41
1:A:11:MET:O	1:A:11:MET:HG3	2.20	0.41
2:E:139:MET:HG3	2:E:186:THR:CG2	2.50	0.41
2:E:174:LEU:HD12	2:E:178:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:183:GLU:HB2	3:F:185:TYR:CE1	2.38	0.41
2:B:181:LEU:HG	2:B:182:SER:N	2.35	0.41
3:C:29:PRO:HG3	3:C:53:THR:O	2.21	0.41
3:C:32:GLN:HA	3:C:80:ALA:H	1.85	0.41
3:C:132:THR:O	3:C:140:PHE:HD2	2.04	0.41
2:E:1:GLU:O	2:E:26:GLY:HA3	2.21	0.41
3:F:34:TYR:HD1	3:F:77:SER:HA	1.86	0.41
3:C:25:TRP:O	3:C:55:THR:HB	2.21	0.41
1:D:94:SER:OG	2:E:59:ILE:HG21	2.20	0.41
1:D:183:LYS:O	1:D:186:TYR:HB3	2.20	0.41
2:E:212:LYS:HA	2:E:212:LYS:HD3	1.85	0.41
3:F:74:ARG:HD3	3:F:94:TYR:CD2	2.56	0.41
3:F:94:TYR:CE2	3:F:96:ASN:OD1	2.74	0.41
2:B:105:ASP:O	2:B:106:TYR:CD2	2.74	0.41
1:D:139:PHE:CE2	1:D:175:MET:HB2	2.52	0.41
2:E:11:LEU:HD21	2:E:13:ARG:NH2	2.36	0.41
2:E:59:ILE:C	2:E:60:TYR:HD1	2.28	0.41
3:F:169:LYS:HE2	3:F:169:LYS:HB2	1.24	0.41
3:F:176:LEU:HD13	3:F:176:LEU:HA	1.84	0.41
2:B:154:VAL:HA	2:B:202:ALA:O	2.21	0.40
3:C:166:LYS:HE2	3:C:166:LYS:HB3	1.93	0.40
1:D:12:TYR:CD2	1:D:105:GLU:HB3	2.57	0.40
2:E:174:LEU:HD12	2:E:174:LEU:HA	1.74	0.40
1:A:155:ARG:H	1:A:155:ARG:HG3	1.65	0.40
2:B:87:THR:O	2:B:89:GLU:N	2.54	0.40
2:B:145:LEU:HD21	2:B:147:LYS:CD	2.48	0.40
2:B:157:THR:O	2:B:200:ASN:OD1	2.40	0.40
3:C:69:GLN:O	3:C:102:PRO:HD2	2.20	0.40
3:C:154:THR:HB	3:C:190:GLN:HG2	2.04	0.40
3:F:51:TYR:CE1	3:F:78:TYR:CE2	3.09	0.40
1:A:92:GLY:C	1:A:93:GLU:HG2	2.47	0.40
2:B:52:ASP:C	2:B:54:GLU:N	2.78	0.40
3:C:204:ASP:OD1	3:C:204:ASP:N	2.54	0.40
3:F:34:TYR:HB3	3:F:75:VAL:HG12	2.02	0.40
1:A:192:TYR:HB2	1:A:209:PHE:CE1	2.56	0.40
2:B:3:GLN:HG2	2:B:25:SER:HB2	2.03	0.40
1:D:131:SER:OG	1:D:180:THR:HG23	2.22	0.40
2:E:117:SER:OG	2:E:118:ALA:N	2.54	0.40
2:E:181:LEU:CG	2:E:182:SER:N	2.84	0.40
1:A:142:LYS:HB2	1:A:173:TYR:CE1	2.57	0.40
2:B:121:THR:O	2:B:149:TYR:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:THR:CG2	2:B:213:LYS:HE3	2.49	0.40
3:C:192:VAL:HA	3:C:200:ARG:O	2.22	0.40
2:E:27:PHE:HD2	2:E:32:TYR:CD2	2.40	0.40
3:F:29:PRO:HA	3:F:34:TYR:OH	2.21	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%)	176 (83%)	29 (14%)	7 (3%)	3	17
1	D	212/214 (99%)	177 (84%)	29 (14%)	6 (3%)	4	21
2	B	212/214 (99%)	177 (84%)	26 (12%)	9 (4%)	2	13
2	E	212/214 (99%)	175 (82%)	30 (14%)	7 (3%)	3	17
3	C	196/219 (90%)	158 (81%)	31 (16%)	7 (4%)	2	16
3	F	196/219 (90%)	161 (82%)	29 (15%)	6 (3%)	3	19
All	All	1240/1294 (96%)	1024 (83%)	174 (14%)	42 (3%)	3	17

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
1	A	153	SER
2	B	41	PRO
2	B	56	GLY
3	C	5	ASN
3	C	51	TYR
3	C	130	GLU
1	D	56	ASP

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Mol	Chain	Res	Type
1	D	153	SER
2	E	10	GLU
2	E	56	GLY
2	E	101	SER
3	F	44	ASP
1	A	154	GLU
2	B	7	SER
2	B	101	SER
2	B	132	SER
1	D	154	GLU
2	E	41	PRO
3	F	42	SER
3	F	81	GLY
3	F	160	SER
1	A	27	GLN
2	B	177	ASP
3	C	40	THR
3	C	160	SER
1	D	110	ASP
1	D	184	ASP
2	E	54	GLU
3	F	40	THR
3	C	124	ASN
2	E	165	SER
2	E	177	ASP
1	A	184	ASP
1	A	204	PRO
2	B	163	LEU
1	D	152	GLY
3	F	161	SER
1	A	16	GLY
2	B	176	SER
3	C	198	VAL
2	B	53	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	191/191 (100%)	149 (78%)	42 (22%)	1	5
1	D	191/191 (100%)	149 (78%)	42 (22%)	1	5
2	B	185/185 (100%)	153 (83%)	32 (17%)	2	10
2	E	185/185 (100%)	161 (87%)	24 (13%)	4	19
3	C	186/200 (93%)	156 (84%)	30 (16%)	2	12
3	F	186/200 (93%)	152 (82%)	34 (18%)	2	9
All	All	1124/1152 (98%)	920 (82%)	204 (18%)	2	9

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	2	ILE
1	A	11	MET
1	A	14	SER
1	A	17	GLU
1	A	22	THR
1	A	29	ILE
1	A	42	LYS
1	A	54	LEU
1	A	56	ASP
1	A	67	SER
1	A	73	LEU
1	A	77	SER
1	A	83	THR
1	A	89	LEU
1	A	102	THR
1	A	104	LEU
1	A	105	GLU
1	A	107	ASN
1	A	108	ARG
1	A	122	SER
1	A	143	ASP
1	A	144	ILE
1	A	145	ASN
1	A	146	VAL
1	A	153	SER
1	A	154	GLU
1	A	155	ARG
1	A	159	VAL
1	A	160	LEU

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Mol	Chain	Res	Type
1	A	165	ASP
1	A	166	GLN
1	A	175	MET
1	A	181	LEU
1	A	184	ASP
1	A	185	GLU
1	A	199	LYS
1	A	200	THR
1	A	203	SER
1	A	205	ILE
1	A	213	GLU
1	A	214	CYS
2	B	5	GLN
2	B	7	SER
2	B	12	VAL
2	B	17	LEU
2	B	18	VAL
2	B	22	CYS
2	B	30	LYS
2	B	41	PRO
2	B	57	ASN
2	B	58	THR
2	B	62	PRO
2	B	74	THR
2	B	77	ASN
2	B	81	LEU
2	B	84	SER
2	B	123	PRO
2	B	135	GLN
2	B	136	THR
2	B	139	MET
2	B	144	CYS
2	B	152	GLU
2	B	154	VAL
2	B	155	THR
2	B	157	THR
2	B	162	SER
2	B	178	LEU
2	B	181	LEU
2	B	189	SER
2	B	195	GLU
2	B	198	THR

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Mol	Chain	Res	Type
2	B	199	CYS
2	B	200	ASN
3	C	4	THR
3	C	7	VAL
3	C	16	SER
3	C	23	LEU
3	C	28	LYS
3	C	33	VAL
3	C	35	THR
3	C	44	ASP
3	C	47	SER
3	C	48	LYS
3	C	53	THR
3	C	56	GLU
3	C	61	ASP
3	C	63	ILE
3	C	102	PRO
3	C	105	GLU
3	C	115	SER
3	C	117	GLU
3	C	130	GLU
3	C	132	THR
3	C	138	ASN
3	C	149	LYS
3	C	152	ILE
3	C	163	SER
3	C	172	THR
3	C	176	LEU
3	C	177	ILE
3	C	195	SER
3	C	203	THR
3	C	210	MET
1	D	1	ASP
1	D	2	ILE
1	D	7	SER
1	D	11	MET
1	D	12	TYR
1	D	17	GLU
1	D	19	VAL
1	D	22	THR
1	D	33	LEU
1	D	42	LYS

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Mol	Chain	Res	Type
1	D	48	ILE
1	D	56	ASP
1	D	67	SER
1	D	73	LEU
1	D	77	SER
1	D	83	THR
1	D	102	THR
1	D	105	GLU
1	D	107	ASN
1	D	108	ARG
1	D	122	SER
1	D	133	VAL
1	D	143	ASP
1	D	145	ASN
1	D	146	VAL
1	D	154	GLU
1	D	155	ARG
1	D	159	VAL
1	D	160	LEU
1	D	165	ASP
1	D	166	GLN
1	D	175	MET
1	D	184	ASP
1	D	185	GLU
1	D	194	CYS
1	D	199	LYS
1	D	200	THR
1	D	203	SER
1	D	204	PRO
1	D	205	ILE
1	D	213	GLU
1	D	214	CYS
2	E	2	ILE
2	E	5	GLN
2	E	17	LEU
2	E	30	LYS
2	E	43	GLN
2	E	48	ILE
2	E	57	ASN
2	E	73	ASP
2	E	77	ASN
2	E	81	LEU

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Mol	Chain	Res	Type
2	E	135	GLN
2	E	136	THR
2	E	139	MET
2	E	144	CYS
2	E	152	GLU
2	E	154	VAL
2	E	165	SER
2	E	175	GLN
2	E	176	SER
2	E	178	LEU
2	E	195	GLU
2	E	198	THR
2	E	199	CYS
2	E	200	ASN
3	F	4	THR
3	F	7	VAL
3	F	13	THR
3	F	27	PRO
3	F	28	LYS
3	F	35	THR
3	F	42	SER
3	F	48	LYS
3	F	53	THR
3	F	61	ASP
3	F	70	THR
3	F	75	VAL
3	F	93	LEU
3	F	101	THR
3	F	115	SER
3	F	117	GLU
3	F	126	THR
3	F	139	THR
3	F	143	LEU
3	F	149	LYS
3	F	152	ILE
3	F	165	LYS
3	F	167	THR
3	F	169	LYS
3	F	172	THR
3	F	174	GLU
3	F	176	LEU
3	F	190	GLN

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Mol	Chain	Res	Type
3	F	194	PRO
3	F	197	THR
3	F	198	VAL
3	F	199	ASN
3	F	201	LYS
3	F	203	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	34	ASN
1	A	91	HIS
1	A	124	GLN
1	A	145	ASN
1	A	156	GLN
2	B	6	GLN
2	B	28	ASN
2	B	57	ASN
2	B	77	ASN
3	C	69	GLN
3	C	118	GLN
3	C	124	ASN
3	C	184	ASN
1	D	34	ASN
1	D	37	GLN
1	D	38	GLN
1	D	124	GLN
1	D	145	ASN
1	D	210	ASN
2	E	3	GLN
2	E	5	GLN
2	E	6	GLN
2	E	28	ASN
2	E	39	GLN
2	E	77	ASN
2	E	175	GLN
3	F	11	ASN
3	F	32	GLN
3	F	37	GLN
3	F	114	GLN
3	F	118	GLN

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Mol	Chain	Res	Type
3	F	124	ASN
3	F	137	ASN
3	F	190	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.