



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:53 AM UTC

PDB ID : 3BYT / pdb_00003byt
Title : A complex between a variant of staphylococcal enterotoxin C3 and the variable domain of the murine T cell receptor beta chain 8.2
Authors : Cho, S.; Eric, J.S.
Deposited on : 2008-01-16
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

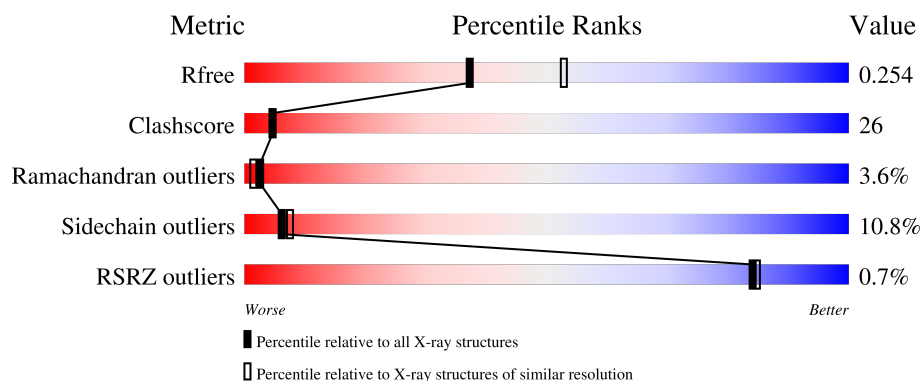
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	109	2% 38% 44% 16% .
1	C	109	39% 35% 22% 5%
1	E	109	31% 51% 15% .
1	G	109	2% 36% 46% 15% .
2	B	239	40% 38% 17% .

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Mol	Chain	Length	Quality of chain
2	D	239	% 37%43%15%
2	F	239	33%44%18%
2	H	239	% 36%43%15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11054 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 T cell receptor beta chain 8.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			
1	C	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			
1	E	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			
1	G	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			

- Molecule 2 is a protein called Enterotoxin type C-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	232	Total	C	N	O	S	0	0	0
			1900	1205	312	373	10			
2	D	233	Total	C	N	O	S	0	0	0
			1906	1208	313	375	10			
2	F	234	Total	C	N	O	S	0	0	0
			1917	1215	315	377	10			
2	H	230	Total	C	N	O	S	0	0	0
			1873	1186	307	370	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	SEE REMARK 999	UNP P0A0L5
B	?	-	GLY	SEE REMARK 999	UNP P0A0L5
B	100B	ALA	-	SEE REMARK 999	UNP P0A0L5
B	101	SER	VAL	SEE REMARK 999	UNP P0A0L5
B	103	TRP	-	SEE REMARK 999	UNP P0A0L5
B	104	HIS	GLY	SEE REMARK 999	UNP P0A0L5
D	?	-	VAL	SEE REMARK 999	UNP P0A0L5
D	?	-	GLY	SEE REMARK 999	UNP P0A0L5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	100B	ALA	-	SEE REMARK 999	UNP P0A0L5
D	101	SER	VAL	SEE REMARK 999	UNP P0A0L5
D	103	TRP	-	SEE REMARK 999	UNP P0A0L5
D	104	HIS	GLY	SEE REMARK 999	UNP P0A0L5
F	?	-	VAL	SEE REMARK 999	UNP P0A0L5
F	?	-	GLY	SEE REMARK 999	UNP P0A0L5
F	100B	ALA	-	SEE REMARK 999	UNP P0A0L5
F	101	SER	VAL	SEE REMARK 999	UNP P0A0L5
F	103	TRP	-	SEE REMARK 999	UNP P0A0L5
F	104	HIS	GLY	SEE REMARK 999	UNP P0A0L5
H	?	-	VAL	SEE REMARK 999	UNP P0A0L5
H	?	-	GLY	SEE REMARK 999	UNP P0A0L5
H	100B	ALA	-	SEE REMARK 999	UNP P0A0L5
H	101	SER	VAL	SEE REMARK 999	UNP P0A0L5
H	103	TRP	-	SEE REMARK 999	UNP P0A0L5
H	104	HIS	GLY	SEE REMARK 999	UNP P0A0L5

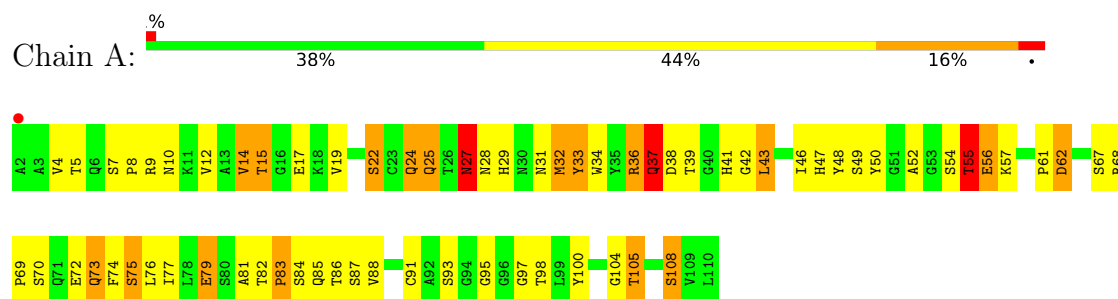
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	21	Total O 21 21	0	0
3	C	14	Total O 14 14	0	0
3	D	27	Total O 27 27	0	0
3	E	12	Total O 12 12	0	0
3	F	23	Total O 23 23	0	0
3	G	10	Total O 10 10	0	0
3	H	28	Total O 28 28	0	0

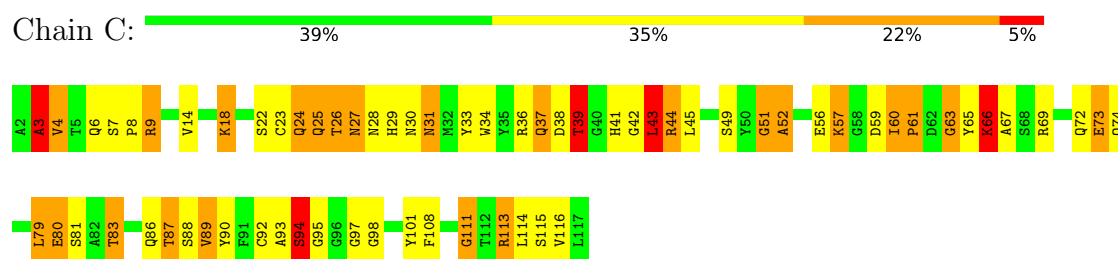
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

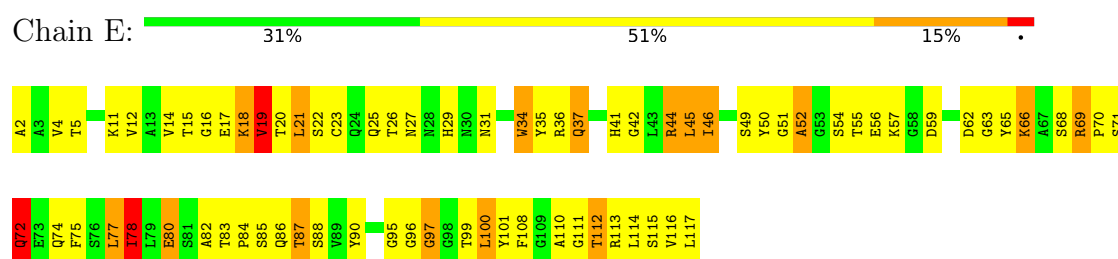
- Molecule 1: T cell receptor beta chain 8.2



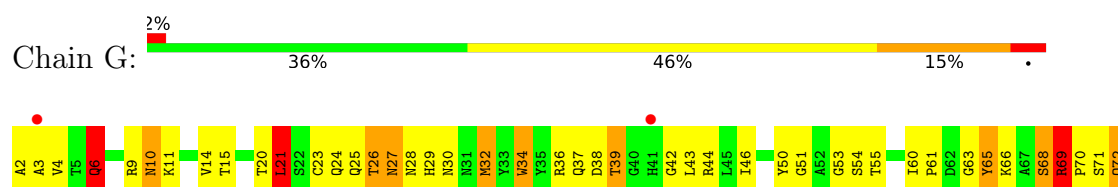
- Molecule 1: T cell receptor beta chain 8.2

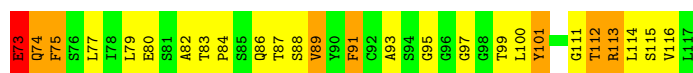


- Molecule 1: T cell receptor beta chain 8.2



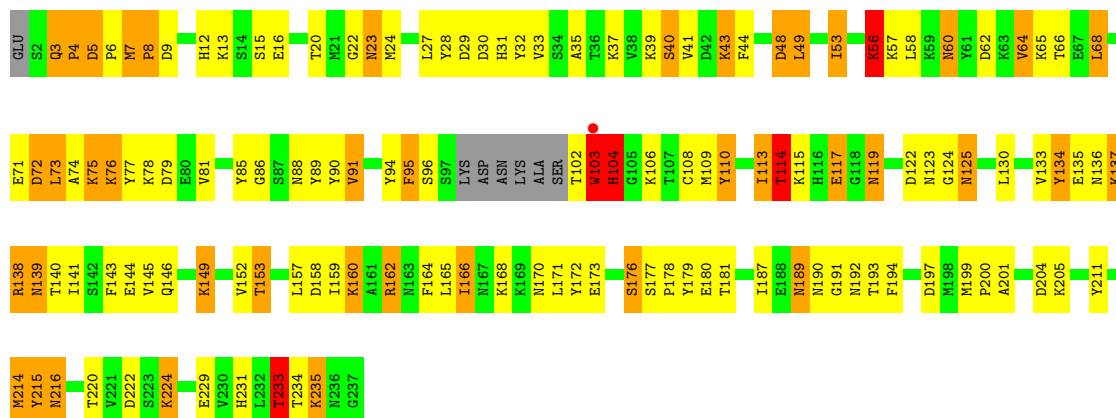
- Molecule 1: T cell receptor beta chain 8.2





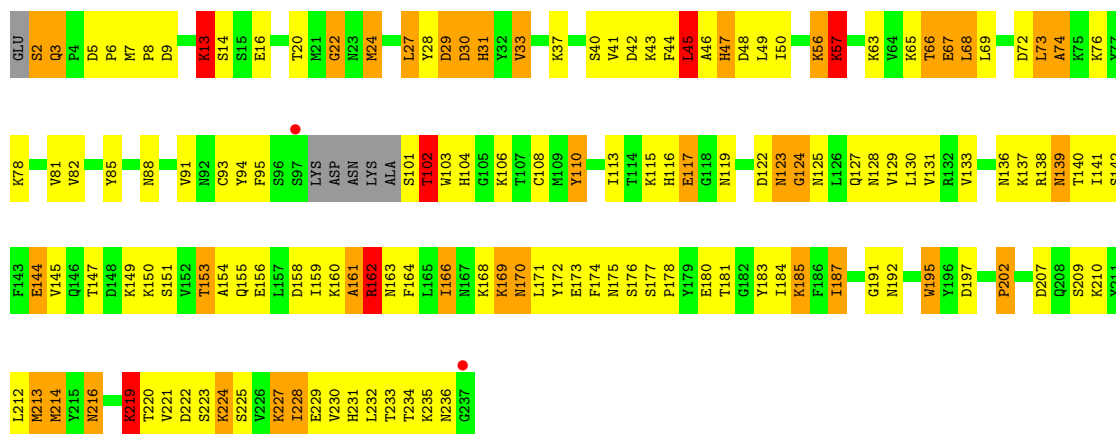
• Molecule 2: Enterotoxin type C-3

Chain B: 40% 38% 17% . .



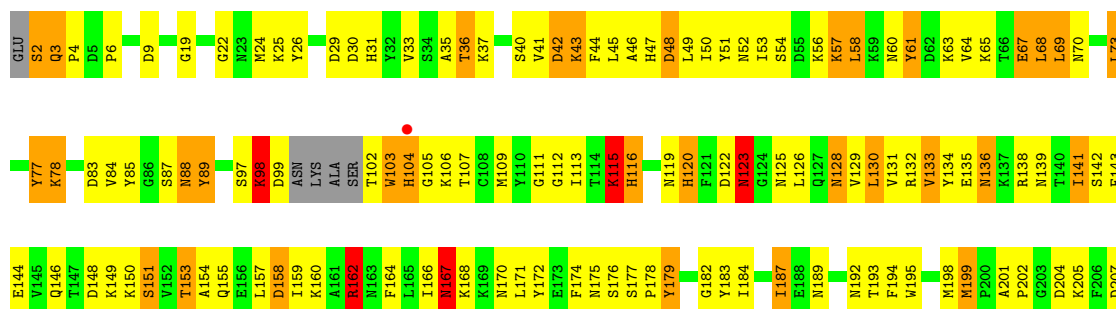
• Molecule 2: Enterotoxin type C-3

Chain D: 37% 43% 15% . .



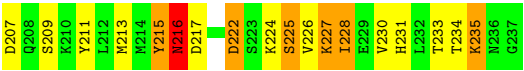
• Molecule 2: Enterotoxin type C-3

Chain F: 33% 44% 18% . .





• Molecule 2: Enterotoxin type C-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.16Å 70.64Å 98.84Å 74.78° 75.16° 88.26°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (30.00-2.30) 95.2 (30.00-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.278 (Not available) , 0.254	Depositor DCC
R_{free} test set	3424 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11054	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.30	34/846 (4.0%)	1.86	26/1145 (2.3%)
1	C	2.41	38/846 (4.5%)	1.92	17/1145 (1.5%)
1	E	2.22	26/846 (3.1%)	1.82	20/1145 (1.7%)
1	G	2.12	25/846 (3.0%)	1.72	12/1145 (1.0%)
2	B	2.05	39/1943 (2.0%)	1.68	28/2617 (1.1%)
2	D	2.22	72/1949 (3.7%)	1.75	28/2625 (1.1%)
2	F	2.12	61/1960 (3.1%)	1.71	34/2639 (1.3%)
2	H	2.06	49/1913 (2.6%)	1.69	22/2574 (0.9%)
All	All	2.16	344/11149 (3.1%)	1.75	187/15035 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (344) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	52	ALA	CA-CB	15.86	1.78	1.53
1	G	101	TYR	C-N	14.80	1.53	1.33
1	C	63	GLY	C-N	13.02	1.50	1.33
1	E	63	GLY	C-N	11.55	1.49	1.33
2	H	184	ILE	CA-CB	10.54	1.65	1.53
1	C	60	ILE	CA-CB	10.36	1.67	1.54
1	A	19	VAL	N-CA	10.27	1.58	1.46
1	A	81	ALA	CA-CB	-10.18	1.36	1.53
1	E	100	LEU	C-O	-9.88	1.12	1.23
1	E	101	TYR	C-N	9.88	1.47	1.33
2	H	230	VAL	CA-CB	-9.74	1.42	1.54
2	F	201	ALA	CA-CB	9.45	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	THR	CB-CG2	9.44	1.83	1.52
1	A	19	VAL	C-O	-9.39	1.14	1.24
2	D	142	SER	C-O	9.37	1.35	1.23
2	D	56	LYS	CA-C	9.25	1.62	1.53
1	A	75	SER	C-O	-9.24	1.12	1.23
2	D	74	ALA	CA-CB	-9.18	1.38	1.53
2	H	39	LYS	N-CA	8.97	1.56	1.46
2	B	143	PHE	C-O	-8.82	1.14	1.23
2	D	166	ILE	C-O	-8.75	1.14	1.24
2	F	97	SER	CA-C	8.65	1.56	1.52
2	F	50	ILE	CA-CB	8.45	1.65	1.54
2	D	235	LYS	N-CA	8.40	1.57	1.46
2	B	204	ASP	C-O	-8.39	1.12	1.23
1	G	54	SER	N-CA	8.36	1.56	1.46
2	F	166	ILE	CA-CB	8.35	1.63	1.54
2	F	22	GLY	C-O	-8.32	1.13	1.23
2	F	56	LYS	C-O	8.31	1.30	1.23
2	B	135	GLU	CA-C	-8.30	1.42	1.52
2	D	164	PHE	C-O	-8.30	1.14	1.24
1	E	86	GLN	CA-C	-8.26	1.41	1.52
1	C	29	HIS	C-O	-8.22	1.14	1.23
1	E	80	GLU	CG-CD	8.22	1.72	1.52
2	D	214	MET	N-CA	-8.20	1.36	1.46
2	F	233	THR	C-O	-8.19	1.13	1.23
2	D	228	ILE	CA-CB	8.02	1.64	1.54
2	H	200	PRO	C-O	8.02	1.32	1.23
2	H	172	TYR	C-O	-7.94	1.15	1.24
2	B	44	PHE	CA-C	7.86	1.59	1.52
1	A	73	GLN	C-O	-7.86	1.14	1.24
2	F	214	MET	CA-C	7.81	1.64	1.52
2	H	179	TYR	N-CA	7.71	1.54	1.45
2	D	145	VAL	CA-CB	7.67	1.65	1.54
1	E	20	THR	C-O	7.53	1.32	1.23
2	D	133	VAL	CA-CB	7.52	1.63	1.54
2	F	60	ASN	CA-CB	7.46	1.64	1.54
1	A	46	ILE	C-O	-7.44	1.15	1.23
1	E	56	GLU	CA-C	7.41	1.61	1.52
1	C	37	GLN	N-CA	7.41	1.55	1.46
1	G	6	GLN	N-CA	7.38	1.55	1.46
2	B	189	ASN	C-O	7.33	1.32	1.24
2	D	129	VAL	C-O	-7.22	1.16	1.24
2	B	49	LEU	C-O	-7.22	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	163	ASN	N-CA	-7.21	1.37	1.46
1	G	30	ASN	CA-C	-7.20	1.42	1.52
1	C	114	LEU	CA-C	-7.14	1.43	1.52
2	F	221	VAL	C-O	7.12	1.32	1.23
1	C	111	GLY	N-CA	7.11	1.51	1.45
1	E	86	GLN	N-CA	7.08	1.55	1.46
1	E	90	TYR	CA-C	-7.04	1.44	1.52
2	D	187	ILE	CA-C	7.04	1.61	1.52
2	D	110	TYR	N-CA	7.04	1.54	1.45
2	H	169	LYS	CA-C	-7.02	1.44	1.52
2	B	201	ALA	CA-CB	-7.00	1.41	1.53
2	D	173	GLU	C-O	6.98	1.32	1.24
2	F	64	VAL	CA-CB	6.97	1.64	1.54
2	H	46	ALA	CA-C	6.96	1.62	1.52
1	E	110	ALA	C-O	-6.93	1.15	1.24
2	D	27	LEU	CG-CD1	6.92	1.75	1.52
2	D	56	LYS	C-O	6.92	1.31	1.23
2	D	42	ASP	CA-C	6.88	1.61	1.52
1	C	39	THR	CB-CG2	6.87	1.75	1.52
2	H	211	TYR	N-CA	6.86	1.55	1.46
1	C	14	VAL	N-CA	6.85	1.54	1.46
2	B	177	SER	CA-C	-6.84	1.45	1.52
2	D	172	TYR	N-CA	6.83	1.54	1.46
2	H	91	VAL	C-O	6.82	1.30	1.23
2	B	114	THR	CA-C	6.82	1.60	1.52
2	D	40	SER	N-CA	6.81	1.54	1.46
2	D	236	ASN	N-CA	6.81	1.54	1.46
1	E	52	ALA	CA-CB	6.78	1.64	1.53
2	D	219	LYS	CA-C	-6.78	1.44	1.52
2	H	209	SER	CA-C	-6.75	1.44	1.52
2	F	176	SER	N-CA	6.75	1.54	1.46
2	D	33	VAL	CA-CB	6.74	1.63	1.54
2	F	130	LEU	N-CA	-6.74	1.37	1.46
2	H	117	GLU	C-O	-6.73	1.15	1.23
2	H	160	LYS	C-O	-6.72	1.16	1.24
2	F	227	LYS	CG-CD	6.70	1.72	1.52
1	A	79	GLU	CG-CD	6.69	1.68	1.52
1	C	41	HIS	C-O	6.67	1.32	1.24
2	H	122	ASP	CA-C	6.64	1.61	1.52
2	F	133	VAL	CA-CB	-6.63	1.46	1.54
2	D	161	ALA	CA-C	-6.63	1.44	1.52
1	A	5	THR	CA-C	6.63	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	147	THR	C-O	-6.63	1.15	1.23
2	H	156	GLU	C-O	-6.63	1.16	1.24
2	D	27	LEU	C-O	6.61	1.32	1.24
1	C	43	LEU	CA-C	-6.59	1.44	1.52
2	F	208	GLN	CA-C	-6.58	1.44	1.52
2	D	45	LEU	CG-CD1	6.58	1.74	1.52
2	H	222	ASP	CA-CB	6.58	1.61	1.53
2	D	137	LYS	CA-C	6.57	1.62	1.52
2	D	229	GLU	C-O	-6.57	1.15	1.23
2	H	207	ASP	CA-C	-6.57	1.44	1.52
1	E	100	LEU	CA-C	-6.56	1.44	1.52
2	D	102	THR	CA-C	6.51	1.61	1.52
2	D	153	THR	CA-CB	6.50	1.63	1.53
2	F	218	ASN	CA-C	6.49	1.61	1.53
1	G	65	TYR	CA-C	6.48	1.60	1.52
2	F	167	ASN	C-O	-6.47	1.16	1.24
2	F	141	ILE	CB-CG1	6.46	1.66	1.53
2	F	44	PHE	CA-C	-6.44	1.48	1.52
2	F	46	ALA	CA-CB	6.43	1.64	1.53
2	F	160	LYS	CA-C	6.42	1.61	1.52
2	B	62	ASP	CA-C	-6.41	1.44	1.52
2	D	195	TRP	CA-C	6.41	1.60	1.52
2	F	77	TYR	N-CA	6.41	1.54	1.46
2	F	184	ILE	CA-CB	6.40	1.61	1.54
1	A	7	SER	CA-C	6.39	1.59	1.53
2	F	201	ALA	N-CA	6.39	1.53	1.45
2	F	162	ARG	CA-CB	-6.38	1.43	1.53
1	A	77	ILE	N-CA	-6.36	1.38	1.46
1	E	54	SER	CA-C	6.35	1.60	1.52
2	B	4	PRO	N-CA	6.34	1.54	1.47
2	D	202	PRO	CA-C	6.34	1.60	1.52
1	C	81	SER	N-CA	-6.33	1.39	1.46
2	B	7	MET	CB-CG	6.30	1.71	1.52
1	A	5	THR	CA-CB	6.29	1.62	1.53
1	C	39	THR	CA-CB	6.26	1.64	1.53
1	G	101	TYR	CA-C	-6.26	1.45	1.52
2	D	192	ASN	N-CA	6.25	1.54	1.46
2	B	197	ASP	N-CA	6.24	1.54	1.46
2	B	233	THR	CA-C	-6.22	1.45	1.52
1	A	39	THR	C-O	6.22	1.31	1.23
2	B	44	PHE	N-CA	6.20	1.52	1.46
2	F	210	LYS	CA-C	-6.20	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	44	ARG	CZ-NH1	6.18	1.41	1.32
2	B	235	LYS	N-CA	6.16	1.54	1.46
2	H	11	LEU	N-CA	6.15	1.53	1.46
2	B	200	PRO	N-CA	-6.12	1.40	1.46
2	F	61	TYR	N-CA	6.11	1.53	1.46
2	F	103	TRP	N-CA	6.11	1.54	1.46
2	D	33	VAL	CA-C	6.11	1.60	1.52
1	C	39	THR	CA-C	6.11	1.60	1.52
2	F	228	ILE	CA-CB	6.07	1.63	1.54
2	F	141	ILE	CB-CG2	6.04	1.72	1.52
1	A	104	GLY	C-O	-6.03	1.16	1.23
2	B	90	TYR	C-N	6.02	1.41	1.33
2	D	223	SER	N-CA	6.01	1.53	1.46
2	H	158	ASP	N-CA	6.00	1.53	1.46
2	D	30	ASP	N-CA	5.99	1.53	1.46
1	E	71	SER	N-CA	5.98	1.53	1.45
2	D	169	LYS	CA-C	5.95	1.60	1.52
2	B	146	GLN	CA-C	-5.95	1.45	1.52
1	E	55	THR	CA-C	-5.94	1.47	1.53
2	B	41	VAL	CA-CB	5.94	1.62	1.54
2	F	179	TYR	CA-C	-5.93	1.45	1.52
2	B	220	THR	CA-C	5.92	1.59	1.52
1	E	5	THR	C-O	-5.92	1.17	1.24
1	C	24	GLN	CG-CD	5.91	1.66	1.52
2	F	53	ILE	CA-CB	5.90	1.61	1.53
2	F	157	LEU	C-O	5.89	1.31	1.24
2	H	72	ASP	C-O	5.89	1.31	1.24
1	A	93	SER	CA-C	5.88	1.59	1.52
2	D	102	THR	CA-CB	5.88	1.63	1.53
2	B	200	PRO	C-O	5.88	1.30	1.23
1	C	33	TYR	C-O	-5.87	1.16	1.23
1	G	111	GLY	N-CA	5.85	1.52	1.45
1	A	70	SER	N-CA	5.83	1.53	1.46
2	F	35	ALA	CA-C	-5.83	1.45	1.52
1	E	85	SER	N-CA	-5.83	1.38	1.46
1	C	89	VAL	CA-C	5.83	1.60	1.52
2	D	149	LYS	N-CA	-5.83	1.38	1.46
1	E	87	THR	C-O	5.83	1.30	1.23
1	A	37	GLN	N-CA	5.82	1.53	1.46
2	H	83	ASP	N-CA	5.80	1.52	1.45
2	D	63	LYS	CE-NZ	5.79	1.66	1.49
1	A	75	SER	CA-C	-5.79	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	86	GLY	C-O	-5.78	1.18	1.23
1	C	25	GLN	CD-OE1	-5.78	1.12	1.23
2	F	70	ASN	CA-CB	5.75	1.61	1.53
2	D	168	LYS	CA-C	5.75	1.60	1.52
1	A	55	THR	C-O	5.75	1.31	1.24
2	D	124	GLY	C-O	5.75	1.31	1.23
1	G	61	PRO	CA-C	5.73	1.60	1.52
1	E	51	GLY	N-CA	5.73	1.50	1.45
1	C	87	THR	CA-CB	5.73	1.62	1.53
2	H	234	THR	CA-C	5.73	1.59	1.52
1	G	20	THR	CA-CB	5.72	1.61	1.52
2	D	185	LYS	N-CA	5.72	1.53	1.46
1	C	113	ARG	N-CA	5.71	1.53	1.46
2	D	57	LYS	CA-C	5.71	1.60	1.52
2	D	46	ALA	CA-CB	5.71	1.62	1.53
2	H	125	ASN	CA-C	5.71	1.60	1.52
1	A	14	VAL	CA-CB	5.68	1.61	1.54
1	C	28	ASN	CA-C	-5.68	1.45	1.52
2	H	171	LEU	C-O	5.68	1.31	1.24
1	C	18	LYS	CE-NZ	5.68	1.66	1.49
1	E	72	GLN	C-O	5.67	1.30	1.24
2	D	24	MET	CA-C	-5.66	1.45	1.52
2	F	87	SER	CA-C	-5.65	1.45	1.52
2	H	225	SER	C-O	5.65	1.29	1.24
2	H	36	THR	CA-C	5.65	1.59	1.52
1	G	91	PHE	N-CA	5.64	1.53	1.46
2	F	78	LYS	CD-CE	5.64	1.69	1.52
1	C	31	ASN	C-O	-5.64	1.17	1.23
2	F	160	LYS	N-CA	5.62	1.53	1.46
1	G	112	THR	CA-CB	5.60	1.62	1.53
1	G	69	ARG	CA-C	5.60	1.59	1.52
1	E	57	LYS	CD-CE	5.57	1.69	1.52
2	B	117	GLU	CA-C	5.56	1.60	1.52
1	G	53	GLY	CA-C	-5.56	1.44	1.51
1	A	36	ARG	N-CA	-5.56	1.39	1.46
2	H	122	ASP	N-CA	5.56	1.53	1.46
2	D	29	ASP	C-O	-5.54	1.16	1.23
2	D	221	VAL	CA-C	5.53	1.59	1.52
1	A	25	GLN	N-CA	-5.53	1.39	1.46
1	A	15	THR	N-CA	-5.51	1.39	1.46
2	D	88	ASN	CG-ND2	-5.51	1.21	1.33
2	D	129	VAL	CA-CB	5.51	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	161	ALA	CA-CB	5.50	1.61	1.53
1	A	108	SER	CA-C	-5.49	1.46	1.52
2	H	79	ASP	CA-CB	-5.49	1.46	1.54
2	H	168	LYS	CG-CD	5.49	1.69	1.52
2	D	161	ALA	CA-CB	-5.49	1.45	1.53
2	H	49	LEU	N-CA	5.49	1.52	1.45
2	F	158	ASP	C-O	5.47	1.30	1.24
1	A	43	LEU	C-O	-5.47	1.17	1.24
1	E	77	LEU	C-O	5.47	1.30	1.24
1	G	71	SER	C-O	-5.46	1.17	1.24
1	G	21	LEU	N-CA	5.45	1.52	1.46
2	H	148	ASP	CA-C	5.45	1.60	1.52
2	F	128	ASN	C-O	-5.43	1.17	1.23
2	D	63	LYS	CB-CG	5.43	1.68	1.52
2	F	89	TYR	CA-C	-5.42	1.46	1.52
2	B	20	THR	CA-C	5.42	1.59	1.52
1	C	45	LEU	CA-C	-5.42	1.45	1.52
1	C	98	GLY	C-O	-5.42	1.16	1.23
2	H	230	VAL	C-O	-5.41	1.18	1.24
2	D	3	GLN	CA-C	5.41	1.59	1.53
2	F	4	PRO	CA-C	5.40	1.58	1.52
1	G	51	GLY	C-O	5.40	1.30	1.23
1	C	25	GLN	CB-CG	-5.39	1.36	1.52
2	H	202	PRO	C-O	5.39	1.30	1.23
2	B	205	LYS	CG-CD	5.39	1.68	1.52
1	E	112	THR	CA-CB	5.39	1.61	1.53
1	C	61	PRO	C-O	-5.39	1.17	1.24
2	D	178	PRO	CA-C	5.38	1.60	1.52
1	A	39	THR	CA-C	5.38	1.59	1.52
1	C	67	ALA	CA-CB	-5.38	1.43	1.54
2	H	68	LEU	N-CA	5.38	1.53	1.45
2	F	151	SER	N-CA	5.37	1.53	1.46
2	F	208	GLN	C-O	-5.37	1.18	1.24
2	H	68	LEU	CG-CD2	-5.37	1.34	1.52
1	C	80	GLU	CA-C	-5.37	1.46	1.52
1	G	21	LEU	C-O	-5.36	1.17	1.24
2	B	9	ASP	CB-CG	5.36	1.65	1.52
1	G	32	MET	SD-CE	-5.36	1.66	1.79
1	A	14	VAL	CA-C	5.35	1.58	1.52
2	H	25	LYS	CA-CB	-5.35	1.44	1.53
2	F	159	ILE	CA-C	-5.33	1.46	1.52
1	A	61	PRO	CG-CD	-5.33	1.32	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	32	TYR	C-O	-5.32	1.16	1.23
1	A	105	THR	CA-CB	5.31	1.62	1.53
2	H	152	VAL	CA-C	5.31	1.58	1.52
2	D	176	SER	CA-C	-5.30	1.48	1.53
2	H	222	ASP	C-O	5.30	1.30	1.24
1	G	75	PHE	CA-C	5.30	1.58	1.52
2	B	104	HIS	N-CA	5.29	1.53	1.46
2	D	236	ASN	CA-C	5.29	1.59	1.52
2	D	31	HIS	CA-C	-5.27	1.46	1.52
2	D	140	THR	N-CA	5.26	1.52	1.46
1	E	52	ALA	C-O	5.26	1.30	1.23
2	D	93	CYS	CA-C	-5.26	1.46	1.52
2	H	38	VAL	CA-CB	5.26	1.64	1.55
2	B	172	TYR	N-CA	5.26	1.52	1.45
2	H	226	VAL	CA-CB	5.25	1.60	1.54
2	F	148	ASP	CA-C	5.25	1.60	1.52
2	H	87	SER	CA-C	-5.24	1.46	1.52
1	A	76	LEU	C-O	-5.24	1.17	1.23
2	H	84	VAL	CA-CB	5.24	1.61	1.54
1	C	8	PRO	N-CA	5.24	1.56	1.47
2	F	116	HIS	C-O	5.24	1.28	1.23
1	C	44	ARG	CA-C	5.23	1.58	1.52
2	H	43	LYS	CD-CE	5.23	1.68	1.52
2	F	229	GLU	CA-C	5.22	1.58	1.52
2	H	142	SER	C-O	-5.22	1.17	1.23
2	B	134	TYR	N-CA	-5.21	1.39	1.46
2	F	36	THR	CA-C	5.21	1.59	1.52
2	H	86	GLY	CA-C	-5.21	1.45	1.51
2	D	63	LYS	N-CA	-5.20	1.39	1.46
2	H	113	ILE	CA-C	5.20	1.58	1.52
2	B	153	THR	CA-C	5.19	1.59	1.52
2	D	154	ALA	CA-C	5.19	1.59	1.52
2	D	13	LYS	C-O	5.18	1.30	1.23
1	A	75	SER	CB-OG	-5.17	1.31	1.42
1	A	62	ASP	CG-OD2	5.17	1.35	1.25
2	B	35	ALA	N-CA	5.17	1.52	1.46
1	C	95	GLY	CA-C	-5.17	1.48	1.52
2	F	115	LYS	CG-CD	5.17	1.68	1.52
1	G	73	GLU	C-O	-5.15	1.17	1.23
2	D	140	THR	CA-C	5.15	1.59	1.52
2	D	232	LEU	C-O	-5.14	1.17	1.23
1	A	47	HIS	C-O	-5.13	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	44	PHE	CA-C	5.13	1.59	1.53
2	B	171	LEU	CA-C	-5.12	1.45	1.52
1	G	77	LEU	C-O	-5.11	1.17	1.24
2	F	235	LYS	N-CA	5.11	1.52	1.46
2	B	123	ASN	CA-C	5.10	1.59	1.52
2	D	22	GLY	C-O	-5.10	1.17	1.23
2	F	205	LYS	C-O	5.10	1.29	1.23
2	B	23	ASN	CG-ND2	-5.09	1.22	1.33
2	F	131	VAL	CA-C	-5.09	1.46	1.52
1	G	3	ALA	CA-C	5.09	1.59	1.52
2	F	153	THR	CA-C	5.08	1.59	1.52
2	F	43	LYS	CA-C	5.08	1.58	1.52
2	D	177	SER	CA-CB	-5.08	1.44	1.54
1	C	92	CYS	C-O	-5.08	1.17	1.23
1	G	34	TRP	N-CA	5.08	1.52	1.46
2	F	64	VAL	C-O	-5.07	1.18	1.24
2	F	98	LYS	CA-C	5.07	1.59	1.52
1	C	83	THR	C-O	-5.07	1.19	1.24
1	G	42	GLY	C-O	5.07	1.32	1.24
2	F	154	ALA	CA-CB	5.06	1.61	1.53
2	D	236	ASN	CA-CB	5.06	1.62	1.53
2	D	2	SER	CB-OG	5.05	1.52	1.42
2	B	166	ILE	CG1-CD1	-5.04	1.32	1.51
1	C	3	ALA	C-O	-5.04	1.17	1.24
2	F	67	GLU	N-CA	-5.04	1.40	1.46
2	H	4	PRO	CA-C	5.04	1.57	1.52
2	D	67	GLU	CA-C	-5.03	1.46	1.52
1	E	19	VAL	N-CA	5.03	1.51	1.46
2	F	175	ASN	CG-OD1	5.03	1.33	1.23
1	C	3	ALA	N-CA	5.03	1.52	1.46
2	D	197	ASP	N-CA	5.02	1.52	1.46
2	B	178	PRO	CA-CB	5.02	1.60	1.53
1	A	61	PRO	C-O	5.02	1.30	1.24
1	E	80	GLU	CD-OE1	5.02	1.34	1.25
1	C	57	LYS	CE-NZ	5.01	1.64	1.49
1	C	28	ASN	CG-ND2	5.01	1.43	1.33
2	H	50	ILE	CA-CB	5.01	1.61	1.54
2	B	110	TYR	C-O	-5.00	1.17	1.23

All (187) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	GLY	O-C-N	-17.24	102.16	122.33
2	H	120	HIS	N-CA-C	9.48	124.33	110.59
1	C	101	TYR	O-C-N	-9.26	111.73	122.84
2	H	57	LYS	N-CA-C	9.13	122.06	111.11
2	H	73	LEU	N-CA-C	-8.92	101.64	111.36
1	E	56	GLU	N-CA-C	8.77	122.60	110.24
1	E	66	LYS	N-CA-C	-8.64	96.13	109.52
2	D	14	SER	N-CA-C	-8.46	102.01	111.82
2	D	72	ASP	N-CA-C	-8.39	101.83	110.97
1	G	60	ILE	CA-C-N	-8.23	111.33	119.64
1	G	60	ILE	C-N-CA	-8.23	111.33	119.64
2	F	36	THR	N-CA-C	8.18	121.85	108.52
2	B	162	ARG	NE-CZ-NH1	-8.03	113.47	121.50
2	B	165	LEU	N-CA-C	7.98	120.88	111.71
1	E	63	GLY	O-C-N	-7.90	112.40	122.43
2	F	228	ILE	N-CA-C	-7.89	96.70	108.46
2	H	201	ALA	CA-C-N	7.89	127.84	120.03
2	H	201	ALA	C-N-CA	7.89	127.84	120.03
2	D	122	ASP	N-CA-C	7.83	119.59	111.14
1	E	95	GLY	N-CA-C	7.72	122.53	110.71
2	F	24	MET	CG-SD-CE	-7.72	83.92	100.90
1	C	26	THR	N-CA-C	-7.70	98.55	110.17
1	G	89	VAL	CB-CA-C	-7.56	102.82	111.59
2	F	113	ILE	CB-CA-C	-7.55	99.46	110.63
2	D	162	ARG	N-CA-C	7.50	120.34	111.71
1	A	93	SER	CA-C-N	-7.49	117.02	122.18
1	A	93	SER	C-N-CA	-7.49	117.02	122.18
2	D	213	MET	N-CA-C	-7.40	104.13	113.01
2	B	53	ILE	N-CA-C	-7.33	97.05	107.75
2	B	106	LYS	N-CA-C	7.32	121.26	108.75
2	F	106	LYS	N-CA-C	7.30	119.98	107.93
2	D	47	HIS	N-CA-C	7.30	121.11	112.93
1	A	104	GLY	N-CA-C	7.27	118.85	111.95
1	A	27	ASN	N-CA-C	7.26	121.83	113.19
1	E	50	TYR	N-CA-C	7.20	121.38	112.59
1	C	108	PHE	N-CA-C	7.19	120.26	110.55
1	E	51	GLY	CA-C-O	-7.19	114.59	122.14
2	B	22	GLY	N-CA-C	-7.10	106.86	114.67
1	A	50	TYR	N-CA-C	7.07	121.51	113.02
2	D	24	MET	N-CA-C	7.07	118.88	111.03
2	F	225	SER	N-CA-C	6.96	122.44	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30	ASN	N-CA-C	6.90	118.49	110.97
2	D	168	LYS	N-CA-C	6.86	118.75	111.28
2	F	58	LEU	N-CA-C	-6.75	100.23	109.95
2	H	156	GLU	N-CA-C	-6.73	104.02	111.36
1	C	63	GLY	CA-C-N	6.71	133.75	121.94
1	C	63	GLY	C-N-CA	6.71	133.75	121.94
2	D	123	ASN	CA-C-N	-6.69	108.30	121.41
2	D	123	ASN	C-N-CA	-6.69	108.30	121.41
2	B	159	ILE	N-CA-C	-6.67	104.26	110.53
2	F	120	HIS	N-CA-C	6.63	120.28	110.46
1	G	63	GLY	CA-C-N	-6.63	111.99	122.73
1	G	63	GLY	C-N-CA	-6.63	111.99	122.73
1	A	83	PRO	CA-C-N	6.62	130.05	120.38
1	A	83	PRO	C-N-CA	6.62	130.05	120.38
1	G	66	LYS	CB-CG-CD	-6.59	96.14	111.30
2	B	60	ASN	N-CA-C	6.59	121.33	113.16
2	B	160	LYS	N-CA-C	6.55	118.42	111.28
2	H	117	GLU	N-CA-C	6.55	119.87	110.24
2	F	113	ILE	N-CA-C	6.53	117.25	108.11
2	B	215	TYR	CA-C-N	6.51	128.90	120.44
2	B	215	TYR	C-N-CA	6.51	128.90	120.44
1	E	97	GLY	N-CA-C	-6.48	97.83	113.18
2	F	201	ALA	N-CA-C	6.45	117.02	109.60
1	A	12	VAL	N-CA-C	6.44	116.96	106.72
2	F	65	LYS	CD-CE-NZ	-6.42	91.36	111.90
2	B	15	SER	N-CA-C	-6.38	105.35	113.01
2	F	104	HIS	N-CA-C	6.33	118.76	108.76
1	E	21	LEU	N-CA-C	-6.32	99.41	109.59
1	E	55	THR	CB-CA-C	-6.25	101.69	112.44
2	D	41	VAL	N-CA-C	6.24	118.10	112.17
1	A	15	THR	OG1-CB-CG2	-6.22	96.86	109.30
2	F	44	PHE	CA-C-O	-6.21	115.27	119.68
1	C	66	LYS	N-CA-C	-6.20	100.06	109.85
2	F	97	SER	O-C-N	6.19	125.41	120.83
1	A	34	TRP	N-CA-C	-6.17	98.22	108.34
2	F	48	ASP	N-CA-C	6.17	118.33	109.14
1	A	46	ILE	CB-CA-C	-6.14	104.56	111.80
1	C	4	VAL	N-CA-C	6.09	117.56	108.23
2	D	138	ARG	CB-CA-C	6.09	119.87	111.23
2	D	176	SER	N-CA-C	6.06	119.85	108.65
2	H	159	ILE	N-CA-C	6.05	117.52	110.62
2	D	63	LYS	CG-CD-CE	6.05	125.21	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	145	VAL	N-CA-C	-6.04	99.84	109.20
2	D	209	SER	CA-C-N	6.03	128.86	120.29
2	D	209	SER	C-N-CA	6.03	128.86	120.29
1	A	55	THR	N-CA-C	-6.02	97.98	110.80
1	A	108	SER	CA-C-N	-6.00	114.95	123.11
1	A	108	SER	C-N-CA	-6.00	114.95	123.11
2	B	177	SER	CA-C-N	5.97	125.85	119.28
2	B	177	SER	C-N-CA	5.97	125.85	119.28
1	E	111	GLY	N-CA-C	5.96	118.96	112.29
1	C	93	ALA	N-CA-C	-5.95	100.73	109.18
1	A	28	ASN	N-CA-C	5.95	119.63	111.54
1	C	60	ILE	CA-C-N	-5.94	113.86	120.45
1	C	60	ILE	C-N-CA	-5.94	113.86	120.45
2	D	166	ILE	CG1-CB-CG2	-5.94	92.89	110.70
2	F	26	TYR	CA-C-N	5.92	128.21	120.28
2	F	26	TYR	C-N-CA	5.92	128.21	120.28
2	F	215	TYR	CA-C-N	5.92	128.68	120.63
2	F	215	TYR	C-N-CA	5.92	128.68	120.63
2	F	226	VAL	N-CA-C	5.87	117.15	109.58
2	F	22	GLY	N-CA-C	-5.86	105.57	113.24
2	B	214	MET	CG-SD-CE	-5.85	88.03	100.90
1	A	95	GLY	N-CA-C	-5.83	99.37	113.18
1	A	93	SER	O-C-N	-5.83	115.66	123.23
1	A	52	ALA	O-C-N	-5.79	115.77	122.95
2	D	192	ASN	N-CA-C	5.79	118.87	110.42
2	H	133	VAL	N-CA-C	5.78	116.91	108.53
2	F	231	HIS	N-CA-C	5.73	118.00	108.20
2	B	113	ILE	N-CA-C	5.73	116.35	107.99
2	F	187	ILE	N-CA-C	5.73	116.39	107.28
2	F	69	LEU	N-CA-C	5.66	117.31	111.03
2	D	108	CYS	CB-CA-C	-5.66	99.10	110.30
1	E	96	GLY	N-CA-C	-5.63	99.83	113.18
2	B	149	LYS	N-CA-C	-5.63	100.22	109.40
2	F	51	TYR	N-CA-C	-5.63	101.00	109.95
2	H	215	TYR	N-CA-C	-5.58	106.47	113.28
2	B	91	VAL	N-CA-CB	5.57	117.59	110.13
2	B	119	ASN	N-CA-C	5.53	119.65	113.01
1	E	36	ARG	NE-CZ-NH2	5.53	124.18	119.20
2	B	48	ASP	N-CA-C	5.52	118.57	109.85
2	F	54	SER	N-CA-C	5.49	118.25	110.50
2	F	3	GLN	CA-C-N	5.49	126.35	119.98
2	F	3	GLN	C-N-CA	5.49	126.35	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	68	SER	N-CA-C	5.49	117.44	108.55
1	E	78	ILE	N-CA-C	5.48	115.75	107.75
2	D	223	SER	N-CA-C	5.47	117.67	111.11
2	H	191	GLY	N-CA-C	-5.46	107.79	115.32
2	H	125	ASN	N-CA-C	5.45	119.12	109.96
2	F	209	SER	N-CA-C	5.44	116.90	110.97
2	B	103	TRP	CA-CB-CG	5.42	123.89	113.60
2	D	162	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	E	55	THR	N-CA-CB	5.39	120.12	110.79
1	G	50	TYR	N-CA-C	5.37	119.46	113.02
2	D	91	VAL	N-CA-CB	5.37	116.66	110.49
2	B	90	TYR	CA-C-O	-5.36	112.29	119.47
1	E	34	TRP	N-CA-C	5.36	117.15	108.41
2	B	5	ASP	CA-C-N	5.36	126.50	120.66
2	B	5	ASP	C-N-CA	5.36	126.50	120.66
1	A	28	ASN	CB-CA-C	-5.34	104.00	111.80
1	E	45	LEU	CA-C-N	5.33	128.37	120.74
1	E	45	LEU	C-N-CA	5.33	128.37	120.74
2	F	164	PHE	N-CA-C	5.33	116.78	110.97
1	A	57	LYS	CA-C-O	-5.31	115.35	121.19
2	B	88	ASN	N-CA-C	5.29	118.62	110.42
2	H	173	GLU	N-CA-C	-5.29	101.72	109.81
2	D	212	LEU	N-CA-C	-5.26	106.83	113.20
1	C	51	GLY	CA-C-O	-5.24	116.40	121.75
1	G	44	ARG	NH1-CZ-NH2	5.23	126.10	119.30
2	B	179	TYR	N-CA-CB	-5.21	101.78	110.23
1	C	79	LEU	N-CA-C	-5.21	99.92	108.41
1	C	18	LYS	N-CA-C	-5.19	100.27	108.73
2	H	148	ASP	N-CA-C	5.19	119.59	113.16
1	A	73	GLN	N-CA-C	5.18	118.06	109.46
2	H	228	ILE	O-C-N	-5.18	117.59	122.98
2	H	160	LYS	CD-CE-NZ	5.18	128.48	111.90
1	A	52	ALA	CA-C-N	-5.18	115.18	123.31
1	A	52	ALA	C-N-CA	-5.18	115.18	123.31
2	B	64	VAL	N-CA-C	5.17	115.51	107.28
2	F	207	ASP	N-CA-C	5.17	117.13	108.23
1	E	69	ARG	CA-C-N	5.17	126.31	119.84
1	E	69	ARG	C-N-CA	5.17	126.31	119.84
1	A	32	MET	CA-C-O	-5.17	115.07	121.11
2	B	216	ASN	CB-CA-C	-5.16	102.78	110.88
1	G	66	LYS	N-CA-C	-5.15	102.53	109.95
1	C	94	SER	N-CA-C	-5.14	100.65	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	212	LEU	N-CA-C	-5.13	106.52	112.89
1	A	9	ARG	NE-CZ-NH2	5.12	123.80	119.20
2	H	87	SER	CB-CA-C	-5.11	101.91	110.19
2	D	170	ASN	N-CA-CB	-5.10	104.42	112.13
2	D	76	LYS	CD-CE-NZ	-5.09	95.61	111.90
2	D	66	THR	N-CA-C	5.09	117.53	109.24
2	H	110	TYR	N-CA-C	5.08	118.03	109.95
1	G	95	GLY	CA-C-N	5.08	125.48	119.94
1	G	95	GLY	C-N-CA	5.08	125.48	119.94
2	F	204	ASP	N-CA-C	-5.07	108.36	114.75
2	H	7	MET	N-CA-C	-5.07	102.37	108.25
2	H	166	ILE	CA-C-N	5.07	127.33	120.44
2	H	166	ILE	C-N-CA	5.07	127.33	120.44
2	F	141	ILE	CB-CG1-CD1	5.06	124.42	113.80
2	H	94	TYR	N-CA-C	5.04	117.12	108.90
2	D	224	LYS	N-CA-C	5.02	117.49	111.71
1	A	22	SER	N-CA-C	5.02	117.16	110.53
1	C	59	ASP	N-CA-C	-5.01	106.33	112.90
1	E	57	LYS	CB-CG-CD	5.01	122.83	111.30
2	D	161	ALA	N-CA-C	-5.01	104.78	111.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	63	GLY	Mainchain

5.2 Too-close contacts [i](#)

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	828	0	788	36	0
1	C	828	0	788	52	0
1	E	828	0	788	57	0
1	G	828	0	788	51	0
2	B	1900	0	1827	93	0
2	D	1906	0	1832	83	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1917	0	1844	106	1
2	H	1873	0	1804	96	0
3	A	11	0	0	0	0
3	B	21	0	0	1	0
3	C	14	0	0	0	0
3	D	27	0	0	0	0
3	E	12	0	0	0	0
3	F	23	0	0	0	0
3	G	10	0	0	1	0
3	H	28	0	0	0	0
All	All	11054	0	10459	554	1

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 26.

All (554) 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:D:27:LEU:CD1	2:D:27:LEU:CG	1.75	1.60
1:C:52:ALA:CB	1:C:52:ALA:CA	1.78	1.60
1:C:39:THR:CG2	1:C:39:THR:CB	1.75	1.58
1:A:55:THR:CG2	1:A:55:THR:CB	1.83	1.53
2:F:115:LYS:N	2:F:115:LYS:HE3	1.66	1.10
2:F:31:HIS:HA	2:F:57:LYS:NZ	1.68	1.08
1:E:87:THR:HG23	1:E:115:SER:HA	1.27	1.07
2:F:115:LYS:HE3	2:F:115:LYS:H	0.92	1.04
1:E:21:LEU:HD22	1:E:112:THR:HG21	1.39	1.02
2:F:115:LYS:H	2:F:115:LYS:CE	1.72	1.02
1:C:26:THR:O	1:C:27:ASN:HB2	1.59	1.00
2:B:76:LYS:HZ3	2:B:115:LYS:HE2	1.30	0.96
1:C:87:THR:HG23	1:C:115:SER:HA	1.48	0.96
2:H:11:LEU:HD11	2:H:183:TYR:HD2	1.32	0.92
2:H:88:ASN:H	2:H:88:ASN:HD22	1.18	0.92
2:F:99:ASP:HA	2:F:102:THR:CG2	2.02	0.90
2:D:123:ASN:O	2:D:125:ASN:N	2.07	0.88
1:E:26:THR:HG1	1:G:2:ALA:N	1.69	0.88
2:D:45:LEU:HD12	2:D:48:ASP:OD2	1.75	0.85
1:G:55:THR:HG23	2:H:20:THR:HG21	1.59	0.85
1:C:26:THR:O	1:C:27:ASN:CB	2.22	0.84
1:C:22:SER:HB3	1:C:24:GLN:NE2	1.92	0.84
2:F:31:HIS:HA	2:F:57:LYS:HZ1	1.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:88:ASN:H	2:F:88:ASN:HD22	1.24	0.83
2:D:119:ASN:HD21	2:D:151:SER:H	1.25	0.83
1:A:8:PRO:O	1:A:105:THR:HG23	1.78	0.82
1:E:37:GLN:O	1:E:37:GLN:HG3	1.78	0.82
1:G:27:ASN:HB3	3:G:127:HOH:O	1.80	0.81
2:B:102:THR:HG22	2:B:103:TRP:H	1.44	0.81
1:G:36:ARG:HH11	1:G:88:SER:HB2	1.44	0.80
2:B:56:LYS:HB2	2:B:56:LYS:HZ3	1.45	0.80
2:H:110:TYR:HE2	2:H:213:MET:HG3	1.47	0.80
2:B:136:ASN:O	2:B:137:LYS:HB2	1.78	0.80
2:D:47:HIS:CD2	2:H:45:LEU:HD11	2.16	0.80
2:H:11:LEU:HD11	2:H:183:TYR:CD2	2.16	0.79
1:C:9:ARG:NH2	1:C:111:GLY:O	2.14	0.79
1:G:69:ARG:HH21	1:G:69:ARG:HG3	1.46	0.79
2:D:47:HIS:CE1	2:D:67:GLU:HG2	2.19	0.78
2:D:31:HIS:HA	2:D:57:LYS:HE2	1.65	0.77
1:E:87:THR:CG2	1:E:115:SER:HA	2.13	0.77
2:H:110:TYR:CD2	2:H:213:MET:HA	2.19	0.77
2:H:66:THR:HG21	2:H:113:ILE:HD11	1.68	0.76
2:B:43:LYS:HZ2	2:B:43:LYS:HB2	1.49	0.76
2:F:213:MET:O	2:F:216:ASN:HB2	1.85	0.76
1:G:69:ARG:HH21	1:G:69:ARG:CG	1.99	0.76
1:C:22:SER:HB3	1:C:24:GLN:HE22	1.49	0.76
2:B:76:LYS:NZ	2:B:115:LYS:HE2	2.02	0.75
2:H:110:TYR:CE2	2:H:213:MET:HG3	2.22	0.74
2:H:88:ASN:H	2:H:88:ASN:ND2	1.84	0.74
2:B:173:GLU:HB2	2:B:176:SER:O	1.88	0.74
2:B:43:LYS:HE3	2:B:75:LYS:HZ1	1.53	0.74
2:H:115:LYS:HG3	2:H:115:LYS:O	1.86	0.74
2:B:33:VAL:O	2:B:85:TYR:HA	1.88	0.74
1:G:73:GLU:O	1:G:74:GLN:HB2	1.88	0.73
1:E:2:ALA:N	1:G:26:THR:HG1	1.84	0.73
1:G:69:ARG:HG3	1:G:69:ARG:NH2	2.00	0.73
2:B:187:ILE:HA	2:B:193:THR:HG22	1.71	0.73
2:H:8:PRO:O	2:H:13:LYS:NZ	2.22	0.73
2:B:13:LYS:HB3	2:B:180:GLU:OE1	1.89	0.73
2:B:233:THR:HG23	2:B:235:LYS:NZ	2.04	0.73
1:A:32:MET:HE2	1:A:74:PHE:HB3	1.70	0.72
2:B:40:SER:HB3	2:B:78:LYS:O	1.88	0.72
1:G:79:LEU:HD23	1:G:86:GLN:OE1	1.89	0.72
2:D:184:ILE:HG13	2:D:230:VAL:HG22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:GLN:HE21	1:E:72:GLN:HA	1.54	0.71
2:H:35:ALA:HB2	2:H:53:ILE:HD12	1.71	0.71
2:F:99:ASP:HA	2:F:102:THR:HG22	1.73	0.71
2:F:138:ARG:HG2	2:F:138:ARG:HH11	1.54	0.70
1:E:68:SER:C	1:E:70:PRO:HD3	2.17	0.70
1:A:27:ASN:HD22	1:C:27:ASN:ND2	1.90	0.69
2:D:128:ASN:HD22	2:D:144:GLU:HG2	1.58	0.69
2:F:123:ASN:N	2:F:123:ASN:HD22	1.89	0.69
2:F:199:MET:HA	2:F:199:MET:HE2	1.75	0.69
2:B:43:LYS:HD3	2:B:48:ASP:O	1.92	0.69
2:H:110:TYR:N	2:H:110:TYR:CD1	2.57	0.68
2:H:120:HIS:O	2:H:150:LYS:HE3	1.93	0.68
1:A:27:ASN:HD22	1:C:27:ASN:HD21	1.42	0.68
1:C:69:ARG:HD2	1:C:74:GLN:O	1.94	0.68
2:F:99:ASP:HA	2:F:102:THR:HG23	1.73	0.67
2:B:190:ASN:HD21	2:B:192:ASN:HB2	1.60	0.67
2:B:139:ASN:C	2:B:139:ASN:HD22	2.01	0.67
2:F:41:VAL:HG21	2:F:52:ASN:OD1	1.95	0.67
1:G:36:ARG:NH1	1:G:88:SER:HB2	2.10	0.67
2:F:77:TYR:HE2	2:F:115:LYS:HE2	1.60	0.67
2:D:8:PRO:O	2:D:13:LYS:HE3	1.96	0.66
1:G:87:THR:HG23	1:G:114:LEU:O	1.96	0.66
1:E:83:THR:O	1:E:116:VAL:HG11	1.95	0.65
1:A:67:SER:O	1:A:69:PRO:HD3	1.95	0.65
1:C:37:GLN:OE1	1:C:42:GLY:O	2.15	0.65
2:F:89:TYR:HD1	2:F:212:LEU:HD12	1.62	0.65
2:H:35:ALA:CB	2:H:53:ILE:HD12	2.26	0.65
1:C:66:LYS:NZ	1:C:80:GLU:OE1	2.29	0.65
2:D:27:LEU:CD1	2:D:27:LEU:CD2	2.72	0.65
1:E:25:GLN:HE22	1:E:29:HIS:H	1.45	0.65
2:H:213:MET:O	2:H:216:ASN:HB2	1.96	0.65
2:D:27:LEU:CD1	2:D:27:LEU:CB	2.73	0.65
2:H:83:ASP:HB2	2:H:114:THR:OG1	1.96	0.64
1:E:65:TYR:HA	1:E:78:ILE:O	1.97	0.64
2:H:222:ASP:OD1	2:H:225:SER:OG	2.12	0.64
2:F:31:HIS:CA	2:F:57:LYS:HZ1	2.09	0.64
2:D:219:LYS:HD3	2:D:220:THR:N	2.13	0.64
2:D:33:VAL:O	2:D:85:TYR:HA	1.97	0.64
2:D:37:LYS:HZ2	2:D:37:LYS:HB3	1.63	0.64
2:H:110:TYR:N	2:H:110:TYR:HD1	1.96	0.64
2:B:37:LYS:HB3	2:B:37:LYS:HZ2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:GLN:HE21	1:G:72:GLN:HA	1.62	0.64
2:H:199:MET:HE2	2:H:199:MET:HA	1.79	0.63
2:F:155:GLN:NE2	2:F:215:TYR:HB3	2.13	0.63
2:F:167:ASN:N	2:F:167:ASN:HD22	1.94	0.63
2:H:18:THR:OG1	2:H:204:ASP:HB3	1.98	0.63
2:B:68:LEU:HD11	2:B:113:ILE:HD12	1.80	0.63
2:B:3:GLN:HG3	2:B:194:PHE:HA	1.80	0.63
2:H:152:VAL:HG11	2:H:157:LEU:HD21	1.81	0.63
1:A:55:THR:HG22	2:B:23:ASN:OD1	1.99	0.62
2:F:31:HIS:HA	2:F:57:LYS:HZ2	1.61	0.62
1:G:73:GLU:O	1:G:74:GLN:CB	2.47	0.62
1:A:4:VAL:HG21	1:A:100:TYR:O	1.98	0.62
2:D:94:TYR:O	2:D:95:PHE:HB3	1.99	0.61
2:D:213:MET:O	2:D:216:ASN:HB2	2.00	0.61
1:E:68:SER:O	1:E:70:PRO:HD3	2.01	0.61
2:H:137:LYS:HB2	2:H:137:LYS:NZ	2.16	0.61
1:A:22:SER:HB3	1:A:73:GLN:HE22	1.65	0.61
1:C:57:LYS:HB3	1:C:61:PRO:HG3	1.81	0.61
1:G:37:GLN:HG2	1:G:38:ASP:N	2.15	0.61
1:A:36:ARG:CG	1:A:36:ARG:O	2.49	0.60
2:D:47:HIS:HE1	2:D:67:GLU:HG2	1.61	0.60
1:E:26:THR:HG21	1:G:2:ALA:HB2	1.83	0.60
2:B:43:LYS:CE	2:B:75:LYS:NZ	2.63	0.60
2:F:40:SER:HB3	2:F:49:LEU:HD22	1.83	0.60
2:D:130:LEU:HB2	2:D:144:GLU:OE2	2.01	0.60
2:F:194:PHE:CE2	2:F:219:LYS:HE3	2.37	0.60
2:B:24:MET:HE1	2:B:28:TYR:HE1	1.66	0.60
1:E:26:THR:OG1	1:G:2:ALA:N	2.34	0.60
1:E:87:THR:O	1:E:88:SER:HB2	1.99	0.60
1:C:57:LYS:NZ	2:D:175:ASN:HD21	2.00	0.59
2:B:43:LYS:HE2	2:B:75:LYS:HZ3	1.67	0.59
2:B:134:TYR:HD2	2:B:137:LYS:O	1.85	0.59
2:B:233:THR:CG2	2:B:235:LYS:NZ	2.65	0.59
2:D:16:GLU:HB3	2:D:202:PRO:HB3	1.84	0.59
2:H:28:TYR:CE1	2:H:162:ARG:NH1	2.70	0.59
2:F:138:ARG:HG2	2:F:138:ARG:NH1	2.16	0.59
1:C:36:ARG:HD3	1:C:60:ILE:HD12	1.85	0.59
2:F:167:ASN:N	2:F:167:ASN:ND2	2.51	0.59
1:C:80:GLU:OE2	1:C:80:GLU:N	2.35	0.58
2:B:136:ASN:HD21	2:B:234:THR:H	1.51	0.58
2:B:130:LEU:HA	2:B:144:GLU:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:GLN:HE21	1:E:72:GLN:CA	2.15	0.58
1:C:66:LYS:HB2	1:C:66:LYS:HZ3	1.67	0.58
2:H:7:MET:HB3	2:H:8:PRO:HD2	1.84	0.58
1:G:21:LEU:HD22	1:G:112:THR:HG21	1.84	0.58
2:H:34:SER:HA	2:H:84:VAL:O	2.04	0.58
2:H:110:TYR:CE2	2:H:213:MET:HA	2.38	0.58
2:D:123:ASN:C	2:D:125:ASN:N	2.61	0.58
2:F:226:VAL:O	2:F:227:LYS:HE2	2.04	0.58
2:B:4:PRO:O	2:B:5:ASP:C	2.46	0.57
2:D:117:GLU:HA	2:D:117:GLU:OE1	2.04	0.57
2:D:139:ASN:CG	2:D:139:ASN:O	2.46	0.57
1:E:72:GLN:HA	1:E:72:GLN:NE2	2.18	0.57
2:F:49:LEU:HD21	2:F:78:LYS:HA	1.85	0.57
1:C:36:ARG:HD3	1:C:60:ILE:CD1	2.34	0.57
2:F:130:LEU:HD11	2:F:142:SER:HB3	1.86	0.57
2:D:130:LEU:O	2:D:227:LYS:NZ	2.36	0.57
2:B:24:MET:CE	2:B:28:TYR:HE1	2.17	0.57
2:B:94:TYR:O	2:B:95:PHE:HB3	2.04	0.57
2:F:128:ASN:HD22	2:F:144:GLU:CD	2.13	0.57
2:D:187:ILE:HB	2:D:227:LYS:HB3	1.85	0.57
1:G:113:ARG:CZ	1:G:113:ARG:HB3	2.34	0.57
2:H:184:ILE:HD11	2:H:228:ILE:CG2	2.35	0.57
1:E:25:GLN:NE2	1:E:29:HIS:H	2.02	0.56
2:H:91:VAL:O	2:H:92:ASN:HB2	2.05	0.56
1:A:82:THR:HG22	1:A:85:GLN:HG3	1.87	0.56
1:C:36:ARG:CG	1:C:60:ILE:HD11	2.35	0.56
2:B:43:LYS:HE2	2:B:75:LYS:NZ	2.21	0.56
2:D:136:ASN:ND2	2:D:233:THR:HA	2.19	0.56
2:F:88:ASN:H	2:F:88:ASN:ND2	1.99	0.56
2:F:172:TYR:HE2	2:F:199:MET:HE3	1.71	0.56
2:H:119:ASN:O	2:H:150:LYS:HG3	2.05	0.56
1:C:51:GLY:O	1:C:69:ARG:HG2	2.05	0.56
1:E:87:THR:HG23	1:E:114:LEU:O	2.06	0.56
2:B:189:ASN:C	2:B:191:GLY:H	2.12	0.56
1:C:65:TYR:CZ	1:C:86:GLN:HG2	2.41	0.56
1:C:66:LYS:HG3	2:D:174:PHE:CG	2.40	0.56
2:D:123:ASN:C	2:D:125:ASN:H	2.13	0.56
1:G:25:GLN:O	1:G:73:GLU:HB3	2.06	0.56
1:E:23:CYS:H	1:E:74:GLN:HE22	1.52	0.56
1:E:14:VAL:HG12	1:E:15:THR:O	2.06	0.56
2:H:121:PHE:CZ	2:H:127:GLN:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:GLN:NE2	2:F:195:TRP:NE1	2.54	0.56
2:D:95:PHE:CZ	2:D:106:LYS:HB2	2.41	0.56
2:F:183:TYR:CE2	2:F:231:HIS:HB2	2.40	0.56
1:A:32:MET:HE2	1:A:74:PHE:CB	2.36	0.56
2:D:73:LEU:O	2:D:73:LEU:HD13	2.06	0.56
2:F:158:ASP:CG	2:F:162:ARG:HH11	2.13	0.56
2:D:207:ASP:HB3	2:D:210:LYS:HB3	1.87	0.55
2:F:42:ASP:OD2	2:F:43:LYS:N	2.31	0.55
2:H:74:ALA:O	2:H:78:LYS:HB2	2.07	0.55
2:B:164:PHE:C	2:B:164:PHE:CD2	2.85	0.55
2:F:129:VAL:HG12	2:F:130:LEU:N	2.21	0.55
1:A:37:GLN:C	1:A:38:ASP:OD1	2.49	0.55
2:D:158:ASP:OD1	2:D:162:ARG:HD3	2.06	0.55
1:A:15:THR:HG23	1:A:15:THR:O	2.07	0.55
1:G:99:THR:HG22	1:G:100:LEU:N	2.21	0.55
2:F:189:ASN:HB3	2:F:225:SER:HB2	1.89	0.55
1:A:87:SER:OG	1:A:88:VAL:N	2.40	0.55
1:A:33:TYR:N	1:A:33:TYR:CD1	2.75	0.54
2:F:84:VAL:HA	2:F:112:GLY:O	2.06	0.54
1:E:83:THR:C	1:E:116:VAL:HG11	2.31	0.54
2:F:89:TYR:CZ	2:F:209:SER:HB2	2.43	0.54
2:D:156:GLU:O	2:D:160:LYS:HG3	2.07	0.54
1:G:73:GLU:H	1:G:73:GLU:CD	2.16	0.54
2:B:75:LYS:HE3	2:B:75:LYS:HA	1.90	0.54
2:D:119:ASN:ND2	2:D:150:LYS:HB2	2.23	0.54
2:F:99:ASP:CA	2:F:102:THR:HG22	2.37	0.54
2:F:171:LEU:HD21	2:F:198:MET:HE2	1.90	0.54
2:F:120:HIS:O	2:F:150:LYS:NZ	2.40	0.54
2:F:129:VAL:HG12	2:F:130:LEU:H	1.72	0.54
2:B:43:LYS:HE3	2:B:75:LYS:NZ	2.20	0.54
1:E:14:VAL:O	1:E:15:THR:C	2.51	0.53
1:E:25:GLN:HE22	1:E:29:HIS:N	2.07	0.53
2:H:7:MET:O	2:H:8:PRO:C	2.51	0.53
2:D:29:ASP:O	2:D:30:ASP:C	2.50	0.53
2:D:48:ASP:C	2:D:48:ASP:OD1	2.51	0.53
2:H:187:ILE:HG23	2:H:193:THR:HG22	1.91	0.53
2:B:89:TYR:CE1	2:B:108:CYS:HB2	2.44	0.53
2:F:214:MET:C	2:F:216:ASN:H	2.16	0.53
2:H:158:ASP:OD2	2:H:215:TYR:OH	2.24	0.53
2:B:75:LYS:HE2	2:B:78:LYS:HD2	1.91	0.53
2:B:13:LYS:HD3	2:B:16:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:LYS:HB2	2:B:56:LYS:NZ	2.20	0.53
2:H:134:TYR:CE2	2:H:139:ASN:HB2	2.44	0.53
2:B:24:MET:CE	2:B:28:TYR:CE1	2.91	0.52
2:H:222:ASP:HB3	2:H:225:SER:OG	2.09	0.52
2:B:181:THR:OG1	2:B:233:THR:HB	2.07	0.52
2:D:50:ILE:HD12	2:D:65:LYS:HB2	1.92	0.52
1:E:66:LYS:HA	2:F:174:PHE:CE2	2.44	0.52
2:F:123:ASN:C	2:F:125:ASN:H	2.17	0.52
2:H:184:ILE:HD11	2:H:228:ILE:HG23	1.92	0.52
1:C:65:TYR:OH	1:C:86:GLN:HG2	2.09	0.52
2:D:170:ASN:O	2:D:171:LEU:C	2.50	0.52
2:B:39:LYS:HE3	2:B:79:ASP:OD1	2.10	0.52
2:F:123:ASN:HD22	2:F:123:ASN:H	1.54	0.52
2:D:5:ASP:OD2	2:D:185:LYS:NZ	2.42	0.52
2:F:57:LYS:HB3	2:F:58:LEU:HD22	1.91	0.52
2:F:135:GLU:O	2:F:136:ASN:HB2	2.08	0.52
2:F:194:PHE:CD2	2:F:219:LYS:HE3	2.44	0.52
2:F:31:HIS:CE1	2:F:88:ASN:ND2	2.78	0.52
2:B:56:LYS:HZ3	2:B:56:LYS:CB	2.20	0.52
1:G:14:VAL:O	1:G:15:THR:C	2.51	0.52
1:A:86:THR:HG23	1:A:108:SER:HA	1.92	0.51
2:F:42:ASP:CG	2:F:43:LYS:H	2.16	0.51
2:F:182:GLY:HA2	2:F:231:HIS:O	2.11	0.51
2:H:82:VAL:HB	2:H:114:THR:O	2.09	0.51
1:C:36:ARG:HG2	1:C:60:ILE:HD11	1.92	0.51
2:H:28:TYR:CZ	2:H:162:ARG:NH1	2.79	0.51
2:B:53:ILE:HB	2:B:64:VAL:CG2	2.40	0.51
2:B:138:ARG:HG2	2:B:138:ARG:HH11	1.76	0.51
2:B:139:ASN:C	2:B:139:ASN:ND2	2.63	0.51
2:H:24:MET:HE2	2:H:28:TYR:CE1	2.45	0.51
1:E:26:THR:HG21	1:G:2:ALA:N	2.25	0.51
2:F:40:SER:CB	2:F:49:LEU:HD22	2.41	0.51
2:H:182:GLY:HA2	2:H:231:HIS:O	2.10	0.51
2:B:136:ASN:O	2:B:137:LYS:CB	2.54	0.51
2:B:166:ILE:O	2:B:170:ASN:HA	2.09	0.51
2:B:12:HIS:HB2	2:B:199:MET:HB2	1.94	0.50
2:F:162:ARG:HD2	2:F:198:MET:HE3	1.94	0.50
1:C:38:ASP:CG	1:C:44:ARG:HH11	2.20	0.50
2:F:130:LEU:HD12	2:F:143:PHE:O	2.12	0.50
2:B:43:LYS:CE	2:B:75:LYS:HZ1	2.20	0.50
2:B:37:LYS:HB3	2:B:37:LYS:NZ	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:ILE:CG2	1:E:65:TYR:CD2	2.94	0.50
2:F:3:GLN:NE2	2:F:195:TRP:CE2	2.80	0.50
2:B:158:ASP:O	2:B:162:ARG:HG3	2.12	0.50
2:B:214:MET:HE3	2:B:215:TYR:CE2	2.47	0.50
2:D:214:MET:C	2:D:216:ASN:H	2.20	0.50
1:E:23:CYS:HB2	1:E:34:TRP:CZ2	2.47	0.49
2:H:44:PHE:HB3	2:H:48:ASP:OD2	2.11	0.49
2:D:110:TYR:CD1	2:D:110:TYR:N	2.80	0.49
2:F:178:PRO:O	2:F:234:THR:HG22	2.12	0.49
2:H:95:PHE:CZ	2:H:106:LYS:HB2	2.46	0.49
2:B:152:VAL:HG13	2:B:157:LEU:HD11	1.93	0.49
2:F:61:TYR:HA	2:F:105:GLY:CA	2.42	0.49
1:E:34:TRP:O	1:E:46:ILE:HG13	2.12	0.49
2:H:88:ASN:HD22	2:H:88:ASN:N	1.98	0.49
2:H:133:VAL:HB	2:H:141:ILE:HG23	1.94	0.49
1:C:22:SER:CB	1:C:24:GLN:HE22	2.24	0.49
2:B:66:THR:HA	2:B:109:MET:O	2.13	0.49
1:C:3:ALA:HA	1:C:26:THR:OG1	2.12	0.49
1:C:83:THR:C	1:C:116:VAL:HG11	2.38	0.49
2:H:135:GLU:O	2:H:138:ARG:HB3	2.12	0.49
1:C:25:GLN:O	1:C:25:GLN:HG3	2.07	0.49
1:C:39:THR:CG2	1:C:39:THR:HB	2.17	0.49
2:H:115:LYS:O	2:H:115:LYS:CG	2.59	0.48
1:A:36:ARG:O	1:A:36:ARG:HG3	2.12	0.48
1:A:48:TYR:CE1	1:A:56:GLU:HB3	2.48	0.48
2:D:101:SER:HA	2:D:103:TRP:CZ3	2.48	0.48
2:B:27:LEU:HA	2:B:31:HIS:HD2	1.78	0.48
2:B:71:GLU:O	2:B:74:ALA:N	2.46	0.48
2:D:68:LEU:HD23	2:D:74:ALA:HA	1.95	0.48
2:D:48:ASP:O	2:D:49:LEU:HD23	2.13	0.48
2:D:13:LYS:HB3	2:D:180:GLU:OE2	2.14	0.48
2:F:214:MET:HE3	2:F:215:TYR:CE2	2.49	0.48
1:G:83:THR:HG22	1:G:86:GLN:NE2	2.29	0.48
2:H:134:TYR:HA	2:H:138:ARG:O	2.13	0.48
1:G:68:SER:O	1:G:70:PRO:HD3	2.14	0.48
2:B:66:THR:HG21	2:B:113:ILE:HD11	1.94	0.48
2:B:222:ASP:OD2	2:B:224:LYS:HG2	2.14	0.47
1:C:9:ARG:HA	1:C:9:ARG:NE	2.29	0.47
2:B:43:LYS:HZ2	2:B:43:LYS:CB	2.23	0.47
2:D:13:LYS:HD2	2:D:181:THR:HG22	1.96	0.47
1:E:19:VAL:HG23	1:E:82:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:158:ASP:CG	2:F:162:ARG:NH1	2.73	0.47
2:B:53:ILE:HB	2:B:64:VAL:HG21	1.97	0.47
1:A:25:GLN:OE1	1:A:29:HIS:N	2.44	0.47
1:C:52:ALA:CB	1:C:52:ALA:C	2.78	0.47
1:E:31:ASN:HA	1:E:49:SER:O	2.15	0.47
1:E:74:GLN:HE21	1:E:75:PHE:C	2.23	0.47
2:F:77:TYR:CE2	2:F:115:LYS:HE2	2.45	0.47
2:F:89:TYR:CD1	2:F:212:LEU:HD12	2.47	0.47
2:F:158:ASP:OD2	2:F:162:ARG:NH1	2.47	0.47
1:G:25:GLN:O	1:G:25:GLN:HG3	2.15	0.47
2:H:109:MET:C	2:H:110:TYR:CD1	2.93	0.47
2:H:184:ILE:HD12	2:H:186:PHE:CE1	2.49	0.47
2:B:229:GLU:HB3	2:B:231:HIS:HE2	1.80	0.47
1:G:23:CYS:HB2	1:G:34:TRP:CZ2	2.50	0.47
1:A:41:HIS:O	1:A:43:LEU:N	2.47	0.47
2:D:82:VAL:HG21	2:D:113:ILE:HG23	1.96	0.47
1:E:11:LYS:HD3	1:E:19:VAL:CG1	2.45	0.47
2:H:187:ILE:HA	2:H:193:THR:HG22	1.97	0.47
2:B:27:LEU:HA	2:B:31:HIS:CD2	2.50	0.46
2:D:6:PRO:HD3	2:D:195:TRP:CE2	2.50	0.46
2:F:3:GLN:HE21	2:F:195:TRP:NE1	2.13	0.46
2:D:131:VAL:HG22	2:D:228:ILE:HG13	1.97	0.46
1:E:16:GLY:N	1:E:82:ALA:O	2.45	0.46
2:F:48:ASP:CB	2:F:67:GLU:HA	2.45	0.46
2:F:158:ASP:O	2:F:162:ARG:HG2	2.15	0.46
2:H:127:GLN:NE2	2:H:224:LYS:HB3	2.31	0.46
2:H:184:ILE:HG23	2:H:184:ILE:O	2.13	0.46
1:G:87:THR:HG23	1:G:115:SER:HA	1.96	0.46
1:A:67:SER:C	1:A:69:PRO:HD3	2.40	0.46
2:D:155:GLN:O	2:D:159:ILE:HG13	2.16	0.46
1:G:36:ARG:HE	1:G:36:ARG:HB2	1.61	0.46
1:E:27:ASN:HB3	1:E:29:HIS:NE2	2.30	0.46
2:H:171:LEU:O	2:H:177:SER:OG	2.34	0.46
2:B:152:VAL:HG11	2:B:157:LEU:HD21	1.97	0.46
2:D:6:PRO:HB3	2:D:195:TRP:CZ2	2.51	0.46
1:E:11:LYS:HD3	1:E:19:VAL:HG11	1.98	0.46
2:H:21:MET:O	2:H:21:MET:HG3	2.16	0.46
1:A:15:THR:O	1:A:15:THR:CG2	2.64	0.46
2:D:37:LYS:HG3	2:D:81:VAL:HG11	1.98	0.46
2:B:29:ASP:O	2:B:30:ASP:C	2.59	0.46
2:B:37:LYS:HG3	2:B:81:VAL:CG1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TRP:O	2:B:104:HIS:C	2.59	0.46
1:G:24:GLN:HE22	1:G:74:GLN:CD	2.22	0.46
2:H:123:ASN:HB2	2:H:125:ASN:OD1	2.16	0.46
2:H:227:LYS:NZ	2:H:227:LYS:HA	2.31	0.46
1:A:38:ASP:OD1	1:A:38:ASP:N	2.50	0.45
1:C:39:THR:CG2	1:C:39:THR:CA	2.85	0.45
2:D:219:LYS:HD3	2:D:220:THR:H	1.81	0.45
2:H:43:LYS:HA	2:H:50:ILE:HD12	1.98	0.45
2:H:65:LYS:HE2	2:H:95:PHE:HB3	1.97	0.45
1:A:98:THR:HG23	1:G:100:LEU:O	2.16	0.45
2:B:89:TYR:CZ	2:B:108:CYS:HB2	2.51	0.45
2:D:227:LYS:HZ3	2:D:227:LYS:HA	1.81	0.45
2:F:49:LEU:HD12	2:F:68:LEU:HD21	1.97	0.45
2:B:133:VAL:HB	2:B:141:ILE:HG23	1.97	0.45
1:C:43:LEU:HD12	1:C:43:LEU:HA	1.73	0.45
1:E:2:ALA:O	1:G:2:ALA:HB3	2.16	0.45
2:F:29:ASP:O	2:F:30:ASP:C	2.57	0.45
1:A:25:GLN:NE2	1:A:32:MET:SD	2.89	0.45
1:A:36:ARG:HH21	1:A:36:ARG:HD3	1.52	0.45
1:A:79:GLU:H	1:A:79:GLU:HG3	1.45	0.45
1:E:35:TYR:HA	1:E:44:ARG:O	2.17	0.45
2:F:162:ARG:CD	2:F:198:MET:HE3	2.46	0.45
1:A:24:GLN:NE2	1:A:24:GLN:N	2.64	0.45
1:E:77:LEU:C	1:E:78:ILE:HD12	2.40	0.45
2:F:136:ASN:HD21	2:F:234:THR:H	1.64	0.45
1:C:31:ASN:HA	1:C:49:SER:O	2.17	0.45
1:G:27:ASN:HD22	1:G:27:ASN:C	2.25	0.45
2:B:170:ASN:N	2:B:170:ASN:HD22	2.15	0.45
2:D:166:ILE:HG21	2:D:166:ILE:HD13	1.64	0.45
2:F:177:SER:C	2:F:179:TYR:H	2.25	0.45
2:D:43:LYS:HG3	2:D:48:ASP:O	2.17	0.45
2:F:61:TYR:CD2	2:F:107:THR:CG2	3.00	0.45
2:F:172:TYR:HE2	2:F:199:MET:CE	2.29	0.45
1:C:23:CYS:HB2	1:C:34:TRP:CZ2	2.52	0.45
2:F:224:LYS:HE3	2:F:224:LYS:HB2	1.67	0.45
2:H:24:MET:HG2	2:H:172:TYR:CE2	2.52	0.45
2:H:33:VAL:O	2:H:85:TYR:HA	2.17	0.45
1:G:88:SER:OG	1:G:89:VAL:N	2.50	0.45
2:B:136:ASN:ND2	2:B:233:THR:HA	2.32	0.44
2:H:29:ASP:O	2:H:30:ASP:C	2.61	0.44
2:B:140:THR:O	2:B:141:ILE:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LYS:NZ	1:C:66:LYS:HB2	2.32	0.44
2:D:20:THR:HG22	2:D:22:GLY:H	1.82	0.44
2:F:123:ASN:O	2:F:125:ASN:N	2.51	0.44
1:E:46:ILE:HG21	1:E:65:TYR:CD2	2.52	0.44
1:C:6:GLN:O	1:C:9:ARG:HD2	2.18	0.44
2:F:88:ASN:HD22	2:F:88:ASN:N	1.96	0.44
2:B:58:LEU:HD12	2:B:60:ASN:HD21	1.83	0.44
2:B:75:LYS:CE	2:B:78:LYS:HD2	2.47	0.44
1:C:113:ARG:HG3	1:C:113:ARG:HH11	1.83	0.44
1:E:12:VAL:HA	1:E:115:SER:O	2.17	0.44
2:B:37:LYS:NZ	2:B:37:LYS:CB	2.79	0.44
2:H:112:GLY:HA2	2:H:153:THR:HG21	1.98	0.44
1:C:57:LYS:HZ3	2:D:175:ASN:HD21	1.66	0.44
2:D:119:ASN:ND2	2:D:151:SER:H	2.05	0.44
1:E:69:ARG:HD2	1:E:74:GLN:O	2.17	0.44
2:F:109:MET:HE2	2:F:111:GLY:O	2.18	0.44
1:G:27:ASN:O	1:G:29:HIS:N	2.50	0.44
2:B:190:ASN:OD1	2:B:192:ASN:N	2.40	0.43
2:H:123:ASN:CB	2:H:125:ASN:OD1	2.66	0.43
2:B:56:LYS:NZ	2:B:56:LYS:CB	2.79	0.43
2:F:33:VAL:O	2:F:85:TYR:HA	2.18	0.43
2:H:87:SER:OG	2:H:159:ILE:HD13	2.18	0.43
1:C:25:GLN:HG2	1:C:73:GLU:HA	2.00	0.43
2:F:134:TYR:CE2	2:F:139:ASN:HB2	2.53	0.43
2:F:212:LEU:O	2:F:213:MET:C	2.59	0.43
2:H:170:ASN:O	2:H:178:PRO:HD3	2.18	0.43
2:B:65:LYS:HE2	2:B:108:CYS:SG	2.59	0.43
2:B:168:LYS:HB2	2:B:168:LYS:HE2	1.84	0.43
2:D:7:MET:O	2:D:9:ASP:N	2.51	0.43
2:F:123:ASN:N	2:F:123:ASN:ND2	2.61	0.43
1:G:38:ASP:O	1:G:39:THR:C	2.62	0.43
2:D:28:TYR:CD2	2:D:162:ARG:HG3	2.54	0.43
1:E:100:LEU:HD13	1:E:108:PHE:CZ	2.53	0.43
1:G:32:MET:HE2	1:G:75:PHE:HB3	2.01	0.43
2:B:73:LEU:O	2:B:76:LYS:HB3	2.19	0.43
1:C:4:VAL:CG2	1:C:94:SER:HB3	2.49	0.43
2:H:49:LEU:HD21	2:H:78:LYS:HA	2.00	0.43
2:H:70:ASN:OD1	2:H:73:LEU:HD23	2.18	0.43
1:A:31:ASN:HA	1:A:49:SER:O	2.18	0.43
2:B:110:TYR:CD1	2:B:110:TYR:N	2.86	0.43
2:D:85:TYR:C	2:D:85:TYR:CD2	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:LYS:O	2:D:170:ASN:HB2	2.19	0.43
1:E:26:THR:HG21	1:G:2:ALA:CB	2.47	0.43
2:H:11:LEU:CD1	2:H:183:TYR:HD2	2.17	0.43
2:H:200:PRO:HB3	2:H:206:PHE:CE1	2.53	0.43
2:D:119:ASN:HD22	2:D:119:ASN:HA	1.63	0.43
2:F:25:LYS:HB2	2:F:172:TYR:HB2	2.01	0.43
2:H:222:ASP:CG	2:H:225:SER:HG	2.20	0.43
2:B:71:GLU:O	2:B:72:ASP:C	2.61	0.43
1:C:24:GLN:HA	1:C:73:GLU:O	2.19	0.43
1:E:25:GLN:CD	1:E:29:HIS:H	2.26	0.43
2:F:77:TYR:O	2:F:78:LYS:C	2.62	0.43
2:F:187:ILE:HG12	2:F:193:THR:HG22	2.00	0.43
2:H:86:GLY:HA3	2:H:109:MET:HE3	2.01	0.43
2:D:185:LYS:HE2	2:D:187:ILE:CD1	2.48	0.43
2:F:61:TYR:CG	2:F:107:THR:HG22	2.54	0.43
2:F:99:ASP:N	2:F:102:THR:HG22	2.33	0.43
2:H:28:TYR:CE2	2:H:162:ARG:HD2	2.53	0.43
2:H:35:ALA:CB	2:H:53:ILE:CD1	2.96	0.43
2:H:201:ALA:HB1	2:H:202:PRO:HD3	2.01	0.43
2:D:136:ASN:HD22	2:D:233:THR:HG22	1.84	0.42
1:E:65:TYR:HB3	1:E:77:LEU:HD11	2.00	0.42
2:H:95:PHE:O	2:H:106:LYS:NZ	2.41	0.42
2:H:197:ASP:OD1	2:H:198:MET:N	2.52	0.42
1:A:54:SER:HB2	2:B:91:VAL:HG21	2.02	0.42
2:D:131:VAL:HA	2:D:228:ILE:HB	2.01	0.42
2:H:216:ASN:HD22	2:H:216:ASN:HA	1.38	0.42
2:B:7:MET:O	2:B:8:PRO:C	2.59	0.42
2:B:119:ASN:O	2:B:149:LYS:HA	2.18	0.42
1:C:57:LYS:HZ2	2:D:175:ASN:HD21	1.65	0.42
2:D:127:GLN:OE1	2:D:224:LYS:HA	2.19	0.42
1:G:46:ILE:HG21	1:G:65:TYR:CD2	2.54	0.42
2:H:75:LYS:HD3	2:H:75:LYS:HA	1.58	0.42
2:H:136:ASN:OD1	2:H:233:THR:HA	2.19	0.42
2:D:183:TYR:CE2	2:D:231:HIS:HB2	2.54	0.42
2:F:126:LEU:HD12	2:F:146:GLN:NE2	2.34	0.42
2:F:132:ARG:HA	2:F:142:SER:OG	2.19	0.42
2:H:24:MET:CE	2:H:28:TYR:HE1	2.32	0.42
1:E:52:ALA:HA	1:E:69:ARG:HG3	2.01	0.42
1:G:83:THR:HG22	1:G:86:GLN:CD	2.44	0.42
1:G:93:ALA:CB	1:G:101:TYR:O	2.67	0.42
1:A:14:VAL:O	1:A:17:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:PRO:HB3	2:F:195:TRP:CH2	2.55	0.42
1:C:86:GLN:O	1:C:90:TYR:OH	2.25	0.42
1:G:93:ALA:HB1	1:G:101:TYR:O	2.19	0.42
2:H:81:VAL:O	2:H:116:HIS:HB3	2.19	0.42
1:C:66:LYS:HG3	1:C:66:LYS:HZ2	1.57	0.42
2:F:155:GLN:HG3	2:F:215:TYR:CE1	2.55	0.42
2:H:6:PRO:HB3	2:H:10:ASP:HB2	2.01	0.42
2:B:5:ASP:HA	2:B:6:PRO:HD3	1.89	0.42
2:B:211:TYR:O	2:B:214:MET:HG2	2.20	0.42
2:F:158:ASP:OD1	2:F:162:ARG:NH1	2.45	0.42
2:H:195:TRP:O	2:H:196:TYR:HD2	2.03	0.42
2:H:201:ALA:HB1	2:H:202:PRO:CD	2.50	0.42
1:C:18:LYS:HA	1:C:79:LEU:O	2.20	0.42
1:E:23:CYS:HB3	1:E:75:PHE:O	2.19	0.42
2:F:61:TYR:HA	2:F:105:GLY:C	2.45	0.42
2:F:170:ASN:O	2:F:171:LEU:C	2.59	0.42
2:H:157:LEU:HD13	2:H:228:ILE:HD11	2.02	0.42
2:B:229:GLU:HB3	2:B:231:HIS:NE2	2.34	0.41
2:D:27:LEU:HA	2:D:31:HIS:HD2	1.85	0.41
2:D:113:ILE:HG21	2:D:113:ILE:HD13	1.52	0.41
2:D:227:LYS:NZ	2:D:228:ILE:H	2.18	0.41
1:E:46:ILE:HG21	1:E:46:ILE:HD13	1.77	0.41
1:E:78:ILE:HD12	1:E:78:ILE:N	2.35	0.41
2:F:119:ASN:HD21	2:F:149:LYS:HB3	1.85	0.41
2:H:55:ASP:HB3	2:H:58:LEU:O	2.20	0.41
1:A:33:TYR:O	1:A:91:CYS:HA	2.20	0.41
1:A:37:GLN:HE21	1:A:37:GLN:HB2	1.63	0.41
2:F:43:LYS:HE2	2:F:48:ASP:O	2.20	0.41
1:G:82:ALA:HB1	1:G:116:VAL:HG11	2.02	0.41
2:D:219:LYS:HD3	2:D:220:THR:O	2.20	0.41
1:E:45:LEU:O	1:E:59:ASP:N	2.50	0.41
2:H:170:ASN:O	2:H:171:LEU:C	2.63	0.41
2:F:123:ASN:C	2:F:125:ASN:N	2.77	0.41
2:F:230:VAL:O	2:F:230:VAL:HG12	2.19	0.41
1:G:6:GLN:OE1	1:G:91:PHE:HA	2.21	0.41
1:G:55:THR:CG2	2:H:20:THR:HG21	2.40	0.41
2:B:77:TYR:O	2:B:78:LYS:C	2.63	0.41
2:B:114:THR:HG22	2:B:153:THR:HG23	2.02	0.41
2:F:2:SER:N	2:F:192:ASN:OD1	2.54	0.41
2:H:128:ASN:HB3	2:H:144:GLU:OE1	2.20	0.41
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ILE:O	1:C:60:ILE:HG13	2.21	0.41
2:D:153:THR:HA	2:D:220:THR:HA	2.03	0.41
2:F:37:LYS:HB2	2:F:116:HIS:CE1	2.56	0.41
2:F:129:VAL:O	2:F:144:GLU:HA	2.20	0.41
1:G:9:ARG:HG3	1:G:9:ARG:HH11	1.86	0.41
2:B:68:LEU:N	2:B:68:LEU:HD22	2.36	0.41
2:D:13:LYS:N	2:D:13:LYS:HD3	2.36	0.41
1:G:10:ASN:O	1:G:11:LYS:HB2	2.20	0.41
2:H:71:GLU:O	2:H:71:GLU:HG2	2.21	0.41
1:C:88:SER:HB3	1:C:89:VAL:H	1.68	0.41
1:E:12:VAL:HG12	1:E:117:LEU:HD12	2.02	0.41
1:E:84:PRO:HA	1:E:116:VAL:HB	2.02	0.41
2:H:184:ILE:CD1	2:H:228:ILE:HG23	2.50	0.41
2:H:200:PRO:HB3	2:H:206:PHE:CD1	2.56	0.41
2:D:37:LYS:HB2	2:D:116:HIS:CE1	2.56	0.41
1:E:69:ARG:HD2	1:E:69:ARG:HA	1.88	0.41
1:E:100:LEU:HD23	1:E:100:LEU:HA	1.71	0.41
2:F:48:ASP:HB2	2:F:67:GLU:HA	2.02	0.41
1:G:26:THR:HG22	1:G:27:ASN:H	1.86	0.41
1:G:69:ARG:CG	1:G:69:ARG:NH2	2.63	0.41
1:A:25:GLN:HG2	1:A:72:GLU:HA	2.03	0.40
2:F:41:VAL:O	2:F:42:ASP:HB2	2.20	0.40
2:F:43:LYS:HD3	2:F:45:LEU:O	2.21	0.40
2:F:172:TYR:OH	2:F:198:MET:O	2.29	0.40
2:D:158:ASP:O	2:D:161:ALA:HB3	2.21	0.40
2:D:222:ASP:OD1	2:D:225:SER:HB3	2.21	0.40
1:E:87:THR:CG2	1:E:114:LEU:O	2.68	0.40
2:F:36:THR:HG23	2:F:83:ASP:OD2	2.21	0.40
1:G:100:LEU:HA	1:G:100:LEU:HD23	1.87	0.40
2:B:49:LEU:HD23	2:B:49:LEU:HA	1.86	0.40
2:B:160:LYS:HD3	3:B:252:HOH:O	2.22	0.40
1:C:38:ASP:O	1:C:39:THR:C	2.64	0.40
2:D:37:LYS:HB3	2:D:37:LYS:NZ	2.35	0.40
2:F:119:ASN:O	2:F:119:ASN:CG	2.65	0.40
1:C:36:ARG:CD	1:C:60:ILE:CD1	3.00	0.40
2:D:20:THR:C	2:D:22:GLY:N	2.76	0.40
2:D:48:ASP:HB2	2:D:66:THR:O	2.21	0.40
1:E:17:GLU:HG2	1:E:18:LYS:N	2.36	0.40
2:H:24:MET:HE2	2:H:28:TYR:HE1	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:LYS:NZ	2:F:123:ASN:OD1[1_554]	2.08	0.12

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	107/109 (98%)	98 (92%)	7 (6%)	2 (2%)	6	5
1	C	107/109 (98%)	97 (91%)	6 (6%)	4 (4%)	2	1
1	E	107/109 (98%)	90 (84%)	14 (13%)	3 (3%)	4	2
1	G	107/109 (98%)	93 (87%)	9 (8%)	5 (5%)	2	1
2	B	228/239 (95%)	183 (80%)	34 (15%)	11 (5%)	2	1
2	D	229/239 (96%)	195 (85%)	30 (13%)	4 (2%)	7	7
2	F	230/239 (96%)	183 (80%)	35 (15%)	12 (5%)	1	1
2	H	226/239 (95%)	197 (87%)	22 (10%)	7 (3%)	3	2
All	All	1341/1392 (96%)	1136 (85%)	157 (12%)	48 (4%)	2	1

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	57	LYS
2	B	104	HIS
2	B	125	ASN
2	F	57	LYS
2	F	236	ASN
1	G	28	ASN
1	G	74	GLN
2	H	122	ASP
2	H	235	LYS
2	B	122	ASP
2	B	137	LYS
2	B	224	LYS

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Mol	Chain	Res	Type
1	C	3	ALA
1	C	39	THR
2	D	102	THR
2	D	124	GLY
2	F	19	GLY
2	F	98	LYS
2	F	122	ASP
2	F	136	ASN
2	F	217	ASP
2	H	217	ASP
2	B	96	SER
1	C	27	ASN
2	F	9	ASP
2	F	42	ASP
2	F	47	HIS
1	G	27	ASN
2	H	216	ASN
1	E	62	ASP
1	G	39	THR
2	H	116	HIS
2	H	137	LYS
2	B	56	LYS
2	B	95	PHE
2	D	57	LYS
2	H	8	PRO
2	B	124	GLY
1	E	42	GLY
1	E	97	GLY
2	F	73	LEU
2	F	123	ASN
1	G	97	GLY
1	C	97	GLY
1	A	42	GLY
2	B	8	PRO
2	D	191	GLY
1	A	97	GLY

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	88/88 (100%)	76 (86%)	12 (14%)	3	4
1	C	88/88 (100%)	79 (90%)	9 (10%)	7	8
1	E	88/88 (100%)	75 (85%)	13 (15%)	3	3
1	G	88/88 (100%)	76 (86%)	12 (14%)	3	4
2	B	214/220 (97%)	196 (92%)	18 (8%)	10	14
2	D	215/220 (98%)	194 (90%)	21 (10%)	7	10
2	F	216/220 (98%)	189 (88%)	27 (12%)	4	5
2	H	211/220 (96%)	193 (92%)	18 (8%)	10	13
All	All	1208/1232 (98%)	1078 (89%)	130 (11%)	6	7

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	24	GLN
1	A	27	ASN
1	A	33	TYR
1	A	37	GLN
1	A	55	THR
1	A	56	GLU
1	A	62	ASP
1	A	68	ARG
1	A	75	SER
1	A	83	PRO
1	A	84	SER
2	B	3	GLN
2	B	40	SER
2	B	43	LYS
2	B	56	LYS
2	B	68	LEU
2	B	72	ASP
2	B	73	LEU
2	B	75	LYS
2	B	76	LYS
2	B	103	TRP
2	B	114	THR
2	B	117	GLU

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Mol	Chain	Res	Type
2	B	125	ASN
2	B	138	ARG
2	B	139	ASN
2	B	176	SER
2	B	216	ASN
2	B	233	THR
1	C	7	SER
1	C	9	ARG
1	C	39	THR
1	C	43	LEU
1	C	56	GLU
1	C	66	LYS
1	C	72	GLN
1	C	73	GLU
1	C	94	SER
2	D	2	SER
2	D	3	GLN
2	D	13	LYS
2	D	24	MET
2	D	45	LEU
2	D	68	LEU
2	D	69	LEU
2	D	73	LEU
2	D	78	LYS
2	D	102	THR
2	D	104	HIS
2	D	115	LYS
2	D	117	GLU
2	D	139	ASN
2	D	141	ILE
2	D	144	GLU
2	D	162	ARG
2	D	216	ASN
2	D	219	LYS
2	D	227	LYS
2	D	234	THR
1	E	4	VAL
1	E	18	LYS
1	E	19	VAL
1	E	22	SER
1	E	37	GLN
1	E	41	HIS

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Mol	Chain	Res	Type
1	E	44	ARG
1	E	46	ILE
1	E	72	GLN
1	E	78	ILE
1	E	80	GLU
1	E	99	THR
1	E	113	ARG
2	F	2	SER
2	F	63	LYS
2	F	68	LEU
2	F	69	LEU
2	F	73	LEU
2	F	88	ASN
2	F	98	LYS
2	F	103	TRP
2	F	104	HIS
2	F	115	LYS
2	F	123	ASN
2	F	133	VAL
2	F	141	ILE
2	F	151	SER
2	F	153	THR
2	F	162	ARG
2	F	167	ASN
2	F	168	LYS
2	F	199	MET
2	F	202	PRO
2	F	209	SER
2	F	216	ASN
2	F	218	ASN
2	F	220	THR
2	F	224	LYS
2	F	229	GLU
2	F	235	LYS
1	G	4	VAL
1	G	6	GLN
1	G	10	ASN
1	G	21	LEU
1	G	26	THR
1	G	43	LEU
1	G	69	ARG
1	G	72	GLN

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Mol	Chain	Res	Type
1	G	73	GLU
1	G	80	GLU
1	G	84	PRO
1	G	113	ARG
2	H	3	GLN
2	H	41	VAL
2	H	56	LYS
2	H	58	LEU
2	H	68	LEU
2	H	84	VAL
2	H	88	ASN
2	H	97	SER
2	H	110	TYR
2	H	117	GLU
2	H	137	LYS
2	H	153	THR
2	H	184	ILE
2	H	194	PHE
2	H	205	LYS
2	H	216	ASN
2	H	227	LYS
2	H	235	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	27	ASN
1	A	30	ASN
1	A	37	GLN
1	A	71	GLN
1	A	73	GLN
2	B	47	HIS
2	B	88	ASN
2	B	136	ASN
2	B	139	ASN
2	B	167	ASN
2	B	170	ASN
2	B	216	ASN
1	C	24	GLN
1	C	27	ASN
1	C	30	ASN

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Mol	Chain	Res	Type
1	C	72	GLN
2	D	47	HIS
2	D	88	ASN
2	D	92	ASN
2	D	116	HIS
2	D	119	ASN
2	D	125	ASN
2	D	128	ASN
2	D	136	ASN
2	D	155	GLN
2	D	167	ASN
2	D	175	ASN
2	D	216	ASN
1	E	24	GLN
1	E	30	ASN
1	E	72	GLN
1	E	74	GLN
2	F	3	GLN
2	F	88	ASN
2	F	92	ASN
2	F	123	ASN
2	F	128	ASN
2	F	136	ASN
2	F	139	ASN
2	F	163	ASN
2	F	167	ASN
2	F	170	ASN
2	F	216	ASN
2	F	236	ASN
1	G	27	ASN
1	G	28	ASN
1	G	30	ASN
1	G	31	ASN
1	G	37	GLN
1	G	72	GLN
2	H	3	GLN
2	H	52	ASN
2	H	88	ASN
2	H	92	ASN
2	H	139	ASN
2	H	163	ASN
2	H	167	ASN

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Mol	Chain	Res	Type
2	H	175	ASN
2	H	216	ASN

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	109/109 (100%)	-0.29	1 (0%) 81 82	24, 39, 60, 68	0
1	C	109/109 (100%)	-0.44	0 100 100	21, 34, 55, 64	0
1	E	109/109 (100%)	-0.29	0 100 100	25, 39, 60, 71	0
1	G	109/109 (100%)	-0.15	2 (1%) 67 69	26, 46, 67, 76	0
2	B	232/239 (97%)	-0.27	1 (0%) 88 89	23, 44, 75, 88	0
2	D	233/239 (97%)	-0.40	2 (0%) 81 82	18, 38, 62, 84	0
2	F	234/239 (97%)	-0.10	1 (0%) 88 89	26, 46, 76, 105	0
2	H	230/239 (96%)	-0.24	2 (0%) 81 82	25, 43, 72, 90	0
All	All	1365/1392 (98%)	-0.27	9 (0%) 84 85	18, 42, 69, 105	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	3.9
2	B	103	TRP	3.1
2	D	97	SER	2.7
2	F	104	HIS	2.6
1	G	41	HIS	2.4
1	G	3	ALA	2.2
2	H	96	SER	2.2
2	H	104	HIS	2.1
2	D	237	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.